


AN ABSTRACT OF THE DISSERTATION OF

Douglas H. Ernst for the degree of Doctor of Philosophy in Bioresource Engineering presented on April 17, 2000. Title: AquaFarm: Simulation and Decision-Support Software for Aquaculture Facility Design and Management Planning.

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Abstract approved: _____

 John P. Bolte

A simulation and decision-support software product for aquaculture facility design and management planning is described (AquaFarm, Oregon State University©), including comprehensive documentation and applications to practical problems. AquaFarm provides (1) simulation of physical, chemical, and biological unit processes, (2) simulation of facility and fish culture management, (3) compilation of facility resource and enterprise budgets, and (4) a graphical user interface and data management capabilities. These analytical tools are combined into an interactive, decision support system, for the analysis and development of facility design specifications and management strategies. Intended user groups include aquaculture research, engineering, education, and production. As guided by the user, aquaculture facilities can be of any type, configuration, and management objectives, for purposes of broodfish maturation, egg incubation, and/or growout of finfish or crustaceans in cage, single pass, serial reuse, water recirculation, or solar-algae pond systems. User-accessible specifications include (1) site climate and water supplies, (2) components and configurations of fish culture systems, (3) fish and facility management strategies, (4) unit costs for budget items, (5) production objectives (species, time schedules, and fish numbers and weights), and (6) parameters of unit-process and fish performance models. Based on these specifications, aquaculture facilities are simulated, resource requirements are compiled, and operation schedules are determined so that production objectives are achieved. Facility performance is reported to the user as management schedules, summary reports, resource and

graphical compilations of time-series data for unit process, fish, and water quality variables. If unsatisfactory resource requirements or unattainable production objectives are found, procedures of iterative design and management refinement are supported. To provide this analytical capacity, a wide range of existing and newly developed, quantitative methods and models are assembled and synthesized into an integrated analytical framework, including aquatic chemistry, aquatic biology, fish biology, aquacultural engineering, and simulation techniques. Unit-process and system-level validation exercises are demonstrated for a wide range of aquaculture facilities, in which (1) facilities are constructed according to reported studies, (2) simulation trials are accomplished, and (3) good agreement between predicted performance and empirical observations is demonstrated, given that sufficient specification of site-specific variables is provided.

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**AquaFarm: Simulation and Decision-Support Software
for Aquaculture Facility Design and Management Planning**

by

Douglas H. Ernst

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APPROVED:

Redacted for Privacy

Major Professor, representing Bioresource Engineering

Redacted for Privacy

Head of Department of Bioresource Engineering

Redacted for Privacy

Dean of Graduate School

I understand that my dissertation will become part of the permanent collection of Oregon State University libraries. My signature below authorizes release of my dissertation to any reader upon request.

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Douglas H. Ernst, Author

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DEDICATION

In memory of my mother, to whom this work is dedicated, and to my father, who ensured that I would get the educational opportunities he could not.

AquaFarm: Simulation and Decision-Support Software for Aquaculture Facility Design and Management Planning

1. Introduction

A review of global aquaculture shows both continuing expansion of production levels and current development constraints. From these constraints, the challenge faced in the application of aquacultural engineering to the design and management of aquaculture facilities is brought forward. To address this challenge, the development of a computerized simulation and decision support system for aquaculture engineering is proposed. Previous work relevant to this task is reviewed.

1.1 Aquaculture status and development constraints

People have been farming fish for thousands of years, but the emergence of aquaculture as a global source of food and income has been especially rapid in the last half of the twentieth century. Currently, a wide range of aquatic plants and animals are produced, including algae, mollusks, crustaceans, and finfish (Table 1.1). Many cultivated species are exotic to the regions in which they are grown and/or highly domesticated through selective breeding. Aquaculture is carried out in freshwater, brackish water, and marine environments, spanning from the equator to the temperate northern and southern temperate latitudes. Global aquaculture production data since 1984 and projections to 2010 have been compiled by the FAO (1999a), with additional analyses of these data by Rana and Immink (1999), the FAO (1999b), and New (1999). Historical production data for aquaculture and capture fisheries, together with agricultural production data, show that aquaculture has been the fastest growing food production sector in the world over the last few decades. Since 1984, global aquaculture output has increased at an average annual rate of about 10%, compared with a 3% increase for livestock meat and a 1.6% percent increase for capture fisheries. Aquaculture provided 8% of global fishery production (11% of food fish) in 1984, increasing to 22% (29% of food fish) in 1996. Of the world's top 13 species produced by capture fisheries and aquaculture in 1996, five were almost entirely derived from aquaculture. Finfish continued to be the dominant global aquaculture activity in 1996, accounting for about 49% of total aquaculture production by weight and 55% by value.

Table 1.1. Aquaculture production categories and major species

Production categories	Major species
Freshwater finfish	Carp, tilapia, catfish, trout, eels
Marine finfish	Salmon, milkfish, mullet, amberjacks
Freshwater crustaceans	Freshwater prawn, crayfish
Marine crustaceans	Shrimp, lobster, crab
Marine bivalve mollusks	Oysters, clams, mussels
Marine gastropod mollusks	Abalone, conch
Freshwater and marine algae	Red and brown seaweeds (e.g. <i>Gracillaria</i> and kelp), freshwater micro algae (e.g. <i>Spirulina</i>)
Integrated aquaculture-hydroponics	Finfish and leafy greens and herbs

Table 1.2. A coarse breakdown of aquaculture practices according to management intensity

Type of aquaculture	Management intensity	Gross fish yields (kg/ha) ¹
Extensive	Static water ponds with makeup of water losses, pond fertilization, and high reliance on natural fish foods	50 – 3,000
Semi-intensive	Water aeration, limited water exchange, some utilization of natural foods, and application of prepared feeds	3,000 – 20,000
Intensive	Continuous water exchange on a flow through, reuse, or recirculation basis, and high application rates of prepared feeds	20,000 – 1,000,000+

¹ Ranges in gross fish yields for a given intensity level reflect differences in the fish species used and intensities of prepared feed application rates and water quality management.

While advanced economies such as Japan, Norway and the United States are among the top producers, aquaculture production is predominantly performed in low-income, food-deficit countries (includes China). In 1996, for example, the latter comprised 82% of the total world finfish, shellfish, and aquatic plant production (FAO, 1999b). In 1996, North America accounted for only 2.3% of world aquaculture food fish production. Asia is currently the world leader in aquaculture production by a good margin, with China alone producing about two-thirds of the world's total. For the period 1987 to 1996, global aquaculture increased 250%, but this value is only 150% when production from China (360% growth) is not included (percentages based on weight; New, 1999). In terms of value, relatively low value carp and seaweeds dominate production in China, and China's contribution to the world value of aquaculture production was much less (45%).

The expanding role of aquaculture in food fish production will likely continue, as widespread unsustainable fishing practices have left capture fisheries with a shrinking resource base worldwide. FAO (1999a) estimates that 11 of the world's 15 major fishing areas and 69% of the world's major fish species are in decline and in need of urgent management. Development and pollution have also had major impacts, given that about a third of the world's six billion people live near the sea. These environmental, economic, and social issues present a major challenge. While increasing protein needs of a growing global human population must be met, depleted fisheries must be allowed to recover and intact fisheries protected. Aquaculture provides alternative work for displaced fishers, alternative sources of food fish, and mechanisms for fishery enhancement, but aquaculture does not represent a substitute for good fishery management.

For current global production (1998), in terms of weight and excluding seaweeds, about 57% of aquaculture was performed in freshwater, 37 % in marine waters (mariculture), and 6% in brackish waters (mainly Penaeid shrimp) (FAO, 1999b). Major aquaculture production species were all low in the food chain, consisting of primary producers (e.g. kelp), filter feeders (e.g. bivalves and carp), or finfish that as adults are herbivores or omnivores (e.g. carp and tilapia). Globally, almost all aquaculture production is extensive or semi-intensive, in outdoor, solar-algae pond environments (Table 1.2), which may be integrated with agricultural practices with respect to water, animal manures, and other resources (Hopkins and Cruz, 1982). Intensive fish production, in which fish are grown in flowing-water tanks or raceways supplied by water transport and treatment systems, is a relatively new development compared to pond production. Given the relatively higher production costs, intensive practices are generally limited to higher value species or specialty markets (e.g. live fish markets). In terms of fish biomass produced, the contribution of intensive production to global fish production is relatively insignificant, and extensive and semi-intensive practices are likely to continue to dominate for some time.

In addition to the direct production of food fish, artificial propagation is widely used for genetic conservation and enhancement of fisheries. Perhaps the most notable example of this is the multitude of salmon hatcheries ringing the north Pacific ocean, most of which have been in operation for many decades. More recent developments in fishery enhancement include the wild release of artificially reared species such as redfish and striped bass. Artificial propagation efforts can include broodfish maturation and spawning, egg incubation, larval rearing, and fry-to-fingerling growout, culminating with fish release to the wild. In sum, fish culture for fishery enhancement is aquaculture and within the subject area of this dissertation.

While the expanding role of aquaculture in global fishery production is evident, the modern development of this industry has been constrained by a number of factors. Where these constraints are most pronounced, aquaculture has developed at very slow rates (e.g., Caribbean basin; Hargreaves and Alston, 1991). In regions where aquaculture development has been rapid, the long-term environmental and economic sustainability of certain production practices has come into question (Pillay, 1992; New et al., 1995; Barg and Phillips, 1999). Notable examples that have come into wide public attention over the last decade are Penaeid shrimp farming in estuarine and marine environments and Atlantic salmon farming in marine cages. Based on a wide review of the literature, socio-economic and technological impediments to aquaculture development include:

- 1) Modification of traditional social values and lack of local familiarity: for example, the transition of fishers to fish farmers
- 2) Resource use conflicts and privatization of common property resources: land and water resource conflicts with industries such as tourism, fishing, and navigation; and the privatization of public resources (e.g., mangrove lagoons)
- 3) Potential and real environmental degradation: the development of sensitive coastal areas, nutrient discharge from marine cage systems and certain types of land based systems, and the culture of exotic and potentially invasive species (e.g. Atlantic salmon production in British Columbia and tilapia production in the southern US)
- 4) Poor business environment: shortage of development capital and low interest loans, unattractive production costs and risks, lack of marketing infrastructure (e.g., processing and transportation), and downward trending market prices for some species as worldwide production and competition increases (e.g., tilapia)
- 5) Lack of specialized equipment and supplies: facility construction, water transportation and treatment, fry and fingerling production, and growout feeds of reasonable price and quality
- 6) Limited technical knowledge: limited access to data, information, and expertise resources, and unknowns encountered in the development of new aquaculture species, geographical regions, and production methods
- 7) Limited ability to apply knowledge: challenges encountered in the application of engineering and production analyses to informed decision-making regarding aquaculture planning, design, and management.

Alleviation of the last two of these constraints has a positive impact on the other constraints. These impacts include (1) minimization of environmental impacts, resource requirements, and production costs per unit fish production, (2) coordination of production timing to market demand or fish release schedules (to the wild), (3) quantification and minimization of production risk, and (4) an enhanced capacity for the generation of realistic business plans. Such analyses can be used to (1) optimize production output with respect to required management intensity and resource consumption and (2) explore tradeoffs between the fish biomass density levels maintained and fish production throughput (residence time of fish in a facility).

1.2 Problem definition and objectives of work

The purpose of this dissertation is to address elements in the last two of the constraints listed above. These are the challenges encountered in the application of relevant data resources, numerically intensive analytical methods, aquacultural engineering, and fish production planning procedures to aquaculture design and management. A farm-level perspective will be pursued in this work, along with an attempt to include all significant material and energy flows and required physical and biological components at this system level. Four major tasks can be delineated:

- 1) The physical, chemical, and biological process models, management methods, and resource economics used to represent a given aquaculture system must be collected and parameterized.
- 2) Quantitative methods and rule-based procedures are required to combine and simulate these processes for estimating current and future operational constraints and production capacities.
- 3) Management of large datasets is required, including facility and management specifications, projected facility performance and management schedules, and resource and economic budgets.
- 4) Intensive calculation procedures must be adequately supported, as required to (1) consider multiple fish lots and fish rearing units in a given project, (2) generate facility performance and management schedules by simulation, (3) compare alternative design and management strategies, (4) adjust and optimize facility designs through a series of iterative performance tests, and (5) compare production economics over a range of production scales.

Studies documenting specific constraints encountered in the application of good engineering practices to aquaculture were not found in the literature. Furthermore, a formalized process of user group identification and needs assessment was beyond the scope of this dissertation. Therefore, the specific objectives put forth in this dissertation to address issues of aquacultural engineering are built upon some working assumptions:

- 1) Aquaculture research scientists, extension agents, educators and students, facility designers, and production managers share a common need for comprehensive, system level, analytical tools to facilitate the understanding, planning, and management of aquaculture production facilities.
- 2) The level of development of the aquaculture science and engineering literature base, in conjunction with a reasonable amount of additional method development and integration of methods, is sufficient to support rigorous analytical methods over the full range of aquaculture system types and major aquaculture species.
- 3) The application of data resources and analytical methods to problems in aquaculture design and management are ongoing and must be responsive to local, case-specific environmental conditions, resource availabilities, production practices, fishery markets, and user analytical needs.
- 4) Computer software tools developed for aquaculture design and management can embody expertise in aquaculture science and engineering and serve as mechanisms of technology transfer to education, development, and production. In addition, computer tools can assume the burden of data management and calculation processing and thereby reduce the workload of design and planning analyses. In particular, modeling and simulation are powerful analytical approaches to aquacultural engineering. In the US National Oceanic and Atmospheric Administration (NOAA) 1995-2005 Strategic Plan for Aquaculture (released July 1993), the application of computer based tools and technologies to aquaculture was identified as a high priority area of research and development. For both fishery enhancement and food fish production, a range of computer tools for the design and management tasks of aquaculture facilities have been in use since personal computers first became generally available. A compilation of these tools (Ernst, 1998) demonstrates their continuing evolution in conjunction with advances in aquacultural engineering and computer technology.

Building on these working assumptions, the objective of this dissertation is to describe the development and application of AquaFarm (Version 1.0; Microsoft Windows®; Oregon State University©). AquaFarm is a simulation and decision support software product for the design and management planning of finfish and crustacean aquaculture facilities. Major themes in this work are (1) the division of aquaculture production systems into functional components and associated models, including unit processes, management procedures, and resource accounting and (2) the flexible reintegration of these components into system-level simulation models and design procedures that are adaptable to various aquaculture system types, production objectives, and user analytical needs. The preceding review of global aquaculture production summarizes the wide range of possible aquaculture environments, produced species, and system types that are to be considered.

The chapters of this dissertation are organized according to the process by which AquaFarm was developed, including functional components and applications. In Chapter 2, the functionality objectives that guided the development of AquaFarm are itemized, the design procedure supported by AquaFarm is described, and the software architecture, components, and variables comprising AquaFarm are defined. In Chapter 3, building on this structural framework, procedures used to simulate the management, processes, and resource requirements of an aquaculture facility are described. In Chapters 4 – 7, methods and models used for physical, chemical, and biological unit processes are described. Comprehensive documentation is provided given that these methods were collected from a wide range of disparate sources and newly synthesized here and that these methods represent the rigorous, engineering basis of AquaFarm. In Chapter 8, the discussion returns to a system-level perspective, regarding considerations and accomplishments of AquaFarm calibration, validation, and case study applications. In Chapter 9, summary conclusions and ongoing work are described.

1.3 Literature background

A considerable amount of aquaculture science and engineering literature was used in the development of AquaFarm, due to (1) the wide scope of analyses and system types supported, (2) the predominate reliance on existing methods and models in the literature, and (3) the use of the aquaculture production data from the literature. Much of this literature is cited in the body of this dissertation as it is used. The purpose here is to provide an overview of the three major avenues by which the aquaculture literature was applied to the development of AquaFarm.

Studies concerned with the physical, chemical, and biological unit-processes found in aquaculture systems provided quantitative methods and models for these processes that could be adapted for use in AquaFarm. Much of this literature was from the fields of wastewater treatment and environmental engineering (e.g., Chen and Orlob, 1975; Stumm and Morgan, 1981; James, 1984; Fritz, 1985; Tchobanoglous and Schroeder, 1985; Tchobanoglous and Burton, 1991). In addition, a large amount of unit process modeling work was available in the aquaculture literature, for (1) extensive, pond based systems (e.g., Bernard, 1983; Svirezhev, et al., 1984; Cuenco et al., 1985a, b, c; Cuenco, 1989; Piedrahita, 1990; Piedrahita, 1991; Nath, 1996; Piedrahita et al., 1997), (2) intensive flow-through and recirculating systems (e.g., Muir, 1982; McLean et al., 1991; Colt and Orwicz, 1991b; Weatherly et al., 1993; Timmons and Losordo, 1994; Wood et al., 1996;), and (3) general aquaculture (e.g., Allen et al., 1984; Brune and Tomasso, 1991). Overall, a wealth of studies was available regarding unit processes and single reactor (single water body) perspectives. For system-level modeling of flowing-water aquaculture systems, however, prior work concerning flow-through systems (e.g., Fivelstad et al., 1990; Fivelstad et al., 1991; Colt and Orwicz, 1991b) and recirculating systems (e.g., Weatherly et al., 1993) was limited. The large majority of prior work for flowing-water systems was concerned with singular facility units (e.g., fish tanks, solid filters, biofilters, and gas exchangers). No published models were found that (1) represented flowing-water aquaculture facilities as networks of linked facility units, including all relevant types of facility units, and (2) adequately accounted for facility mass and energy transfer processes and corresponding resource needs.

Secondly, environmental engineering, aquacultural engineering, and aquaculture production studies that provided empirical results from research and applied systems were used for the calibration and validation of unit processes (including fish performance) and sets of unit processes (i.e., single reactor systems; e.g., fish ponds). These studies consisted of technical texts, articles, and databases and are cited as they are used in the development and case study applications of AquaFarm. For aquaculture production studies, monitored variables were typically impacted by multiple processes (e.g., dissolved oxygen) and individual unit-processes were often not delineated. This complicated the use of these studies for calibration and validation purposes.

Finally, papers reporting software development for end users in aquaculture have introduced computerized analysis tools and decision support systems to aquaculture educators, developers, and producers (Lannan, 1993; Bourke et al., 1993; Nath, 1996; Leung and El-Gayar, 1997; Piedrahita et al., 1997; Schulstad, 1997; Wilton and Daley, 1997; Stagnitti and Austin, 1998). The software applications developed by these authors range widely in their internal mechanisms and intended

purpose. The software POND (Nath, 1996; Bolte et al., 2000) is most similar to AquaFarm and some program modules have been jointly developed with AquaFarm.

A current listing and description of software for aquaculture siting, planning, design, and management is available on the Internet (Ernst, 1998). Much of this software falls under the general heading of decision support systems (Sprague and Watson, 1986; Hopgood, 1991), in which quantitative methods and models, rule-based planning and diagnostic procedures (expert systems), and databases are packaged into interactive software applications. The application of decision support systems to aquaculture is relatively recent and has been preceded by the development of simulation models for aquaculture research. Foretelling these trends, decision support systems have been developed for agriculture for purposes of market analysis, selection of crop cultivars, crop production, disease diagnosis, and pesticide application (Bolte et al., 2000). The use of decision support systems for aquaculture design and planning is a relatively recent development and available software applications are essentially first-generation products.

Existing publications that are directly related and complementary to the content of this dissertation, for which the author of this dissertation was a primary author or contributor, include the following (see bibliography for full references; listed in order of most to least recent):

- 1) *Simulation and decision support for aquaculture facility design and management planning* (Ernst et al., 2000)
- 2) *Fish performance engineering* (Ernst, 2000)
- 3) *Computer modeling for system planning, design, and management* (Piedrahita et al., 1999)
- 4) *A listing of computer software for aquaculture* (Ernst, 1998)
- 5) *Computer applications in pond aquaculture – modeling and decision support systems* (Piedrahita et al., 1997).
- 6) *Development of a decision support system for pond aquaculture* (Nath, 1996)
- 7) *Decision support for pond aquaculture planning and management* (Nath et al., 1995)
- 8) *A decision support system for finfish aquaculture* (Ernst et al., 1993)
- 9) *Coupling a graphical user interface with an object oriented simulator for salmon hatcheries* (Bolte et al., 1991)
- 10) *Intelligent agent-based optimization of a salmon hatchery model* (Bolte et al., 1991)
- 11) *A salmonid production model* (Ernst et al., 1983)

2. Development Objectives and Architecture

The purpose of this chapter is to describe (1) the design strategies and criteria used in the development of AquaFarm and (2) the architecture and components that comprise AquaFarm. The development of AquaFarm proceeded according to the objectives and assumptions presented in Chapter 1. The structure and program modules of AquaFarm reflect the physical, biological, and management components of aquaculture facilities, and their definition here provides a framework for the modeling and simulation methods presented in subsequent chapters.

2.1 Functionality objectives

AquaFarm was developed according to a number of functionality objectives, i.e. design criteria. The overall objective was to construct an interactive, comprehensive, system level, simulation and decision support system for the design and management of aquaculture facilities. Components of this overall objective were to:

- 1) Support a wide range of facility types and management intensities for fishery-supplementation and food-fish aquaculture facilities, including broodfish maturation, egg incubation, and growout of finfish and crustaceans, in cage, single pass, serial reuse, water recirculation, and solar-algae pond systems.
- 2) Support a wide range of user objectives, including aquaculture site assessment, facility design, evaluation and comparison of alternative design and management strategies, production forecasting for short and long term management planning, and performance assessment of operating facilities.
- 3) Assist users in the specification of parameters, variables, and components used to represent facilities, provide navigational pathways and templates for data management and analytical procedures, and alleviate the user burden of data and calculation processing.
- 4) Provide users with schedules and summaries of facility operation, including:
 - a) Fish culture schedules: generate management task and performance schedules for fish population numbers, growth, feeding, metabolism, and handling, in response to predicted environmental conditions and as required to achieve fish production objectives.

- b) Facility operation schedules: generate water quality regimes and operation schedules for fish rearing units and water transport and treatment systems, as required to provide environmental conditions for fish biomass support.
- c) Resource use schedules: compile resource use (facility input) and fish production (facility output) schedules for use in facility resource and enterprise budgets.

Since simulation periods can be of any length, AquaFarm can be applied to daily management time scopes as well as seasonal and annual planning. AquaFarm can be used to design new systems or determine production capacities for existing systems. AquaFarm can be used to assess actual fish performance relative to predicted fish performance and to confirm or update fish production objectives. However, AquaFarm is not intended to provide complete functionality for day-to-day management, mainly due to the lack of interface screens and database methods for the management of daily operations data.

2.2 Basis of functionality

The aquaculture science and engineering literature provides an adequate mechanistic basis for the physical, chemical, and biological unit-processes used to represent aquaculture systems. The majority of new work was (1) determining which unit processes were to be included, (2) collecting available methods for these processes from a wide range of sources, (3) instantiating these methods as program modules, and (4) combining methods into an integrated simulation framework. Additional development of new or simplified methods was required for some unit processes, to provide comprehensive coverage and avoid excessive levels of complexity and input data requirements. In contrast, system-level modeling of aquaculture facilities, as networks of linked reactors, was poorly represented in the literature and was newly developed here. Similar to the status of unit-processes, the methods, rules, and procedures of fish culture and aquaculture facility management were found scattered throughout the aquaculture literature and specific to particular facility types and production strategies. No studies were found which formulated this management logic into a comprehensive, adaptable, and integrated decision framework, as developed for AquaFarm.

AquaFarm was developed as a single software application, which addresses a range of purposes through an adaptable user interface and internal functionality. An alternative strategy would have been the development of separate software applications for each major type of

aquaculture system, with further possible divisions based on user expertise level. A singular development approach was chosen based on the large overlap in analytical methods, simulation processing, graphical interface, and data management requirements over the range of aquaculture systems and analytical perspectives. In addition, some aquaculture systems are not easily categorized, for example intensive tank-based recirculation systems characterized by significant levels of phytoplankton and semi-intensive pond-based systems using recirculation systems for phytoplankton management. Interest in these hybrid, semi-intensive and intensive systems is growing rapidly, and their simulation requires essentially all of the methods available in AquaFarm.

2.3 Analysis resolution level

The analysis resolution level (ARL; Table 2.1) used in AquaFarm is user controlled, so that the individual components and complexity level used in a given analysis are appropriate for the type of system under design and stage of the design procedure. This is accomplished by user control over the particular variables and processes considered in a given simulation. For example, depending on the selected ARL, dissolved oxygen can be completely ignored or modeled as a function of one or more sources and sinks, including water flow, passive and active gas transfer, fish consumption, and bacterial and phytoplankton processes. Groups of processes can be selected according to the selected ARL level and processes can be selected individually. For example, an ARL level of three can be used while ignoring water mechanics. Typical progressions of ARL that are used over the course of a design project are described later in this chapter. In the development of AquaFarm, this feature was used to isolate individual processes and process groups for functional testing.

2.4 User responsibilities

In the development of AquaFarm, a workable balance was sought between (1) the level of responsibility (input data and decisions) required from users and (2) the level of analytical rigor used to simulate aquaculture systems. However, these two concerns are directly linked, and a considerable degree of user responsibility is typically required. While simpler analysis resolution levels can be used to reduce user responsibilities, this occurs at the potential expense of predictive accuracy regarding the generation of facility management schedules, resource needs, and fish production quantities.

Table 2.1. Variables and processes considered for analysis resolution levels (ARL) I-V *

ARL	Water quality and loading variables	Processes of facility units and fish lots
I	Day length (hr) ¹ Temperature (C) ¹ Salinity (ppt) ¹ Water flow rate (m ³ /d) Hydraulic loading (m ³ /m ² -d) ³ Hydraulic retention (1/d) ¹ Water velocity (cm/s and fish body lengths/s) ¹ Fish biomass density (kg/m ³ or kg/m ²) ¹ Fish biomass loading (kg/m ³ -d) ^{1,4} Feed loading (kg/d per m ³ /d, or kg/m ³) ^{1,4}	Weather, water mechanics and stratification, water and salinity mass balances, and passive/active heat transfer Fish survival, development and growth, feeding on prepared feeds, and natural fish productivity based on fish density
II	Dissolved oxygen (mg O ₂ /L and % saturation) ¹ Cumulative oxygen consumption (COC, mg O ₂ /L) ¹	Oxygen mass balances based on water flow, passive and active gas transfer, and fish metabolism
III	pH (NBS) ^{1,2} Total alkalinity (mg CaCO ₃ /L) ² Hardness (mg CaCO ₃ /L) ² Dissolved nitrogen (mg N ₂ /L and % saturation) Total gas pressure (mm Hg and % saturation) ¹ Carbon dioxide (mg CO ₂ /L and % saturation) ^{1,2} Dissolved inorganic carbon (mg C/L) ² Total ammonia nitrogen (TAN, mg N/L) ² Unionized ammonia (mg NH ₃ -N/L) ^{1,2} Nitrite (mg NO ₂ -N/L) ^{1,2} Nitrate (mg NO ₃ -N/L) ¹ Dissolved inorganic nitrogen (mg N/L) Dissolved inorganic phosphorous (mg P/L) ² Generic fish treatment chemical (mg/L) ¹ Generic water treatment chemical (mg/L) ¹ Suspended, particulate inorganic solids (mg dw/L) ¹ Settleable, particulate inorganic solids (mg dw/L) ¹ Settleable, particulate organic solids (mg dw/L) ¹ Settled inorganic solids (g dw/m ²) Settled organic solids (g dw/m ²)	Mass balances for listed compounds, including acid-base chemistry, gas transfer, solids settling, soil processes, filtration of solids and compounds, compound addition, bacterial processes, and fish metabolite excretion
IV	Phytoplankton density (g C/m ³ and mg chl-a/m ³) Secchi disk visibility depth (cm)	Phytoplankton processes included in mass balances and natural fish productivity
V	Total borate (mg B/L) ² Total silicate (mg Si/L) ² Total sulfate (mg S/L) ² Total sulfide (mg S/L) ^{1,2}	Additional mass balances for listed compounds

Table 2.1. Continued

- * Variables and processes considered at each level include those in lower levels.
- 1 Water quality and loading variables to which fish performance can respond
- 2 Compounds participating in acid-base and precipitation-dissolution chemistry
- 3 Hydraulic loading is based on water surface area and flow rate
- 4 Fish and feed loading are based on water flow rate

User responsibilities required in the use of AquaFarm include facility specifications (independent variables), model parameters (equation coefficients and exponents), and decisions regarding alternative facility designs and management strategies. Facility specifications include items such as facility location (for generated climates) or climatic regimes (for file-based climates), source water variables, components and configurations fish culture systems, and management strategies and production objectives. While approximate environmental conditions, typical facility configurations, and typical management strategies can be provided by AquaFarm, it is not possible to avoid user responsibility for these site-specific variables. In contrast, model parameters for passive unit processes (e.g., heat and gas transfer and biological processes) are ideally independent of site-specific conditions, given the use of sufficiently developed models. Due to the necessity of simplifying assumptions and aggregated processes in aquacultural modeling, however, model parameters may be dependent on site-specific conditions to some degree (Svirezhev et al., 1984). While a considerable effort has been made to minimize this dependency, and standard (default) values are provided for all parameters, most model parameters have been made user accessible for any necessary adjustment. Additional solutions to the dilemma of user responsibility versus analytical capacity and accuracy are addresses in Chapter 9. Finally, the purpose of AquaFarm is to support design and management decisions, but these decisions must still be made by the user. Some level of user responsibility cannot be avoided regarding the underlying processes impacting system performance and implications of alternative decisions on facility performance and economics.

2.5 AquaFarm programming

AquaFarm is a stand-alone computer application, programmed in Borland C++® and requiring a PC-based Microsoft Windows® operating environment. The C++ computer language was chosen for its popularity, portability, availability of software developer tools, compatibility with the chosen graphical user interface (Microsoft Windows®), and support of object oriented programming (OOP; Budd 1991; Bolte et al., 2000). According to OOP methods, all components of AquaFarm

are represented as program “objects”. These objects are used to represent abstract entities (e.g., graphical user interface) and real-world entities (e.g., fish lots and rearing units) and are organized into hierarchical structures. Each object contains data, local and inherited methods, and mechanisms to communicate with other objects as needed. The modular, structured program architecture supported by OOP is particularly suited to the development of complex, flexible system-models such as AquaFarm.

2.6 AquaFarm design procedure

AquaFarm supports interactive design procedures, utilizing progressive levels of analysis complexity, simulation based analyses, and iterative design refinement (James, 1984). These procedures are used to develop design and management specifications, until production objectives are achieved or are determined to be biologically or practically infeasible. This decision making process is user directed and can be used to design new systems or determine production capacities for existing systems. Major steps of a typical design procedure are listed below and flow charted in Figure 2.1. A summary of input and output data considered by AquaFarm is provided in Table 2.2.

- 1) *Resolution*. An analysis resolution level is selected that is compatible with the type of facility and stage of the design procedure.
- 2) *Specification*. Facility environment, design, and management specifications are established, based on known and tentative information.
- 3) *Simulation*. The facility is simulated to generate facility performance summaries and operation schedules over the course of one or more production seasons.
- 4) *Evaluation*. Predicted facility performance and operation are reviewed and evaluated, using summary reports, tabular and graphical data presentation, management logs, and enterprise budgets.
- 5) *Iteration*. As necessary, facility design, management methods, and/or production objectives are adjusted so that production objectives and other desired results are achieved (go to step 1 or 2).

In conjunction with progressive analysis resolution, a design procedure can be staged by the level of scope and detail used in specifying physical components and management strategies of a given facility. For example, design analyses can start with fish performance, using simplified

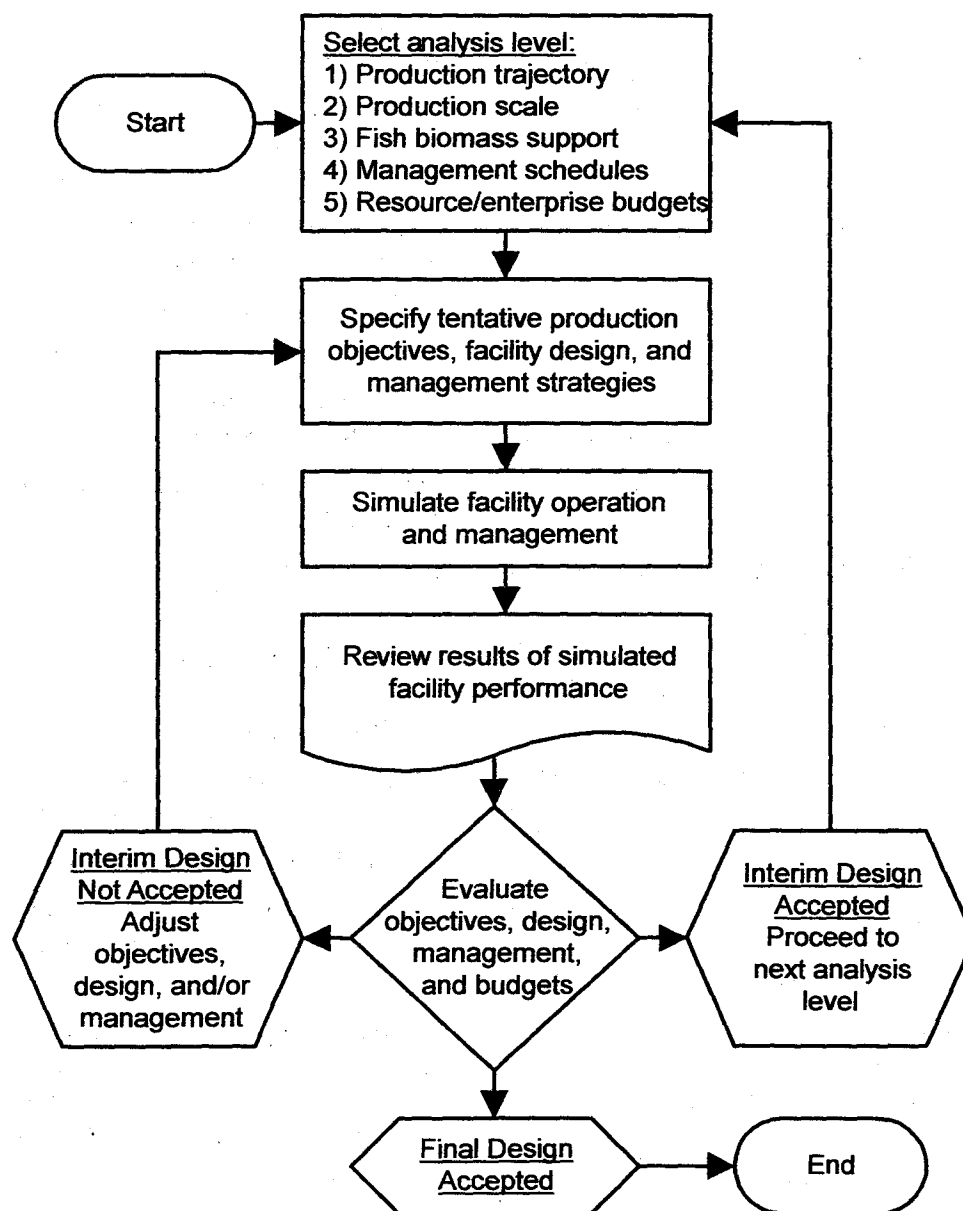


Figure 2.1. Flowchart of the decision support procedure used by AquaFarm for aquaculture facility design and management planning, including progressive analysis levels and iterative procedures of facility and management specification, simulation, and evaluation

Table 2.2. Summary of input specification and output performance data considered by AquaFarm

Input data: facility and management specifications
<ul style="list-style-type: none"> • Selection of alternative methods for some unit processes and possible adjustment of parameters for passive physical, chemical, and biological unit-processes and fish performance models • Facility location (or climate data files), optional facility housing and controlled climate, and water quality and capacity of source water(s) • Configurations of facility units for facility water transport, water treatment, and fish culture systems • Specifications of individual facility units, including dimensions, elevations and hydraulics, soil and materials, housing, and water transport and treatment processes • Fish species, fish and facility management strategies, and production objectives (target fish weights/states and numbers at given future dates) • Unit costs for budget items and additional budget items not generated by AquaFarm
Output data: facility performance and fish production
<ul style="list-style-type: none"> • Fish number and development schedules for broodfish maturation and egg incubation • Fish number, weight, and feed application schedules for fish growout, including optional consideration of fish weight distributions within a fish lot • Fish rearing unit usage and fish lot handling schedules • Tabular and graphical compilations of time-series data for fish performance variables, reported on a fish population and individual fish lot basis, including fish numbers and state, bioenergetic and feeding variables, and biomass loading and water quality variables • Tabular and graphical compilations of time-series data for facility performance variables, reported on a facility and individual facility unit basis, including climate, water quality, fish and feed loading, water flow rates and budgets, compound budgets, process rates, resource use, waste production, and water discharge • Fish production reports, resource use summaries, and enterprise budgets

facilities and a minimum of water quality variables and unit processes. When satisfactory results are achieved at simpler levels, increased levels of complexity for modeling facility performance and management strategies are used. By this approach, the feasibility of rearing a given species and biomass of fish under expected environmental conditions is determined before the specific culture system, resource, and economic requirements necessary to provide this culture environment are developed. Major stages of a typical design procedure are listed below, but this progression is completely user controlled.

- 1) *Production trajectory*. Fish development, growth, and feeding schedules for broodfish maturation, egg incubation, and/or fish growout are determined based on initial and target fish states. Environmental quality concerns are limited to water temperature and day length, and unit processes are limited to water flow and heat transfer.
- 2) *Production scale*. Required water area and volume requirements for fish rearing units are determined, based on initial and target fish numbers, management methods, and biomass density criteria. Natural fish productivity, if considered, is a function of fish density only.
- 3) *Biomass support*. Based on fish feed and metabolic loading, facility water transport and treatment systems are constructed to provide fish rearing units with required water flow rates and water quality. The particular variables and unit processes considered depend on the type of facility. Natural fish productivity, if considered, may consider primary productivity as well as fish density.
- 4) *Management schedules*. Fish and facility management methods and schedules are finalized, including operation of culture systems, fish lot handling, and fish number, weight, and feeding schedules.
- 5) *Resource budgets*. Resource and enterprise budgets are generated and reviewed.

2.7 AquaFarm architecture and components

AquaFarm consists of five major components (Figure 2.2): (1) graphical user interface and data manager, (2) simulation manager, (3) domain experts, (4) facility components, and (5) facility managers. The first two of these are specific to AquaFarm while the last three represent real-world entities and have meaning beyond AquaFarm.

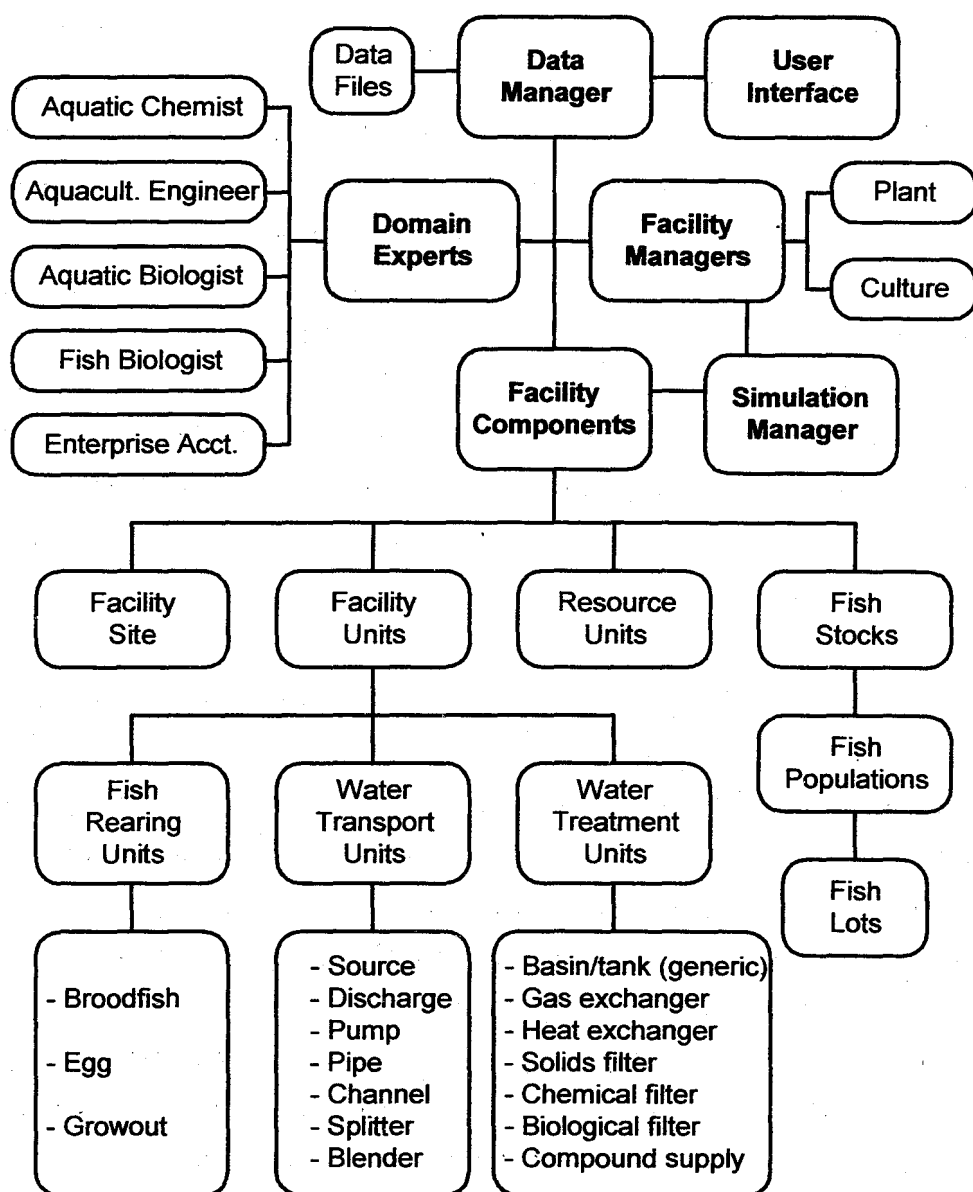


Figure 2.2. Overview of the software architecture and program components that comprise AquaFarm (see Table 3 for facility unit descriptions). Connecting lines denote communication pathways for method and data access.

The *graphical user interface* and *data manager* are described below. The *simulation manager* coordinates and processes facility simulations and is described in Chapter 3. *Domain experts* provide expertise in various knowledge domains of aquaculture science and engineering. Domain expert methods consist of property, equilibrium, and rate calculations of physical, chemical, and biological unit processes and their rules of application. These methods are used to calculate terms in facility-unit and fish-lot state equations and to support management analyses. Domain experts include an enterprise accountant (described below), aquatic chemist (Chapter 4), aquacultural engineer (Chapter 5), aquatic biologist (Chapter 6), and fish biologist (Chapter 7). *Facility components* represent the physical facility and include *facility units*, *resource units*, *fish stocks*, *fish populations*, and *fish lots* (described below). *Facility managers* are responsible for facility management tasks and production scheduling and include a *physical plant manager* and *fish culture manager* (Chapter 3). The italicized text used above denotes terms with specific meanings, as defined here.

2.7.1 Graphical user interface and data manager

The user interface is typical of window-based software, providing a hierarchical menu system and selectable viewing windows that support general-to-specific interface navigation. Types of windows include tool bars, facility maps, specification sheets, output tables and graphs, management schedules, budget spreadsheets, and user help screens. Examples of the interface are shown in Figures 2.3 – 2.12 (see Table 2.3 for key to facility unit names). According to the type of facility under design and analysis resolution level in use, user access to windows, controls, and data fields is limited to relevant items. Data files are used to store and retrieve user projects, with specification and review mechanisms for data files provided within AquaFarm. Output data can be exported in delimited format for use in computer spreadsheets. In total, the user has full control over the modeling, facility, and management specifications itemized in Table 2.2 and full access to all simulation generated data. To support this capacity, the requirements for the graphical user interface and data management capabilities are extensive and represent about one-third of the total program code.

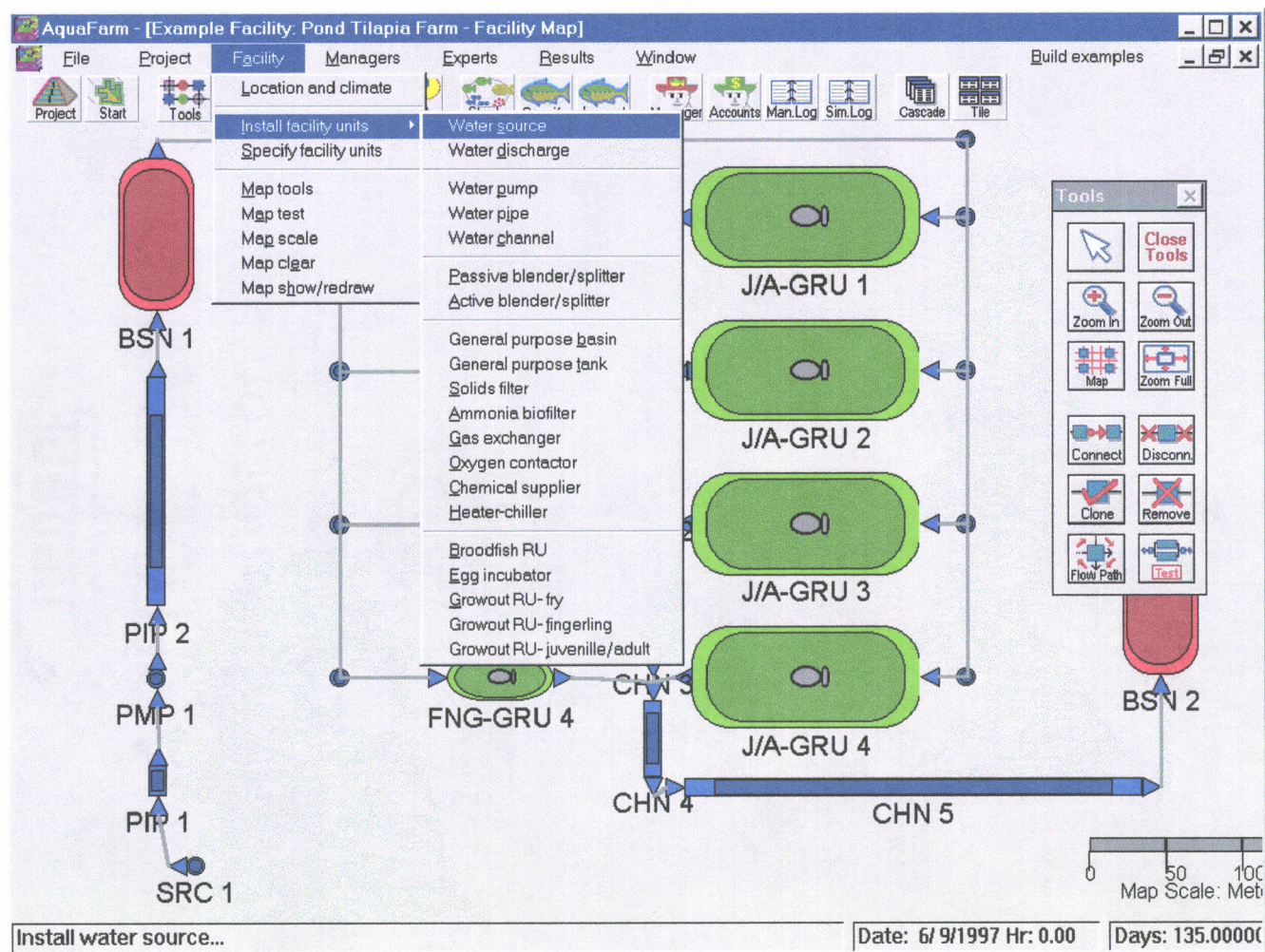


Figure 2.3. Map window: example pond facility, consisting of fish ponds supplied by pumped ground water and gravity flow (head basin, supply pipes, and discharge channels), showing drop-down menu and tool bar for facility construction

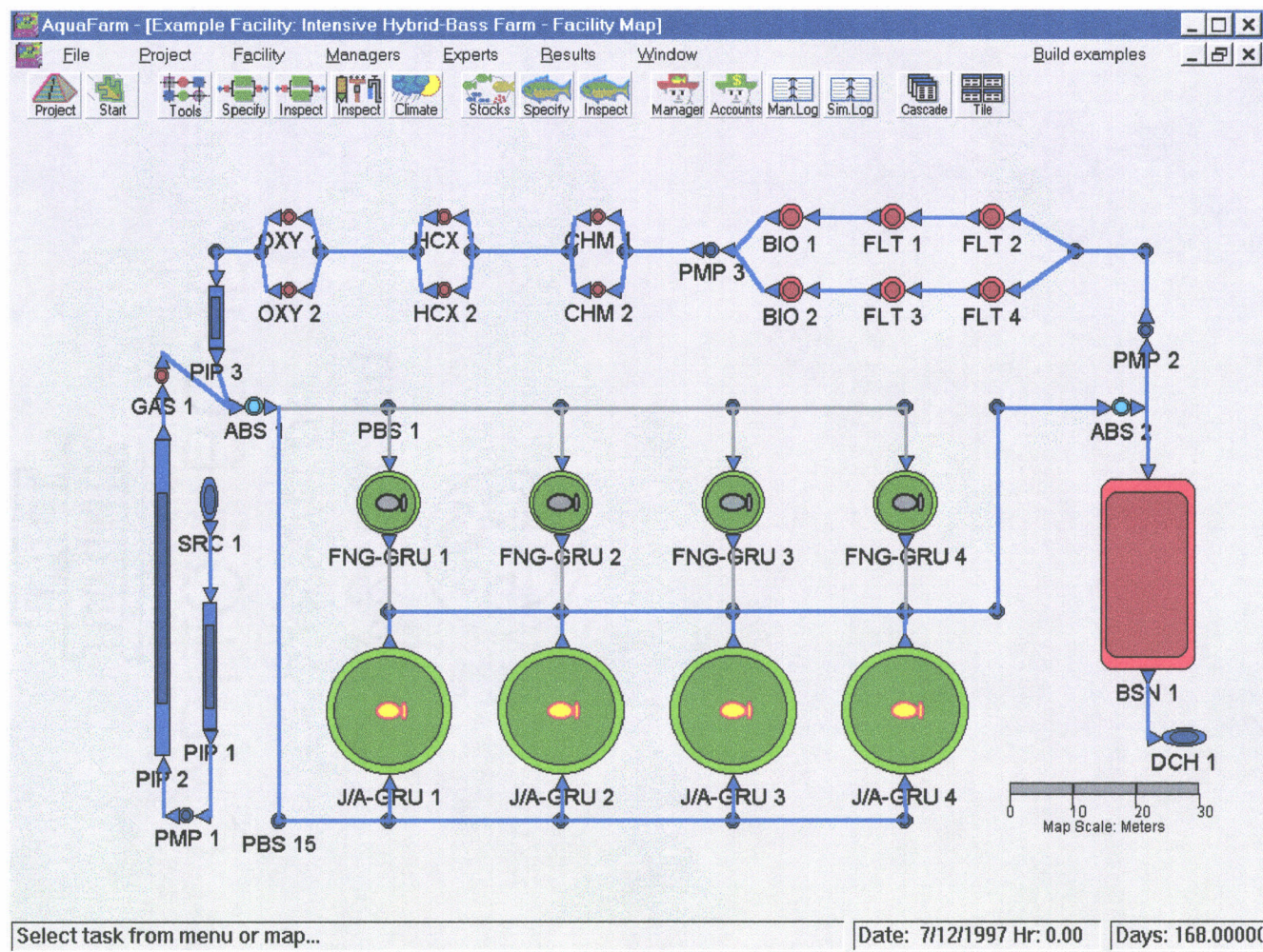


Figure 2.4. Map window: example water recirculation facility, consisting of fish rearing units supplied by a single recirculation loop with water makeup supply and water/solids discharge

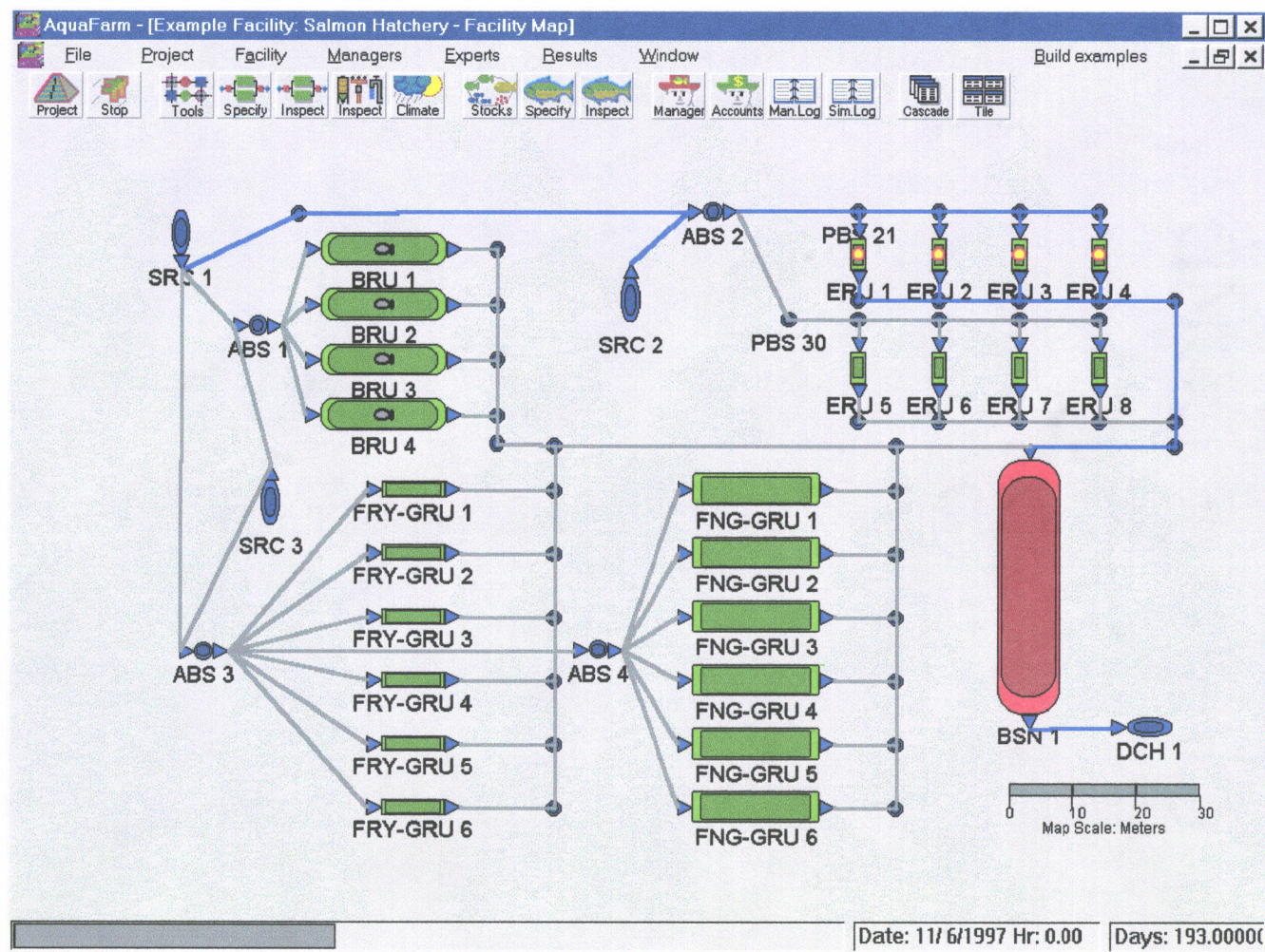


Figure 2.5. Map window: example salmon hatchery, including broodfish maturation, egg incubation, and fry to fingerling growout (current production stage is egg incubation)

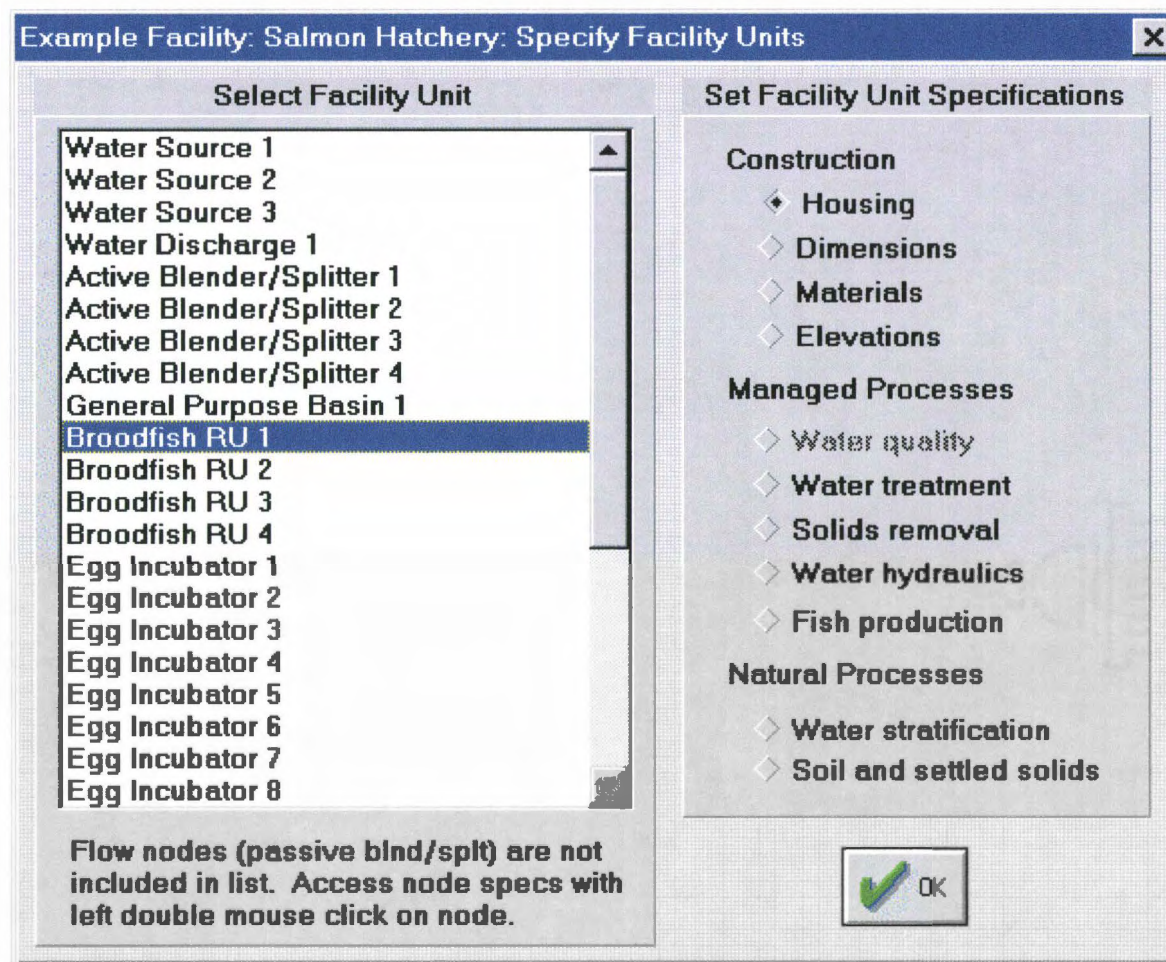


Figure 2.6. Interface screen: access menu for facility-unit specification (e.g., salmon hatchery), for which menu items are enabled/disabled according to the selected facility unit and analysis resolution level in use

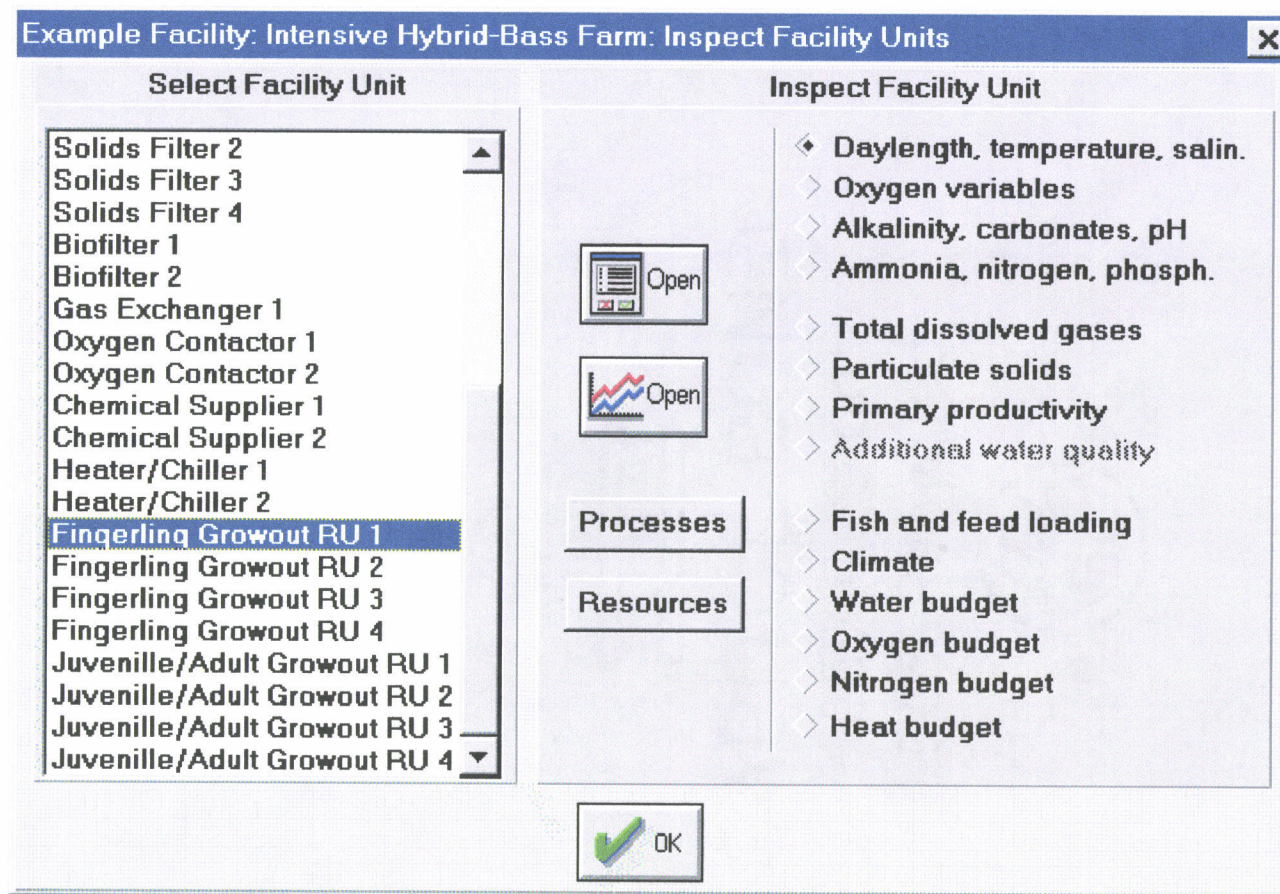


Figure 2.7. Interface screen: access menu for facility-unit inspection (tables and graphs) following a simulation (e.g., recirculation facility), for which menu items are enabled/disabled according to the selected facility unit and analysis resolution level in use

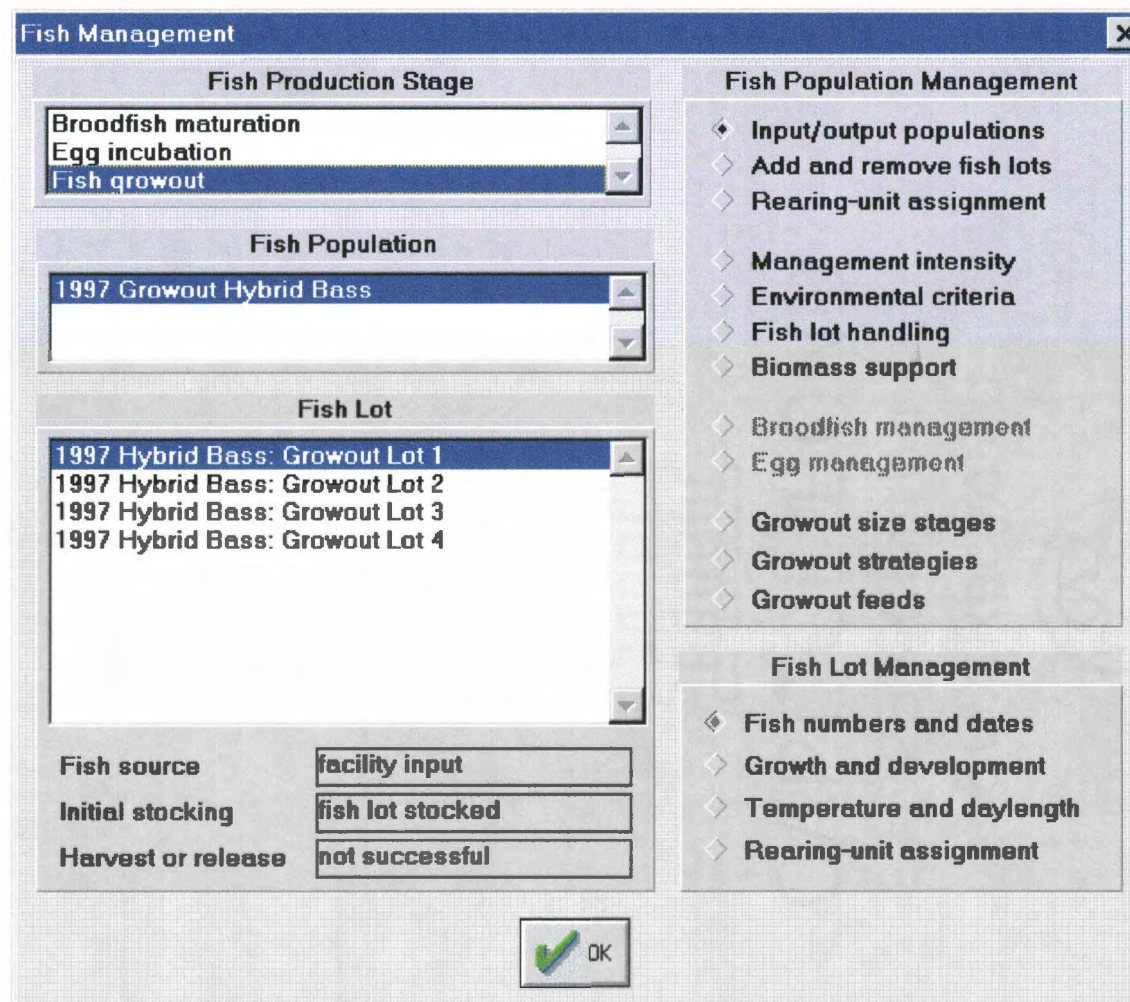


Figure 2.8. Interface screen: access menu for management specification of fish populations and lots, for which menu items are enabled/disabled according to the selected fish lot and analysis resolution level in use

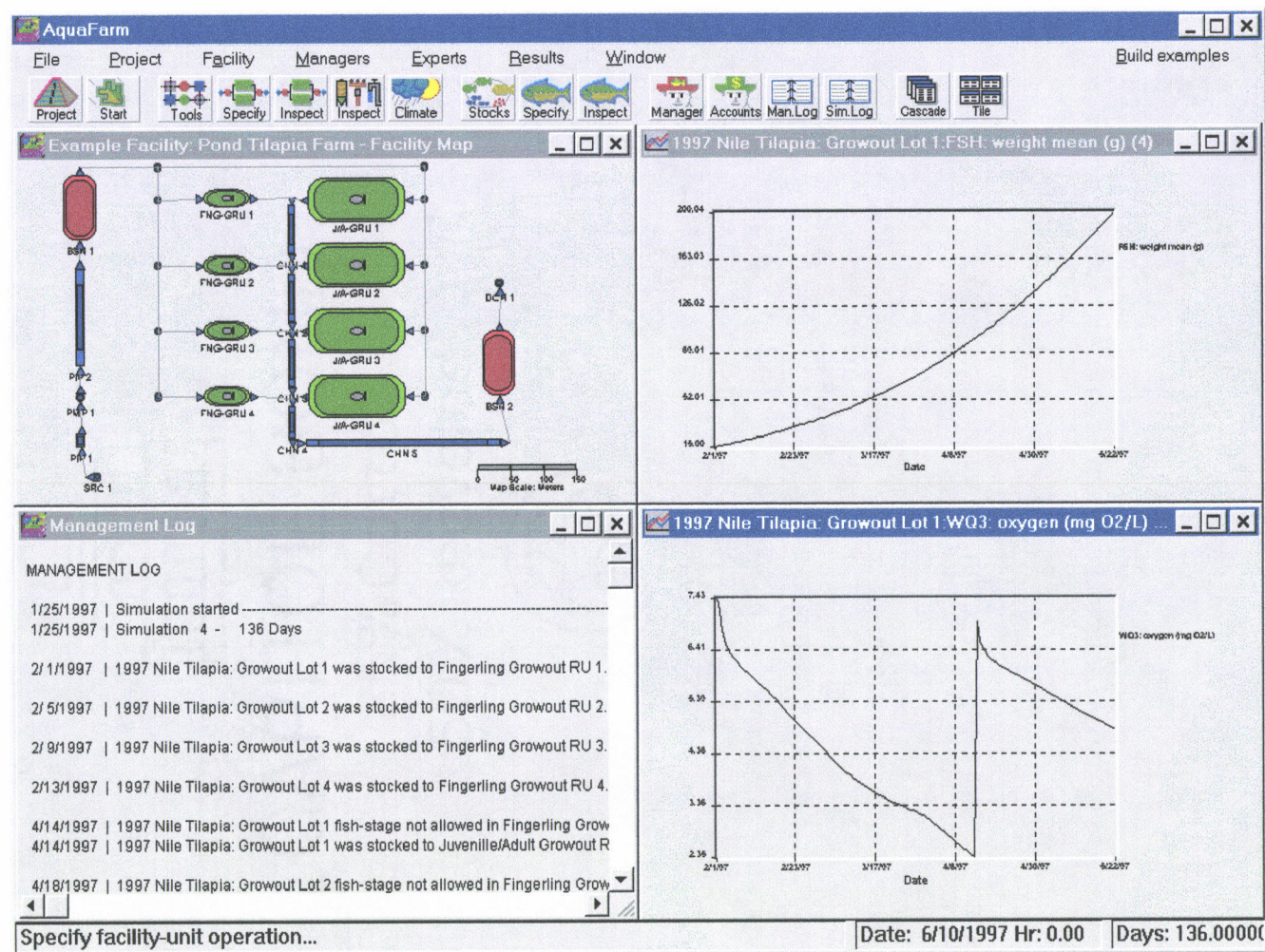


Figure 2.10. Interface screens: example of multiple, tiled screens for review of simulation results (facility map, management log, and fish lot data graphs)

2.7.2 Enterprise accountant

The enterprise accountant is one of the five domain experts, but is not large enough in scope to warrant a separate chapter. The enterprise accountant is responsible for compiling enterprise budgets, which are used to quantify net profit or loss over specified production periods (Meade, 1989; Engle et al., 1997). Enterprise budgets are particularly appropriate for comparing alternative facility designs, in which partial budgets are utilized that focus on cost and revenue items significantly influenced by proposed changes. Additional financial statements (e.g., cash flow and net worth), economic feasibility analyses (e.g., net present value and internal rate of return), and market analyses are required for comprehensive economic analyses (Shang, 1981; Allen et al., 1984; Meade, 1989) but are not supported by AquaFarm.

Individual cost items (e.g., fish feed) and revenue items (e.g., produced fish) can be specified and budgets can be summarized according to various (1) production *bases*, (2) time *periods*, and (3) cost *types* (Figures 2.11 and 2.12):

- 1) Item and budget bases can be per unit production area, per unit fish production, or per production facility. For example, scalable items such as seasonal labor and fish culture equipment can be expressed per unit production or area, while non-scalable items are expressed in terms of the entire facility.
- 2) Item periods, over which cost and income amounts are accrued, can be daily, annual, production cycle (e.g., simulation period), or any user-specified period. The budget reporting period is based on user-specified starting and ending dates, for which the default reporting period is the simulation period. Each budget item may be continuous or discontinuous over the budget period, the latter using specified starting and ending dates of cost/income accrual. The cost or revenue amount of each item in a particular budget is based on its temporal overlap with the budget reporting period, for which continuous items fully overlap the reporting period and the overlap of discontinuous items may be full, partial, or none.
- 3) Cost (or revenue) types include fixed and variable costs, as determined by their independence or dependence on production output, respectively. Fixed costs include items such as management, maintenance, insurance, taxes, interest on owned capital (opportunity costs), interest on borrowed capital, and depreciation for durable assets with finite lifetimes. Variable

costs include items such as seasonal labor, energy and materials, equipment repair, and interest on operational capital. Interest rates for fixed and variable costs may be separately specified.

Enterprise budgets are built by combining simulation-generated and user-specified cost and revenue items. Each item is quantified by a unit cost or price (the cost/income associated with one unit of the item) and the number of units used/produced in the budget period. Simulation generated items are those directly associated with aquaculture production and therefore predicted by AquaFarm (e.g., facility units, energy and material consumption, and produced fish and wastes.) AquaFarm determines total quantities for these items (numbers of units), but the user is responsible for unit costs and other specifications (e.g. interest rates, useful lives, and salvage values). User specified items include additional cost and revenue items (e.g., supplies, equipment, facility infrastructure, and labor). For user specified items that are scalable, the use of unitized cost bases (i.e., per unit production area or production output) alleviates the need to re-specify item quantities when working through multiple design scenarios.

The budget is shown in spreadsheet format for the selected budget basis and period, with cost and revenue items totaled and net profit or loss calculated (Figure 2.12). Net profits can be used as net returns to any cost items that are not included in the budget, e.g. net return to land, labor, and/or management. Cost items are organized under subheadings of 'Fixed Costs', 'Variable Costs', and 'Depreciable-asset Costs'. Revenue items are listed under the subheading 'Income'.

Depreciation costs for durable assets with finite lifetimes are based on their useful lives, salvage values, and length of the budget reporting period. Straight-line depreciation is assumed, i.e. the value of the asset decreases linearly over time. The total depreciation cost accrued is bounded by the useful life of the asset and is scaled to the budget basis (per unit area, fish production, or total facility). It is assumed that depreciable costs occur throughout the budget reporting period, unless the reporting period exceeds the useful life of the asset. The depreciation cost for a given item is calculated by:

$$DC = NU (UC - SV) RP / UL$$

where DC = depreciation cost (\$), NU = number of units, UC = unit cost of item (\$), SV = salvage value (\$), RP = reporting period (years), and UL = useful life (years). If RP is greater than UL, then:

$$DC = NU (UC - SV)$$

The interest cost for a depreciable item for the budget reporting period is based on the depreciation schedule defined above and the average value of the asset over its useful life. The total interest accrued is bounded by the useful life of the asset and is scaled to the budget basis. Interest costs are calculated by:

$$IC = NU [(UC + SV) / 2] (IR / 100) \min\{RP, UL\}$$

where IC = interest cost (\$) and IR = fixed interest rate (%/year).

Cost Parameters (cost.db)

Asset cost, and income items

Name of item..... **Feed -pellet 6-mm (kg)**

☒ Include in budget

<<< >>> Add Copy Remove

Units of item used or produced for the given resource and time bases **20499.8**

Cost or price (\$/unit/.....) **0.20**

Resource basis of cost or price

☐ Per unit production (\$/unit/kg fish)

☐ Per unit water area (\$/unit/m2)

☒ Per total facility (\$/unit/facility)

Type of item

☐ Income

☐ Item used for 'per unit production'

☒ Variable cost (set interest rate at budget)

☐ Fixed cost (set interest rate at budget)

☐ Depreciable asset

Salvage value

Useful life (years)

Time basis of cost or price

Item used throughout production period: (set production period at budget)

☐ Per day (\$/unit/day)

☐ Per year (\$/unit/year)

☐ Per prod. period (\$/unit/period)

Item used over given period:

☐ Per day (\$/unit/day)

☒ Per given period (\$/unit/period)

Period	Begin	End
Month	Jun	Aug
Day	4	19
Year	2000	2000

OK Load from Disk Save to Disk Help Cancel

Figure 2.11. Interface screen: budget item specification sheet

Economic Report

	Item Description	Cost/Unit	# Units	Total Cost
1	Reporting Period: 2/23/2000 - 10/9/2000			
2				
3	INCOME			
4	Fish stage-6 output (fish)	0.00	56000.00	0.00
5	Fish stage-6 output (kg)	2.00	25678.59	51357.18
6	Total Income			51357.18
7				
8	FIXED COSTS			
9	Combined fixed costs	10000.00	1.00	6284.15
10	Interest on Fixed Costs	0.10		
11	Total Fixed Costs			6912.57
12				
13	DEPRECIABLE-ASSET COSTS			
14	Water Source	1000.00	1.00	-
15	Interest			31.51
16	Depreciation			21.00
17	Juvenile/Adult Growout RU	1000.00	1.00	-
18	Interest			31.51
19	Depreciation			21.00
20	Water Discharge	1000.00	1.00	-
21	Interest			31.51
22	Depreciation			21.00
23	Total Depreciable-Asset Costs			250.00
24				
25	VARIABLE COSTS			
26	Fish stage-3 input (fish)	0.00	57205.60	0.00

To add new items, click Edit...
To respecify items, double-click on item name or select item and click Edit...

OK Edit Help Cancel

Interest rates (%/year)

Variable costs 10.00

Fixed costs 10.00

Resource basis of budget

☒ Total facility

☐ Per unit of Area

☐ Per unit of Production

Reporting period of budget

Begin End

Month Feb Oct

Day 23 9

Year 2000 2000

<< Full Year >>

<< Previous Year

Next Year >>

Set reporting period to production period...

Reset

Figure 2.12. Interface screen: enterprise budget (entire budget is viewed by use of the scroll bar)

2.7.3 Fish stocks, populations, and lots

Production fish are represented at three levels of organization: fish stocks, fish populations, and fish lots. A fish stock consists of one or more fish populations, and a fish population is divided into one or more fish lots. A fish stock is a fish species or genetically distinct stock of fish, identified by common and scientific names and defined by a set of biological performance parameters. Parameter values are provided for major aquaculture species and can be added for additional aquaculture species. Fish populations provide a level of organization for the management and reporting tasks of related, cohort fish lots. Fish populations are uniquely identified by their origin fish stock, life stage (broodfish, egg, or growout), and production year. Broodfish, egg, and growout fish populations from the same fish stock are linked by life stage transfers, i.e. from broodfish spawning to egg stocking and from egg hatching to larvae/fry stocking.

Fish lots are fish management units within a fish population. Fish lots are defined by their current location (rearing unit), population size, and development state. The latter consists of accumulated temperature units (ATU) and photoperiod units (APU) for broodfish lots, accumulated temperature units for egg lots, and fish body weights for growout fish lots. At a point in time, fish lot states are maintained as mean values, and fish weights within a growout fish lot can be represented as weight distributions (histograms). Variability in fish weights within a growout fish lot can be due to variability present at facility input, fish lot division and combining, and variability in fish growth rates due to fish sex, genetics, and competition for limited food resources. Target values for fish lot numbers, states, and dates at harvest or release are specified as production objectives. Methods used to manage fish production and achieve production objectives are described in Chapter 3. Methods used to model fish survival, development and growth, feeding, and metabolism are described in Chapter 7.

2.7.4 Facility site, facility units, and resource units

An aquaculture facility is represented by a facility site, facility units, and resource units. A facility site consists of a given location (latitude, longitude, and altitude), ambient or controlled climate, and configuration of facility units. Facility units consist of water transport units, water treatment units, and fish rearing units (Table 2.3). Resource units supply energy and material resources to facility units, maintain combined peak and mean usage rates for sizing of resource supplies, and compile total resource quantities for use in enterprise budgets (Table 2.4).

A facility configuration is completely user specified and can consist of any combination of facility unit types linked into serial and parallel arrays. A facility is built by selecting (from menu), positioning, and connecting facility units on the facility map. Lines connecting facility units on the facility map may represent either a direct connection or an indirect connection via an ignored water transport unit(s). Each type of facility unit is provided with default specifications and characteristic processes at construction, and specifications are adjusted and additional processes are added as needed. Facility units are shown to scale, in plan view, color coded by type, and labeled by name. To visualize the progress of simulations, date and time are shown, colors used for water flow routes denote presence of water flow, and fish icons over rearing units denote presence of fish as they are stocked, removed, and moved within the facility.

Table 2.3. Facility unit types and primary processes *

Facility unit type	Primary processes
Water transport units	
Source (SRC)	Facility influent flow capacity and water quality
Discharge (DCH)	Facility effluent cumulative water and compound discharge
Pump (PMP)	Water pump performance and power/air consumption for centrifugal and airlift pumps
Pipe (PIP)	Pressurized and gravity water flow mechanics
Channel (CHN)	Gravity water flow mechanics
Blender/splitter (ABS)	Active flow stream blending and division for specialized flow rate control, temperature and salinity blending, management of parallel groups of facility units, and water recirculation.
Flow node (PBS)	Passive flow stream blending, division, and redirection
Water treatment units	
Water basin/tank (BSN/TNK)	Water retention for head and sump tanks and a variety of water treatment processes (e.g. parallel plate or tube settling basins)
Gas exchanger (GAS)	Water aeration, degassing, and oxygenation in air-contact units and pure oxygen absorbers, including packed/spray columns, water surface aerators, submerged venturis and diffusers, and oxygenators
Heat exchanger (HCX)	Water heating and chilling using inline and in-tank, elements and exchangers
Mechanical filter (FLT)	Filtration of particulate solids, including granular media filters, porous media filters, micro screens, particle separators (hydroclones, swirl separators), and foam fractionators
Chemical filter (CFL)	Filtration of ammonium by ion-exchange (clinoptilolite) and chlorine by adsorption (granular activated carbon)
Biological filter (BIO)	Bacterial conversion of nitrogen compounds by fixed-film nitrification or denitrification biofilters (trickling, RBC, expandable granular media, and fluidized bed). Wetland and hydroponic units for nutrient uptake (DIN and DIP) and retention of particulate solids.
Compound supplier (CHM)	Addition of water treatment compounds for water conditioning, nutrient supply, disinfection, and fish treatment (see Table 2.4)
Fish rearing units	
Broodfish holding (BRU)	Broodfish maturation: biomass, feed, and metabolic loading
Egg incubator (ERU)	Egg incubation: biomass and metabolic loading
Growout rearing (FRY-, FNG-, J/A-GRU)	Fish growout: biomass, feed, and metabolic loading (default types: fry, fingerling, and juvenile/adult)

* Names in parentheses are abbreviations for facility mapping. Processes in addition to primary processes can be considered depending on facility unit type (e.g. inclusion of gas exchangers and compound suppliers in fish rearing units or hydraulic solids removal in a water splitter)

Table 2.4. Resources produced and consumed by an aquaculture facility that can be calculated by AquaFarm *

Resource Type	Resource Description ¹
Facility units	Total numbers of each type of facility unit and quantities of materials used (m^2 or m^3): metal, wood, concrete, fiberglass, PVC, PE, ABS, acrylic, glass, shade tarp, and insulation (see Chapter 5, Table 5.6)
Supply water	Source water consumption (m^3)
Discharge water	Cumulative discharge water (m^3) and quantities of solids, DIN, DIP, BOD, and COD (kg)
Waste materials	Waste sludge (kg dw), spent filter media (m^3), and dead fish (kg ww)
Energy	Energy consumed by facility lighting, water pumps, gas and heat exchangers, UV sterilizers, etc., expressed as electrical power (kWhr) or energy equivalent of liquid fuels (L; gasoline, methanol, and diesel) or gas fuels (m^3 ; natural gas, propane, and methane)
Compressed air	Compressed air for air-lift pumps, column aerators (optional), air diffusers, and foam fractionators (m^3 air and equivalent energy as kWhr for air compression and delivery)
Water treatment compounds	Compounds added to water for water treatment (kg): (1) Inorganic and organic fertilizers (user specified composition: C, N, P, and organic content), (2) pH and alkalinity adjustment compounds (carbon dioxide, nitric, sulfuric, and phosphoric acid, sodium hydroxide, sodium bicarbonate and carbonate, agricultural limestone, and hydrated and burnt lime), and (3) pure oxygen, sea salt, and various user-defined fish/egg treatment, water conditioning, and water disinfection compounds
Filter media	Filter media for mechanical, chemical, and biological filters (m^3): sand, expanded plastic, plastic beads, gravel/rock, fabric, clinoptilolite, granular activated carbon, and hydroponic and wetland materials. Quantities include original and replacement media, the latter based on the allowed number of regeneration cycles
Fish feed	Prepared fish feeds (kg): larval, flake, mash, pellet sizes 0.5 to 10.0 mm, and broodfish feeds
Stocked and produced fish	Broodfish, eggs, and growout fish (number, kg) input and output by the facility
Labor	To assist specification of required labor, the enterprise budget provides (1) per unit production area and per unit fish production cost bases, (2) total time of fish culture (days), and (3) numbers of management tasks completed for process rate adjustments and fish feeding and handling events

* Additional facility infrastructure, equipment, supplies, and labor resources are the responsibility of the user and are specified at the facility enterprise budget.

¹ Quantitative units given for resources may be reported per day, per year, and/or per production season

2.7.4.1 Facility unit specifications

Facility unit specifications include housing, dimensions and materials, and actively managed processes of water transport, water treatment, and fish production. The purpose of these specifications is to support facility unit modeling. Individual unit processes and associated specifications can be ignored or included, depending on user design objectives and analysis resolution level. Default facility unit specifications are provided during facility construction, but these variables are highly specific to a particular design project and are therefore user accessible. Related considerations of facility unit construction, dimensions, materials, and hydraulics are provided in Chapter 5. Managed (active) processes of water transport, water treatment, and fish production are operated according to the specifications of individual facility units, in addition to management criteria and protocols assigned to facility managers (Chapter 3).

An entire facility, fish rearing system, or individual facility unit can be housed in an opaque structure (no solar radiation; controlled daylength by artificial lighting) or greenhouse structure (ambient solar radiation and daylength). For any structure, air temperature and humidity can be ambient or controlled, wind speed is set to a minimum value (0.1 m/s), and precipitation is zero. Facility units exposed to solar radiation can be equipped with shade cloth of a given rating.

Top, side, and/or bottom walls (walls are optional depending on soil grade) of a facility unit can be constructed from a variety of materials, including structural, insulating, light blocking or passing, water impermeable, and cage mesh materials. Wall materials may be laminated, for example consisting of a water impermeable layer, a structural layer, and an insulation layer. Certain types of facility units (e.g., filters and packed column aerators) are filled with some type of packing media (e.g. sand, plastic beads, or plastic shapes). Media specifications include the proportion of the total water volume to be filled with media (bulk volume), void volume, and surface-volume ratio. For soil lined facility units, soil composition and related variables are not used. Rather, soils are indirectly specified through given water seepage rates and compound uptake and release rates. The quantity of accumulated sediments (settled solids) from prior production seasons can be specified (g dw/m^2). Passive heat transfer between water and soil is ignored.

Facility units can be almost any shape and dimensions, including rectangular (with rounded corners of any radius or completely rounded ends), cylindrical and cylindrical-conical, and tubular (pipes). Irregular polygons are not considered. The top wall of a rectangular or cylindrical-conical facility unit is optional and may consist of a suspended cover that allows airflow over the water

surface or an attached and sealed wall such as used for a pressurized facility unit. Side walls can be sloped (e.g., levee ponds). Facility units are assigned a mean depth capacity and minimum freeboard, but the slope of the facility unit bottom wall is not considered. However, an entire facility unit can be sloped (e.g., water channels), where influent and effluent ends can be assigned elevations with respect to the mean facility elevation. Facility units can be buried (e.g., pipes), placed at soil grade (e.g., ponds), or placed partially or completely above the soil grade (e.g., solid and ammonia filters).

2.7.4.2 Water transport units

Water transport units are used to contain, blend, divide, and control water flow streams (Table 2.3). Water transport units are installed as necessary to adequately represent water transport systems and to determine flow rate capacity limits and pump power requirements. To simplify facility construction, pipe fittings (e.g. elbows, tees, and valves) and short lengths of pipes and channels can be ignored. For clarity in mapping, however, water flow nodes can be used to represent all points of blending, division, and redirection of water flow streams by pipe fittings and channel junctions. Any facility unit can have multiple influent and effluent flow streams. Minor head losses of pipe fittings are calculated as a given proportion of the major head losses of associated pipe lengths and pressurized facility units (see Chapter 5, Water Mechanics). Flow control devices for pipes and channels are assumed to exist, but they are not explicitly defined. Specialized water blenders and splitters are used for designated purposes, such as water flow blending for temperature and salinity adjustment and water flow division to achieve desired water recirculation rates (see Chapter 3).

2.7.4.3 Water treatment units

Water treatment units are used to add, remove, and convert water borne compounds and adjust water temperature (Table 2.3). Water treatment units typically specialize in a particular unit process, but processes can be combined with a single facility unit as desired. Methods used to control process rates of water treatment units are described in Chapter 3 (Process management).

2.7.4.4 Fish rearing units

Fish rearing units can be designated for particular fish stocks (fish species), fish life stages (broodfish, eggs, and growout fish), and fish size stages (e.g. fry, fingerling, and juvenile/adult) (Table 2.3). These designations are used in the management and movement of fish lots within the

facility, as based on fish sizes and management strategies for multiple life-stage, multi-species, and polyculture facilities. Fish rearing units can include most water treatment processes (e.g., fertilization, liming, and aeration) and can utilize process control methods as described for water treatment units.

2.7.4.5 Facility unit state variables

In addition to facility unit specifications, which are fixed for a given simulation, facility units are defined by dynamic state variables that vary over the course of a simulation. These variables consist of operational variables (e.g., water flow rate and process rates) and water quality variables, as typically used in aquacultural engineering. Water quality variables are listed in Table 2.1, and Chapters 4-7 provide additional information on the quantification and practical importance of water quality variables. The variables selected for consideration were chosen due to their potential impact on facility performance for all types of systems. For specific system types and conditions, some variables can have negligible importance and can be ignored.

For facility units other than water sources, water quality variables are determined by simulation. For water sources, water quality is specified, including temperature regimes, gas saturation levels, optional carbon dioxide and calcium carbonate equilibria conditions, and constant values for the remaining variables. Water source temperature regimes may be specified using input data files (similar to climate data files and containing periodic daily mean, minimum, and maximum temperatures) or more simply as annual regimes of monthly mean temperatures and magnitudes and timing of diurnal temperature oscillations.

Water temperature is a fundamental driving variable of aquaculture systems. All physical, chemical, and biological processes respond to temperature, for which process rates increase by factors of about 1.3 to 2.0 for each 10 °C increase in temperature (a temperature range of 0 – 40 °C is considered in AquaFarm). In addition, some biological rates (e.g., primary productivity and fish metabolism) decline as temperatures increase above high optimal levels. Fish performance is particularly dependent on water temperature, where optimal ranges with respect to feeding and growth are typically narrow (e.g., < 8 °C) and fish performance declines rapidly as temperatures diverge beyond optimal ranges.

Fish and feed loading variables and cumulative oxygen consumption (Colt and Orwicz, 1991b) are included to support analyses that use these variables as management criteria and for reporting

purposes. Alkalinity and pH relationships include consideration of dissolved inorganic carbon (DIC; carbon dioxide and carbonates) and additional constituents of alkalinity (conjugate bases of dissociated acids: phosphates, ammonia, silicates, and borates). Constituents of dissolved inorganic nitrogen (DIN) include ammonia, nitrite, and nitrate. Dissolved nitrogen gas is not included in DIN. Dissolved inorganic phosphorous (DIP) is considered equivalent to soluble reactive phosphorous (orthophosphate) and consists of ionization products of orthophosphoric acid (Boyd, 1990). For simplicity, other dissolved forms of phosphorous are not considered and inorganic phosphorous applied as fertilizer is assumed to hydrolyze to the ortho form based on given fertilizer solubilities. Fish and water treatment chemicals are user-defined compounds that may exist or may be used for a variety of reasons, such as control of fish pathogens (e.g., formalin), water disinfection (e.g. ozone), compounds present in source waters (e.g., chlorine), and water conditioning (e.g., sodium thiosulfate for dechlorination). Borate and silicate compounds can have minor impacts on acid-base chemistry, especially for seawater systems, but can normally be ignored. Dissolved organic compounds produced by fish excretion and bacterial processes are ignored. While dissolved organics can impact water clarity and can be oxidized by heterotrophic bacteria with associated impacts on water quality, their sources and sinks are difficult to quantify. Dissolved organics are known to accumulate in recirculation systems, which is indicative of their refractory properties.

Particulate solids include (1) suspended (non-settleable) inorganic solids, (2) settleable inorganic solids, and (3) settleable organic solids in addition to live phytoplankton. These three types of particulate solids are maintained as separate variables, as well as accumulated settled solids. Suspended inorganic solids (clay turbidity) are considered in order to account for their impact on water clarity (expressed as Secchi disk visibility), which is a function of total particulate solid and phytoplankton concentrations. Settleable inorganic and organic solids originate from various sources, e.g., in/organic fertilizers, dead phytoplankton, uneaten feed, and fish fecal material. Particle settling rates and nitrogen and phosphorous contents of organic particulate solids are variable and depend on contributing sources. Particulate solids, whether residing in the water column or accumulated on surfaces, can have a major impact on the performance of aquaculture systems (Chen et al., 1994). Particulate solids in the water column can (1) impact fish performance through gill abrasion and as a substrate for bacteria (especially sensitive fish such as salmonids) and (2) impact primary productivity through water clarity. Organic particulate solids can impact water quality through their oxidation by bacteria and associated oxygen consumption and metabolite production. Particulate solids can also foul biofilters, both mechanically and as a substrate for

heterotrophic bacteria, and are a major concern regarding aquaculture facility effluents. In pond based systems, settled solids can provide local anaerobic conditions that support denitrification.

2.7.4.6 Facility hydraulics

A facility configuration is completely user specified and can consist of any combination of facility units linked into serial and parallel arrays, using flow-through and/or recirculation flow paths and pressurized and/or gravity flow streams. All water flow originates at water sources and terminates at water discharges. Specifications of individual facility units applicable to water flow hydraulics and mechanics include: (1) shape, dimensions, and presence of media, (2) elevations and slope, (3) water flow type (basin, gravity, cascade, or pressurized), (4) water flow direction (longitudinal, lateral, or circular; designated influent and effluent points), (5) minimum and maximum water flow rates, and (6) up and down stream connections to other facility units. Any facility unit can have multiple influent and effluent flow streams, and specialized blenders and splitters provide additional flow control. Specialized blenders include those used to (1) blend two flow streams to achieve a desired temperature or salinity and (2) blend makeup and recirculation flow streams. Specialized splitters include those used to (1) shunt solid waste streams (e.g., double-drain fish tanks, centrifugal solid separators, and micro-screen filters), (2) manage parallel, downstream facility units, and (3) divide a flow stream for recirculation and discharge. All facility units have a minimum (may be zero) and maximum water flow rate, based on water velocity, hydraulic loading rate, and/or water exchange rate constraints. Default minimum and maximum water flow rates are provided and are user accessible. Facility units can have specific head loss considerations (e.g. pressurized media filters) and/or hydraulic loading constraints (e.g. trickling filters, packed columns, and sedimentation basins). Calculations and modeling methods of facility unit hydraulics, water volumes, water velocities, water retention times, and maximum hydraulic loading rates are described in more detail in Chapter 5 (Water mechanics).

If water mechanics are considered, then the hydraulic integrity of a given facility configuration is checked prior to simulation. If unrealistic flow configurations are found, then the simulation does not proceed, problem areas are highlighted on the facility map, and problem explanations are posted to the management log. Unrealistic flow configurations include: (1) gravity flow for a positive hydraulic slope, (2) pressurized flow streams lacking water pumps, (3) entry of a gravity flow stream into a pressurized flow stream, (4) lack of coordination of facility-unit elevations for flow streams loops and branches that diverge and re-converge, and (5) non-allowed placement of specialized water blenders and splitters. Facility configurations specified by users may be

unrealistic and inappropriately complex, which can cause difficulties in the simulation of water flow management. This is particularly problematic for water recirculation systems with multiple, nested water flow loops. For this reason, the system integrity check performed by AquaFarm also requires that only one recirculation blender and one recirculation splitter can exist per recirculation loop (see Chapter 3, Figure 3.1). A *recirculation blender* is defined as having one upstream leg from a makeup water source and one from a recirculation loop. A *recirculation splitter* is defined as having one downstream leg to a water discharge and one to a recirculation loop. Recirculation blenders and splitters must always exist in pairs. For clarity, recirculation blenders and splitters are labeled and assigned a unique color (cyan).

3. Facility and Management Simulation

In this chapter, models and procedures used to simulate the physical and management components of aquaculture facilities are added to the program architecture previously developed. Methods include (1) rule-based procedures for facility and fish culture management, (2) mass and energy balance, differential-equation templates and integration procedures for facility units, and (3) generic, system-level procedures for processing simulations.

3.1 Facility managers

Facility and fish culture management is simulated by AquaFarm using two facility managers, termed the physical plant manager and the fish culture manager. The physical plant manager is responsible for managed (active) mass and energy transfer processes used to maintain water quantity and quality variables at desired levels. Managed processes typically include water flow rates and may include heat transfer, compound addition, and compound removal (see Chapter 2, Table 2.3). The fish culture manager is responsible for the maintenance of fish environmental criteria, feed management, fish lot handling, and fish production objectives and scheduling.

Facility managers are assigned responsibilities in the form of (1) tasks to be completed and conditions (variables) to be monitored, (2) evaluation criteria for monitored conditions, and (3) allowed responses to correct problems. Facility managers utilize domain experts for specific technical tasks, such as adjusting process rates and scheduling operations. A given management task or response can be fully, partially, or not successful, depending on the availability of required resources. The number of possible management responsibilities and responses increases with the analysis resolution level and facility complexity. Facility managers perform their assigned tasks at a regular period, defined by the management time-step (e.g., 1, 8, or 24 hours), so that the desired management intensity is emulated. Facility managers report problems and responses to a management log.

3.2 Water management

Water management strategies include (1) static water management with makeup of water losses to maintain designated minimum volumes, (2) water flow-through with optional serial reuse,

and (3) water recirculation at given recirculation rates. For static systems, if a minimum water volume is reached (specified as percent total volume), then makeup water is added until the facility unit is full at a rate depending on the water supply system. Over the course of a simulation, different sections of a facility can be placed on-line and off-line as they are used, in order to emulate practical methods and avoid unnecessary calculations. When a facility unit is placed off-line, it is emptied of water and the facility unit and its individual water flow stream are not simulated. When a facility unit is placed on-line, its water quality is initialized to the flow stream(s) supplying the facility unit.

For water recirculation systems, recirculation rates are specified as a proportion of the total culture system flow rate and system makeup water comprises the remainder of the total flow rate. Therefore, system water exchange rates (%/day) depend on the recirculating flow rate (Figure 3.1). Recirculation systems also use makeup water to replace water losses (e.g., evaporation and solids removal). For recirculation systems, facility units that are operated in an over-flow mode (e.g., constant-head head tanks and fish rearing units with stand pipes) are often used in conjunction with a system sump tank, the latter providing system water collection and return pumping. The sump tank is where system water losses impact water levels and where makeup water is added (e.g., via a float valve). Therefore, by definition, the sump tank is the recirculation blender in such systems. As described in Chapter 2 (Facility hydraulics), a designated recirculation blender and splitter is required for each recirculation loop.

For all types of flowing water systems (flow-through and recirculating), water flow rates of the flow streams within a facility typically vary over the course of a simulation. Flow rates are determined by requirements of fish rearing units, temperature and salinity blenders, water recirculation rates, and minimum-maximum flow rate constraints of individual facility units. For non-aquaculture facilities, flow rates are controlled at water sources, to give constant or varying flow rate regimes. For aquaculture facilities, flow rates are mainly determined by demands of fish rearing units, as based on fish biomass support and determined by the fish culture manager. Flow rates can be constrained by source water capacities and the water mechanics of individual facility units. Flow rate adjustments are accomplished instantaneously between simulation steps, such that water flow rates over a simulation step are constant. Facility unit water volumes, however, are not necessarily constant over a simulation step. Facility unit specifications applicable to water hydraulics are described in Chapter 2 (Facility hydraulics), and modeling methods of water mechanics are described in Chapter 5 (Water mechanics).

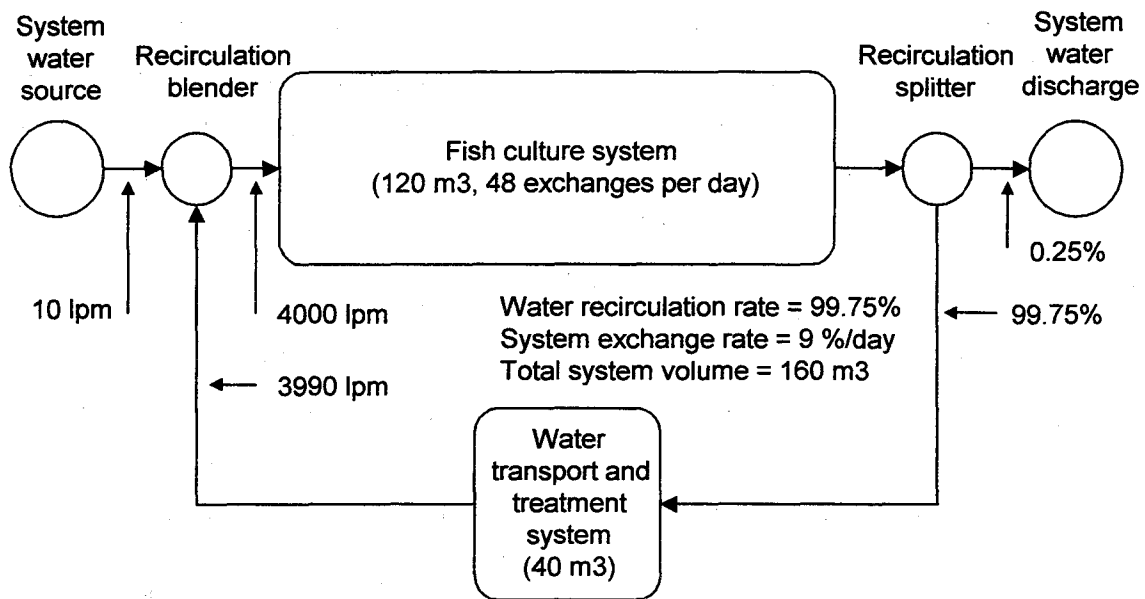


Figure 3.1. Example water recirculation system, illustrating relationships between the system water volume, system water exchange rate, and recirculation rate and showing the placement of the recirculation blender and splitter (water losses ignored)

Algorithms used to adjust water flow rates of individual facility units within systems can be complicated, especially for highly branched systems with diverging and reconverging flow streams and water recirculation systems with multiple recirculation loops. Challenges arise from the need to adjust single flow paths within a system network, using generic procedures adaptable to any facility configuration. These complications are transparent to the user, however, other than the requirement that facility configurations be realistic (see Chapter 2, Facility hydraulics). The procedure used to adjust flow rates is:

- 1) Determine the new flow rate of the facility unit requiring adjustment, e.g., as required to support fish oxygen consumption rates
- 2) Trace up and down stream flow paths of the facility unit to be adjusted, until terminal water sources and discharges are found
- 3) Assess flow paths for flow rate constraints relative to the new flow rate, and limit the new flow rate if required
- 4) Assess and implement parallel facility-unit management
- 5) Implement flow rate adjustments at points of flow rate control, such that the only changes in flow rate are those of the facility unit to be adjusted and its specific flow path.

Flow control points used in AquaFarm include water sources and the distribution of flow streams from facility units with multiple effluent ports. In real systems, flow control points consist of (1) adjustable weirs for open-channel gravity flow, (2) flow control valves for closed-channel gravity flow, and (3) flow control valves and variable-speed or multi-staged (parallel) pumps for pressurized flow. In AquaFarm, these weirs and valves are assumed to exist but are not explicitly defined. Water pumps are made to provide given flow rates, within their given operational constraints. Pump flow-control mechanisms are assumed to exist but are not explicitly defined.

As found in practice, facility units such as water pumps and filters may be arranged in parallel arrays to provide management flexibility. Parallel units can be taken on-line and off-line, depending on the total water flow rate of the parallel units and the flow rate capacities of individual units. Parallel flow management is specified at the water flow splitter upstream of the parallel units.

For flowing water systems, specialized blenders may be used to combine two flow streams such that a given flow rate and temperature or salinity are achieved. The combined flow rate of the two flow streams is determined by downstream demands, which requires that the two influent flow streams be adjusted without changing the combined, total flow rate. Therefore, temperatures or salinities of the influent flow streams (C_1 and C_2) and of the combined flow stream (C_3) and the flow rate of the combined flow stream (Q_3) are given, and the required the flow rates of the two influent flow streams (Q_1 and Q_2) are calculated by:

$$\begin{aligned} Q_3 &= Q_2 + Q_1 \\ Q_3 C_3 &= Q_1 C_1 + Q_2 C_2 \\ Q_1 &= Q_3 (C_3 - C_2) / (C_1 - C_2) \\ Q_2 &= Q_3 - Q_1 \end{aligned}$$

3.3 Process management

Rates of managed (active) process can be controlled by manual or automated mechanisms. *Manual management* is simulated at the management time-step and is used to simulate manual management tasks. These tasks consist of the system operation monitoring and control adjustments typically employed, for example, manual dissolved oxygen monitoring and starting/stopping pond paddlewheel aerators. *Automated management* is simulated at the simulation time-step and is used to simulate automated monitoring and process control, for example, automated dissolved oxygen

monitoring and starting/stopping pure-oxygen injectors. In AquaFarm, automated management is specified via the plant manager specifications, but is operated independently of the plant manager during simulation. When a manual or automated process is adjusted, the adjustment occurs instantaneously, between simulation steps. The rate (or applied effort; e.g., aeration power) of a managed process is constant within a simulation time-step. Management strategies and specifications are given for each managed process used.

For processes that add compounds to water and for temperature adjustment (see Chapter 2, Table 2.3; Chapter 5, Compound addition), process specifications include (1) set-point level (units of controlled variable), (2) set-point tolerance (units of controlled variable) and minimum on-time (hr), (3) efficiency of energy or material transfer (%), (4) process rate increment (infinite or finite) and minimum and maximum process rates (mass or energy / volume or area / time), and (5) process control methods. Process control methods include constant rate, simple on-off, and proportional (throttled) process control. Proportional control allows process rates to vary continuously or in discrete steps over given operational ranges. In addition, “integral-derivative” (ID) process control can be combined with proportional control, to emulate industrial PID controllers. Integral-derivative control accounts for the rate of change of the controlled variable in calculating rate adjustments. As in practice, proportional and integral-derivative controls are used to minimize oscillation of the controlled variable around its set-point level (Heisler, 1984).

For process rate calculations for water heating and chilling, temperature is expressed as kWhr/m^3 , based on heat capacity and water density. Salinity is converted from g/kg to g/m^3 . Other variables are already expressed as g/m^3 (equivalent to mg/L). For on-off control, a process rate is either set to its constant rate or zero, depending on the level of the controlled variable level relative to its set point. For proportional control without integral-derivative control, new process rates (g or $\text{kWhr/m}^3\text{-day}$) for a given state variable C (g or kWhr/m^3) are calculated by:

$$PR_{\text{new}} = PR_{\text{cur}} + (C_{\text{sp}} - C) / t$$

For proportional control with integral-derivative control, new process rates are calculated by:

$$PR_{\text{new}} = PR_{\text{cur}} + [(C_{\text{sp}} - C) / t] - dC/dt$$

where PR_{new} = new process rate, PR_{cur} = current process rate, C_{sp} = set-point of state variable C , C = current level of C , t = time (day), and dC/dt = current rate of change of C . The time (t) over which the desired adjustment is to take place is set to the minimum of the mean hydraulic detention time

and the simulation time step. PR_{new} values are converted to total rates of application for the facility unit (kg or kWhr/ day) based on the water volume, considering mass/energy transfer efficiencies. Finally, if a mass or energy application rate does not vary continuously, then it is adjusted to some integer multiple of a given, discrete step-size, such that the required rate is achieved. Rates can be constrained by designated minimum and maximum rates.

For some conditions, e.g. when both heaters and chillers are present, the controlled variable can be both decreased and increased to achieve a given set point. Typically, controlled variables can only be decreased or increased, for example the addition of a compound to achieve a desired concentration. There may be a singular relationship between a controlled variable and the compound used (e.g., salinity adjustment by salt addition), multiple possible compounds (e.g., pH and alkalinity control), or multiple strategies (e.g., water fertilization can be managed with respect to DIC, DIN, or DIP). For diffusion based processes such as heat and gas transfer (first-order kinetics), as opposed to direct compound addition, the process application effort (applied power) is controlled rather than mass transfer rates, and set-points are not necessarily achieved.

Process specifications in addition to set-points are critical to the capacity of simulations to emulate actual systems. For example, for nightly, on-demand aeration of fish ponds, the aeration effort is typically managed manually, applied in discrete and limited quantities (i.e., a given number of paddle wheel aerator units used in a staged manner), and used continuously over a given time period (e.g., midnight to dawn). For this example, the set-point is used to start aeration (e.g., at 2 mg O_2/L), the set-point tolerance is used to stop aeration (e.g., at 4 mg O_2/L), and manual management is used at a realistic management time-step (e.g., 4-hr). In contrast, diffused aeration in an intensive system is often applied at a continuous, constant rate, and pure-oxygen application to intensive systems is often managed by automated methods.

For filtration processes that remove compounds from the water, processes are primarily defined by given efficiencies. For mechanical and chemical filters, process efficiency is specified as percent removal of the given compound per pass of water through the filter (see Chapter 5; Solids filtration and Chemical filtration). For biological filters, process efficiency is specified as kinetic parameters of bacterial processes (see Chapter 6). For all filters, periodic requirements for media cleaning (removal of accumulated solids) or regeneration (e.g. clinoptilolite and granular activated carbon) over the course of a simulation can be accomplished manually by the facility manager or automatically by the facility unit.

3.4 Fish culture manager

The fish culture manager is responsible for maintaining fish environmental criteria and satisfying fish production objectives. This is accomplished through (1) the control of water flow and water treatment rates, which are determined by the fish culture manager and referred to the physical plant manager for implementation, and (2) a variety of fish lot handling and culture procedures, which are used in response to designated management strategies and objectives. These management tasks are performed according to assigned responsibilities, production targets, and available resources. Fish production objectives are not achieved if they exceed fish performance capacity or available resources. The methods of fish biology described in Chapter 7 provide the biological basis for the fish culture methods described here.

3.4.1 Production objectives

Fish production objectives are defined by designated (1) calendar dates, (2) fish population numbers, and (3) fish states at initial fish stocking and target transfer events. Fish transfer events include fish input to the facility, fish life-stage transfers within the facility (broodfish → eggs and eggs → growout fish), and fish release or harvest from the facility. Production objectives are specified as combined quantities for fish populations and are divided into component values for fish lots. Fish lots within a fish population can be managed uniformly or individually (see Chapter 2, Fish stocks, populations, and lots). If production objectives are not achieved, the fish culture manager can adjust objectives, initial stocking conditions, or culture conditions so that objectives are achieved. These adjustment tasks can occur automatically or under the direction of the user.

Target fish numbers for fish lots are flexible production objectives. Target numbers together with given mortality rates (%/day) and culture period lengths are used to determine required initial fish numbers. For facilities with life-stage transfers (broodfish → eggs → growout fish), the target fish number of the ending life-stage determines the required initial fish number of the starting life-stage. If broodfish are taken from the wild (e.g., salmon hatcheries), then broodfish return (from the wild) and capture rates can be considered in conjunction with initial broodfish numbers.

Target fish lot states represent fixed, biological requirements for broodfish (reproductive maturation) and eggs/larvae (first-feeding fry) and represent flexible production objectives for growout fish (target fish weights). Initial states can be user specified, result from life-stage transfers,

or be determined by the fish culture manager so that target states are achieved. Intermediate states are predicted by simulation. Development rates of broodfish and eggs and growth rates of growout fish can be adjusted by environmental control (temperature and photoperiod). Environmental control is invoked under the direction of the user, and the specific regimes required are determined by the fish culture manager. For growout fish, growth rates can also be controlled by feeding rates, as determined by the fish culture manager.

Target fish lot dates may be flexible production objectives, depending on the type of fish lot and management methods used. Since target states represent fixed requirements for broodfish and eggs, target dates for broodfish and eggs can only be achieved if (1) target states and dates happen to be coincident or (2) environmental control is used to adjust development rates. For growout fish, target states and dates together establish required feeding rates, and thus target dates are typically flexible. If necessary, the fish culture manager can determine initial dates required to achieve target dates or target dates that allow given initial dates. For linked life-stage facilities (e.g., broodfish → eggs → growout fish), this function can span multiple life-stages.

3.4.2 Environmental criteria

Environmental conditions are monitored at each management time-step and evaluated in relation to given criteria. Variables that can be responded to by the fish culture manager include (1) water exchange rate and velocity, (2) fish biomass density (per area or volume), (3) fish biomass loading rate (biomass per water flow rate), (4) feed loading rate (feed applied per water flow rate), (5) cumulative oxygen consumption, (6) dissolved oxygen saturation, (7) carbon dioxide saturation, and (8) concentrations of unionized ammonia and particulate solids (Chapter 2, Table 2.1).

Environmental criteria are based on reported biological criteria for individual fish species (Chapter 7, Table 7.1). Allowed deviations beyond optimal biological ranges are established by management variables. User accessible, biological criteria are provided for major aquaculture species and may be added for additional aquaculture species. For lower analysis resolution levels and systems with known capacities, water exchange rate, fish biomass density and loading rate, and/or feed loading rate can serve as measures of metabolic loading and management response variables. Biomass density limits can consider constraints regarding natural fish productivity and desired limits to production intensity, in addition to metabolic support considerations. For fish stocking, biomass density constraints are used to allocate fish lots among rearing units.

3.4.3 Fish lot handling and biomass management

Fish lot handling events include fish lot stocking, combining, division, and transfer. Handling events can occur in response to (1) fish input to the facility, (2) high variability in fish state within a fish lot, (3) low or high fish biomass density, (4) unacceptable biomass loading, feed loading, or water quality conditions, and (5) achievement of threshold fish size-stages, life-stage transfers, and release or harvest target fish states (Figure 3.2). Fish handling and biomass management responsibilities are defined by the following rules and options:

- 1) The use of rearing units is prioritized such that minimum overall fish densities are maintained and either (a) fish lots are never combined or (b) lots are combined only as required to stock all input fish lots. Alternatively, the use of rearing units is prioritized such that maximum overall fish densities are maintained and either (c) lots are combined as required to stock all input fish lots or (d) lots are combined whenever possible to minimize use of rearing units and maximize fish densities. Input fish lots include facility inputs, life stage transfers, and size stage transfers. If sufficient rearing-unit volume is not available for a given fish lot that is to be stocked, as based on designated management methods and available rearing units, then the fish lot is not stocked (each stocking failure is noted in production reports and management logs).
- 2) If a facility holds multiple fish stocks, then either (a) different stocks are maintained in separate rearing units (multi-species facilities) or (b) designated stocks are combined within rearing units (polyculture facilities).
- 3) Fish lots are divided at stocking events to multiple rearing units as required by fish density constraints (yes/no). During culture, fish lots are transferred to smaller rearing units if fish densities are too low (yes/no), and/or fish lots are transferred whole or divided to larger rearing units if fish density is too high (yes/no).
- 4) Based on specified fish biomass loading, feed loading, and water quality criteria, (a) rearing unit water flow rates are adjusted and/or (b) fish biomass levels are adjusted, for which fish lots may be transferred whole or divided to other rearing units. Mass balance analyses are used in the adjustment of biomass levels and water flow rates. The adjustment of water treatment processes occurring in fish rearing units (e.g., aeration) are implemented by the physical plant manager (described earlier) and set-point levels are based on fish water quality criteria.

- 5) Growout fish lots are graded and divided during culture to reduce excessive variability in fish weight (yes/no) and/or remove culls (yes/no). Growout fish lots are high graded and divided at transfer events to leave low grades for further culture (yes/no) and/or remove culls (yes/no).

The last set of these listed management options (item 5) can be used when growout fish lots are modeled using weight distributions rather than mean weights (see Chapter 7, Fish weight distributions). The use of weight distributions provides a basis for dividing fish lots based on the fish size range, for which fish are size-graded and low grades (e.g., low grade culling) or high grades (e.g., high grade harvesting) are removed. The use of distributions also provides a basis for the management of fish weight ranges within single fish lots over the culture period. Such management is established by the rules listed above and additional specifications that are used to control management intensity:

- 1) Minimum change in fish density for fish lot move based on density (e.g., 50%; lower values give higher intensity)
- 2) Minimum proportion of fish removed for fish lot division (e.g., 25%; lower values give higher intensity)
- 3) Maximum proportion fish removed for fish lot division (e.g., 75%; used to prevent unacceptably low numbers of remaining fish)
- 4) Maximum fish-size variability (coefficient of variation, e.g., 30%; lower values give higher intensity)
- 5) Maximum number of fish handling events allowed per fish lot over its culture history (e.g., 5; higher values give higher intensity; includes fish lot stocking, transfers, and divisions).

3.4.4 Management intensity and risk

Levels of management intensity and risk are established by multiple specifications, including the type of facility, fish production objectives, fish lot handling strategies, fish biomass loading relative to maximum capacities, and degree of production staging and maximization of cumulative production. Based on these specifications, management intensity can range from simple batch stocking and harvest practices to staged, continuous culture, high grade harvesting and restocking practices. For example, “hands-off” or “grow-into-space” type management is typical of salmon hatcheries, where to minimize fish handling, fish are initially stocked at low levels and allowed to grow into their available volume. In addition, since a narrow window of release dates must be achieved for all fish, fish lots of a fish population are reared together, in a uniform manner.

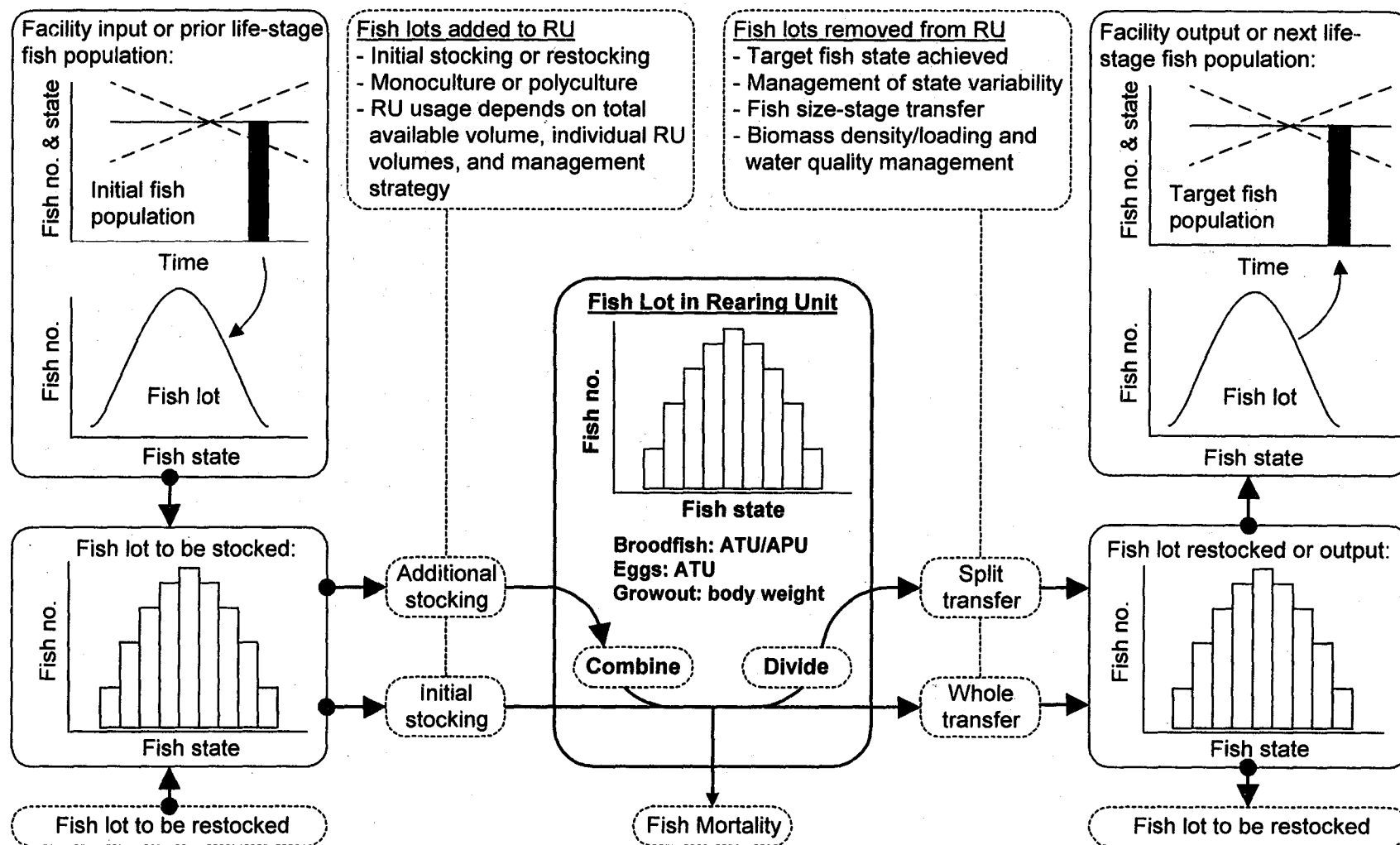


Figure 3.2. Management of fish lot stocking, division, combining, and transfer, as based on fish input and output for the facility, life stage transfers within the facility, and fish management strategies used within a life stage

In contrast, for intensive food fish production, fish lots within a fish population can be managed individually for temporal staging (sequential rearing) of fish production (Watten, 1992; Summerfelt et al., 1993). Such management can be used to maximize the total, cumulative fish production of a facility and to operate the facility at its biomass capacity for as much of the time as possible. Management intensity is also defined by the size of the management time-step, allowed variability in growout fish weights, minimum adjustment increments of process rates, and allowed tolerances for environmental variables to exceed optimal biological ranges.

Management risk is quantified as a failure response time (FRT, hr) for fish rearing units. FRT values are maintained by the fish culture manager for each rearing unit. FRT is the predicted time between the failure of biomass support processes (e.g., water flow or in-pond aeration) and occurrence of high fish stress or mortality due to the decline of dissolved oxygen (DO) below the low tolerance value (see Chapter 7). Management risk is controlled by establishing a minimum allowed FRT for the facility. If a rearing unit FRT value falls below this minimum, then fish biomass density is reduced, using the given fish lot handling rules. FRT values are a function of the rearing unit volume (V ; m^3), current DO (DO_{cur} ; $g\ O_2/m^3$), critical DO (DO_{crit} ; $g\ O_2/m^3$), and the total oxygen consumption rate of fish in the rearing unit (OCR; $g\ O_2/day$):

$$FRT = V (DO_{cur} - DO_{crit}) (24\ hr/day) / OCR$$

3.4.5 Broodfish maturation and egg incubation

The reproductive maturation state of broodfish is defined by accumulated temperature units (ATU; degree-days) and/or accumulated photoperiod units (APU; hour-days). Starting with given, initial ATU/APU values, current values are maintained over the course of a simulation based on water temperature and photoperiod regimes. These regimes may be adjusted to achieve desired development rates. Spawning occurs when required ATU/APU levels are achieved. Fish number calculations account for required female-male sex ratios, egg production per female, and fish spawning characteristics (i.e., spawn once per year, repeat spawn, or death after spawning). For eggs, development state is defined by accumulated temperature units (ATU). Achievement of development stages during incubation (eyed egg, hatched larvae, and first-feeding fry) is based on the ATU requirements of each stage. Egg handling can be restricted during sensitive development stages, and temperature regimes may be adjusted to achieve desired development rates.

3.4.6 Fish growout

Feeding strategies for fish growout can be based on (1) endogenous (natural) food resources only, (2) natural foods plus supplemental prepared feeds, or (3) prepared feeds only. Natural food resources can be managed indirectly, by control of fish densities and maintenance of nutrient levels for primary productivity. Prepared feeds are defined by their proximate composition and pellet size. Prepared feeds are applied over daylight hours, according to the specified length of the feeding day in relation to sunrise and sunset. Fish management size-stages can be specified for growout lots to support fish-size based assignment of (1) designated rearing units (e.g. fry, fingerling, and on-growing), (2) types of fish feed (pellet size and composition), and (3) length of the feeding day. The impact of feed allocation strategies and application rates on food conversion efficiency and fish growth variability (due to competition for limited food resources) can be simulated, but the fish culture manager always controls feed rates based on target growth rates.

Target growth rates for fish growout are based on initial and target, fish weights and dates, which are user designated production objectives. Prepared feeds are applied as necessary to achieve target growth rates, considering any contributions from natural foods. When environmental conditions (e.g., temperature) are variable, as is typically the case, a direct procedure to determine feeding rates that achieve target weights is not possible, and solutions are achieved by iterative simulations and adjustments. These “internal” iterative simulations are not under the control of the user, but tolerance values regarding the degree of accuracy by which target dates and weights must be achieved (\pm %) can be set by the user to control the number of iterative simulations required (e.g., 2 to 5). Once feed rate regimes are established according to predicted environmental conditions, subsequent simulations do not require internal iterations unless production targets or environmental conditions are changed. As an alternative to this entire approach, growout production targets can be based on dates or weights only (not both), using a given feed application intensity level (percent of maximum ration; 1 – 100%).

3.5 Facility unit modeling

State variables, heat energy transfer rates, and compound mass transfer rates are maintained separately for each facility unit. Together, these variables, rates, and modes of transfer determine the number and structure of the differential equations used to model an individual facility unit. A single, generic, differential equation, is used as a template for all possible differential equations, where one or more terms may be dropped from the template equation for a specific use. Therefore, integration procedures for individual differential equations, as well as sets of simultaneous equations, can be processed in a generic manner by a single set of program modules.

3.5.1 Mass and energy transfer processes

Physical, chemical, and biological unit processes and associated compound sources and sinks that can occur in facility units are listed in Table 3.1. In addition to these mass transfer processes, water flow mechanics and heat transfer are represented by energy transfer processes. Unit processes can be individually selected for consideration, according to the analysis resolution level. Methods used to model unit processes are described in Chapters 4 – 7. The water contained in a facility unit is subject to mass transfer, including influent and effluent flow (advection), seepage infiltration and loss, precipitation and runoff, and evaporation (see Chapter 5, Water budgets). Settled solids can accumulate depending on rates of contributing sources and bacterial oxidation. Settled solids can be removed by periodic manual procedures (e.g. rearing unit vacuuming and filter cleaning) or continuous hydraulic procedures (e.g. dual-drain effluent configurations).

Unit processes can be passive, active (managed), or both passive and active. Examples of passive processes are heat and gas transfer, bacterial processes, and primary productivity. Passive processes may be uncontrolled or indirectly controlled, e.g., primary productivity can be indirectly managed through the control of nutrient levels. Actively managed processes are directly controlled to maintain water quantity and quality variables at desired levels. Examples of active processes are water flow rate, heating, aeration, solids filtration, and compound addition. Air-water gas transfer of a fish pond is an example of a combined, passive and active process, in which aeration is used in response to low oxygen levels but passive air-water gas transfer is also significant. Generally, passive processes are defined by model parameters and active processes are defined by facility unit specifications.

Table 3.1. Presence of sources (+, added) and sinks (-, removed) of the listed compounds for the physical, chemical, and biological mass transfer processes occurring in facility units¹

Compound	Facility Unit Processes												
	FLO	DIF	CMP	FLT	CHM	SOL	SST	OXD	NIT	DNT	NPP	FSM	FSC
DO	+/-	+/-	+	0	0	-	0	-	-	0	+	-	0
DN	+/-	+/-	0	0	0	0	0	0	0	+	0/-	0	0
Salinity	+/-	0	+	0	0	0	0	0	0	0	0	0	0
Alkalinity	+/-	-	+	0	+/-	+/-	0	0	-	+	+/-	+	0
Hardness	+/-	0	+	0	+/-	0	0	0	0	0	0	0	0
DIC	+/-	+/-	+	0	+/-	+/-	0	+	-	+	-	+	0
TAN	+/-	-	+	-	0	+/-	0	+	-	0	-	+	0
Nitrite	+/-	0	0	-	0	+/-	0	0	+/-	0	0	0	0
Nitrate	+/-	0	+	-	0	+/-	0	+	+	-	-	+	0
DIP	+/-	0	+	-	0	+/-	0	+	0	0	-	+	0
Partic. solids	+/-	0	+	-	0	0	-	-	0	-	+	+	-
Settled solids	0	0	0	0	0	0	+	-	0	-	0	0	-
Phytoplankton	+/-	0	0	-	0	0	0	0	0	0	+	0	-
Treat. chem..	+/-	-	+	-	-	0	0	0	0	0	0	0	0
Sulfide	+/-	-	0	0	0	+	0	0	0	0	0	0	0
Borate, silicate, sulfate	+/-	0	0	0	0	0	0	0	0	0	0	0	0

¹ See Chapter 2, Table 2.1 for definitions of compound names. Use of "0" denotes absence of mass transfer or lack of consideration by AquaFarm.

FLO Influent (+) and effluent flow (-) (also water seepage and precipitation; see text)

DIF Passive and active, air-water gas diffusion (DIC as DC and TAN as NH₃)

CMP Compound addition to water

FLT Mechanical, chemical, and hydroponic/wetland biological filters (other biological filters under NIT and DNT)

CHM Calcium carbonate dissolution (+) and precipitation (-) and decay of treatment chemicals (e.g., chlorine and ozone)

SOL Soil release (+) and uptake (-)

SST Solids settling (in/organic particulate solids; no settling of live phytoplankton)

OXD Heterotrophic bacterial processes

NIT Nitrification bacterial processes (passive and biological filters)

DNT Denitrification bacterial processes (passive and biological filters)

NPP Phytoplankton processes for NPP > 0 (if NPP < 0, reverse signs). Alkalinity is removed for TAN uptake and added for nitrate uptake. DN use depends on presence of blue-green algae. At death, phytoplankton become particulate organic solids.

FSM Fish metabolic processes: compound excretion (+) and consumption (-)

FSC Fish consumption of endogenous food resources

3.5.2 Reactor modeling

Each facility unit (reactor) is assigned unit processes according to the analysis resolution level, reactor type, and specifications. Unit process rates are collected into differential equations that represent heat energy and mass balances for the reactor. By this procedure, the model structure used to represent a facility unit is responsive to its specifications as well as the conditions of a particular simulation. This flexibility includes the differential equations used, the terms used in the differential equations, and the independent variables applied to the terms of the differential equations.

In general, the structure of mass and energy balance differential equations depends on the reactor hydraulic model used (Levenspiel, 1972; James, 1984; Tchobanoglous and Schroeder, 1985; Montgomery, 1985). For zero-order processes, process kinetics are independent of state and of the hydraulic model used. For first-order processes, however, mean process rates are typically higher under plug-flow conditions, due to higher mean concentration gradients. In AquaFarm, differential equations are based on the simplifying assumption that all types of facility units can be adequately represented as completely-mixed reactors (CMR; also termed completely-stirred tank reactors, CSTR), as opposed to plug-flow reactors (PFR) or some combination of mixed and plug flow hydraulics. This assumption is rationalized below, but an assessment of its impact on simulation accuracy is not provided in this dissertation.

CMR and PFR hydraulics represent idealized conditions. Under practical applications, intermediate conditions between CMR and PFR are typically found, due to water flow short-circuiting, dead space, longitudinal dispersion, and influent and effluent hydraulics (Levenspiel, 1972). The mean of the residence time distribution (RTD) of a given compound is equivalent to the mean hydraulic retention time (θ ; day), but the shape of the RTD profile is a function of reactor hydraulics (Levenspiel, 1972). To determine RTD profiles, theoretical based methods are typically not practical and stimulus-response tracer studies are used (Montgomery, 1985). In summary, input data requirements, modeling complexity, and calculation intensity are increased considerably for non-ideal reactor models and such models are not practical for the purposes of AquaFarm.

Facility units in aquaculture systems that may show PFR characteristics include fish raceways and sufficiently long pipes, channels, and packed columns. These facility units are characterized by low hydraulic retention times (e.g., ≤ 30 min) and high ratios of length to cross-sectional flow area (e.g., $\geq 10 \text{ m/m}^2$). Due to the following considerations, PFR modeling is not used in AquaFarm:

- 1) Since PFR water exchange rates are typically high, the impact of first-order processes such as passive heat and gas transfer are typically minor. For example, in a typical salmon hatchery raceway with a 30-minute retention time, water temperatures change little from influent to effluent (e.g. < 1-2 °C) and oxygen budgets are composed primarily (e.g. > 90%) of water advection and fish consumption (see Chapter 8).
- 2) Raceways are typically used in flow-through, cold and clean water systems, where biological processes other than fish metabolism tend to be negligible. In addition, water quality is normally maintained at high levels, where fish metabolism is not responding to water quality variables other than temperature (zero-order kinetics).
- 3) If fish are characterized by first-order kinetics, process dynamics are complicated by the fact that fish often concentrate at the influent end of the raceway. At the least, fish do not tend to disperse uniformly in a raceway. During feeding, when metabolic rates are at maximum levels, fish swimming action increases longitudinal water mixing and fish distribution in the raceway depends on how the feed is applied.
- 4) Pipes and channels are the most likely facility units to show PFR characteristics. Long lengths of these units are most common in facility water supply systems, where if ambient, equilibrated water is used, then first-order processes are typically minimal.

Using the CMR model, a generic, mass balance, differential equation (dC_e/dt ; g C/m³/day), expressed in terms of concentration (mass / volume) for a given compound C, is:

$$dC_e/dt = Q_i C_i / V - Q_e C_e / V - dV/dt C_e / V + K_{Lac} (C_s - C_e) + K_{rc} C_e + M_c$$

or
$$dC_e/dt = Q_i C_i / V - (Q_e + dV/dt) C_e / V + K_{Lac} (C_s - C_e) + K_{rc} C_e + M_c$$

where influent and effluent flow rates are constant (may be zero) but not necessarily equal, water volume may change, Q_i = influent flow rate (m³/day), Q_e = effluent flow rate (m³/day), V = water volume at end of time interval (m³), t = time (days), Q/V = mean hydraulic retention time (θ ; day), C_i = influent concentration (g C/m³), C_e = effluent concentration (g C/m³), C_s = equilibrium concentration (for diffusing gases; g C/m³), K_{Lac} = overall mass transfer coefficient for diffusing gas C (1/day), K_{rc} = first-order exponential decay coefficient for compound C (e.g., chlorine, ozone, and user defined treatment chemicals; 1/day), M_c = combined mass transfer term for various zero-order and first-order unit processes (g C/m³/day), and dV/dt represents the change in water volume

over the time interval t (m^3/day ; may be zero). In the application of this equation to particulate solids, solid settling is modeled equivalent to first-order exponential decay.

Integration with respect to time yields:

$$C_{et} = C_{eo} e^{-tA} + (B/A)(1 - e^{-tA})$$

where $A = (Q_e + dV/dt)/V + K_{Lac} - K_{rc}$

and $B = Q_i C_i / V + K_{Lac} C_s + M_c$

This analytical integration is not typically achieved under rigorous methods. In order to achieve this solution, it is often necessary to include some first-order processes in the M_c term and to represent some variables by constants rather than by additional terms or equations (e.g., C_i). However, as explained later in this chapter and applied in Chapter 8, analytical solutions can provide good results at the typically small time-steps used in simulations. Alternatively, if numerical integration is used, then the CMR differential equation given above is used as a finite difference equation (all processes are zero-order) and solutions are as rigorous as the numerical procedure used.

The heat balance differential equation given in Chapter 5 (Heat transfer; H , $kWhr/m^3/day$) is similar to the generic, mass balance differential equation, for which heat-energy content and transfer are analogous to compound concentration and transfer ($WJ = kWhr/3600$ kJ):

$$dH/dt = Q_i \rho_i HC_i T_i WJ / V - [(Q_e + dV/dt) \rho_e HC_e T_e WJ / V] + \phi_{net}$$

The dV/dt term in both the mass and heat-energy equations is used to correct for changes in water volume due to influent and effluent flow rates, seepage infiltration and loss, precipitation and runoff, and evaporation (see Chapter 5, Water budgets) (McDuffie, 1991). Since transfer by advective flow is included in the differential equation, the dV/dt term must include changes in volume due to advective flow. For example, this occurs when influent flow is in use to makeup a low water volume, and thus the effluent flow rate is zero. For seepage water, the simplifying assumption is made that seepage water quality is equivalent to that of the water volume and has no impact on water quality. Therefore, seepage transfer is not included in any transfer terms or in the dV/dt term. If the impacts of precipitation and evaporation on water quality are to be considered, then they are included in the dV/dt term, and any mass transfer by these water flow routes is included in the M_c term. For this purpose, evaporation water is considered pure, and precipitation/runoff water is considered pure except for saturation with atmospheric gases ($20^\circ C$;

zero alkalinity; pH 5.63). High levels of precipitation and evaporation can significantly impact water quality, which in turn are based on estimated climatic conditions. Therefore, to simplify simulations, consideration of the impacts of precipitation and evaporation on water quality is optional. Heat-energy transfer by precipitation is always ignored and the latent heat of vaporization is used for evaporative heat loss. Thus, the dV/dt term for the heat balance differential equation is always limited to advection-based volume changes only.

3.5.3 Water stratification

In the development of AquaFarm, it was found that consideration of water stratification was necessary to achieve sufficiently accurate modeling of thermally stratified (vertically stratified) water bodies such as solar-algae ponds. Thermal stratification of the water column develops when heat input rates to the water surface (radiation and conduction) are high relative to the mixing energy imparted by wind and water movement (James, 1984). Stratification is especially characteristic of tropical solar-algae ponds (Losordo and Piedrahita, 1991; Piedrahita et al., 1993; Culberson and Piedrahita, 1994). Stratification also occurs in temperate ponds during warmer months, and while stratification tends to increase with water turbidity (e.g., phytoplankton concentration), stratification can develop when significant turbidity is not present. Stratification profiles vary both diurnally and seasonally (Cathcart and Wheaton, 1987). When significant stratification exists, processes acting in a stratified manner cause water quality variables other than temperature to also become stratified. Possible stratified processes include (1) physical processes (e.g., surface heat and gas transfer), (2) chemical processes (e.g., compound uptake and release by soils), and (3) biological processes (e.g., settled solid oxidation and primary productivity as a function of depth). Possible stratified water quality variables include temperature, dissolved gases, pH and alkalinity, nitrogen and phosphorous compounds, and organic particulate solids. Because of these stratified processes and variables, stratified water bodies show significantly different kinetics and states compared to non-stratified water bodies.

Rigorous, fully mechanistic heat transfer and stratification models divide the water column into multiple, horizontal layers (e.g., 5 layers for a 90-cm deep pond) and require complete, local, diurnal climate data (Losordo and Piedrahita, 1991; Piedrahita et al., 1993; Culberson and Piedrahita, 1992). These studies show that solar radiation, water turbidity, wind speed, and wind direction with respect to pond dimensions and orientation are critical driving variables. Wind data required for rigorous modeling are particularly demanding, where they must be local to the water

surface, are dependent on pond type (e.g. use of levees) and surrounding structures and topography, and typically show pronounced diurnal regimes. In sum, rigorous stratification modeling is calculation and data intensive and was avoided in the development of AquaFarm.

The thermal stratification model developed for AquaFarm represents a considerable simplification of previously developed models. Stratification is modeled using two, completely-mixed, horizontal water layers of equal depth (termed top and bottom layers). State variables and processes are separately accounted for each of these layers, and mass and energy transfers between layers occur by mixing. Mixing rates between layers are based on temperature differentials between layers and given values for the water mixing index (WMI; 1/day). WMI values represent combined molecular and turbulent diffusion, are interpolated from given annual regimes of monthly mean values, and are used to quantify the potential for stratification development. WMI values less than about 3.0/day represent strong stratification and almost complete mixing occurs at about 24.0/day and above. During simulation, when surface temperatures exceed bottom temperatures, stratification is allowed to build according to given WMI values. When surface temperatures are less than or equal to bottom temperatures, complete vertical mixing occurs. By this method, daily and/or seasonal stratification development and turnover of the water column turnover are modeled, including temperature and other water quality variables. Transitions between stratified and unstratified conditions are considered to be instantaneous by this method, where these transitions have been observed to be abrupt and this simplification has been used by others (e.g., James, A., 1984c). In order to control calculation intensity, salinity, dissolved nitrogen gas, borate, silicate, sulfide, sulfate, treatment chemicals, and chlorine are considered to always be completely mixed, due to their lack of stratified processes or relative unimportance.

An example WMI regime for a pond at 30° N latitude is (12 months; Jan. – Dec.): 32, 16, 8, 4, 2, 1, 1, 2, 4, 8, 16, 32 (1/day). An empirical basis for specifying WMI regimes is presented in Chapter 8. Simulation of stratification is normally performed for static ponds only, where influent flow is limited to water makeup. If water exchange rate exceeds 0.1/day, the current WMI value is increased linearly to complete vertical mixing (48.0/day) as water exchange rates increase to 2.0/day. In addition, water mixing capacities can be specified for water aerators and destratifiers (m^3/kWhr ; see Chapter 5, Gas transfer). According to the power application rate (kWhr/day), the resulting water movement (m^3/day) is expressed as an internal water exchange rate (1/day) and used to adjust WMI values similar to advective flow.

Stratification in the relatively shallow ponds typical of aquaculture systems (e.g., 0.8 – 2.0m) is mainly a diurnal process, and daily simulations (time-step ≥ 1 day) that include stratification lack meaning. If a daily simulation is used with stratification, an internal, hourly simulation loop for heat transfer and stratification is used to approximate stratification, while the designated simulation time-step is used for all other processes.

The procedure of the two-layer stratification model used in AquaFarm, for a given state variable of the top (C_t) and bottom (C_b) layers is given below, where C is used to represent the concentration of a compound (g/m^3) or of heat energy (kWhr/m^3):

- 1) By the same approach used for non-stratified reactors, zero-order and first-order transfer rates of top and bottom layers, other than those first-order processes represented by individual terms in the CMR equation, are combined to single terms: M_{t0} and M_{b0} (g or $\text{kWhr}/\text{m}^3/\text{day}$).
- 2) For the given time-step (t ; day), ignoring advection and diffusion transfer, new, temporary values for C are approximated by: $C_{t1} = C_{t0} + M_{t0} t$ and $C_{b1} = C_{b0} + M_{b0} t$.
- 3) The whole-column equilibrium state is based on complete mixing: $C_{eq} = (C_{t1} + C_{b1}) / 2.0$.
- 4) Temporary C values are updated again by modeling mixing as a first-order, reversible reaction: $C_{t2} = C_{eq} - (C_{eq} - C_{t1}) e^{(-WMI t)}$ and $C_{b2} = C_{eq} - (C_{eq} - C_{b1}) e^{(-WMI t)}$.
- 5) Layer M terms are adjusted by: $M_{t1} = M_{t0} + (C_{t2} - C_{t1}) / t$ and $M_{b1} = M_{b0} + (C_{b2} - C_{b1}) / t$.
- 6) Using the adjusted M terms, each layer is modeled by the CMR equation given earlier, using original values for C .

For the two layers combined, the rules of mass/energy balance are upheld (mass/energy is neither created nor destroyed). As for non-stratified waters, advection, gas diffusion, and solids settling are maintained as first-order processes. Water advection is divided evenly between the layers. For passive (p) and active (a) gas transfer, top layer diffusion coefficients for gas i ($K_{pt,i}$ and $K_{at,i}$) are calculated by normal procedures. Corresponding coefficients for the bottom layer ($K_{pb,i}$ and $K_{ab,i}$) are calculated assuming serial resistance to gas diffusion:

$$K_{pb,i} = 1.0 / (1.0 / K_{pt,i} + 1.0 / WMI)$$

$$K_{ab,i} = 1.0 / (1.0 / K_{at,i} + 1.0 / WMI)$$

Diffusion concentration gradients and all transfer calculations are specific to the water quality of the layer being modeled. Aeration AE and OTR values (expressed per volume; see Chapter 5, Gas transfer) are applied evenly to both layers. For settling of particulate solids, top layer solids settle to the bottom layer and bottom layer solids settle to the bottom wall/soil surface. Mixing of particulate solids between layers by water advection or forced convection is not considered. Phytoplankton concentrations are assumed to always be vertically mixed. Phytoplankton cells can control their buoyancy and depth in response to light levels, but prediction of their depth distribution is not attempted. Phytoplankton cells are assumed to die before any settling can occur, at which time they are converted to particulate organic solids. The light scalar method used for primary productivity assumes a uniform phytoplankton distribution over the water column (see Chapter 6, Phytoplankton processes).

3.6 Facility and management simulation

Following facility and management specification, facility units and fish lots are integrated and facility managers, fish populations, and resource units are updated over a series of time-steps that total the simulation period. Facility components and managers are classified as *simulation objects* at their highest level of hierarchical abstraction in the object oriented programming architecture. The simulation of these objects is administered by the *simulation manager*. The simulation manager (1) maintains a simulation time clock, (2) sends update commands to simulation objects based on their time-steps, and (3) for purposes of numerical integration, maintains arrays of state variables and finite difference terms for the differential equations of facility units and fish lots. The simulation manager processes these simulation objects in a generic manner and has no need to be concerned with the specific details of individual objects.

Manual procedures of the physical plant and fish culture managers are discontinuous, discrete events. Managers respond to update commands over a series of management time-steps by reviewing their assigned responsibilities, responding as facility resources allow, and logging management problems and completed tasks to a management log. In contrast, facility units and fish lots consist of continuous processes, represented by sets of simultaneous differential equations. Facility units and fish lots are simulated by solving state equations, updating state variables, and logging state variable and process rate data over a series of simulation time-steps. At each simulation step, domain experts are used to calculate property, equilibrium, and process rate terms used by the differential equations and management tasks.

3.6.1 Deterministic simulation

Simulations performed by AquaFarm are deterministic, in which identical results are predicted given the same set of input parameters and variable values, and all parameters and variables are expressed as mean values. Deterministic simulations can be based on worst, best, and mean case scenarios, however, as controlled by the use of worst, best, and mean expected values for input parameters and variables. Stochastic simulations are not currently supported by AquaFarm and their potential utility to AquaFarm users is under review. Stochastic simulations require multiple simulation runs (e.g., 30 - 100) to generate probability distributions of predicted state variables, in which selected parameters and input variables vary stochastically within and between simulations (e.g. Griffin et al., 1981; Straskraba and Gnauck, 1985; Cuenco, 1989; Lu and Piedrahita, 1998). For aquaculture systems characterized by stochastic processes, the use of deterministic simulations represents a considerable simplification. For example, solar-algae ponds are subject to stochastic climate variables (e.g., solar radiation, cloud cover, and wind speed) and similarly managed ponds can show significant variability in primary productivity and related variables. However, the additional complexity and input data requirements of accomplishing and interpreting stochastic simulations is considerable and prolonged computer processing times are required. As in most aquacultural modeling studies, it is assumed that deterministic simulations are useful for facility design and for short and long term management planning, even when significant stochastic behavior exists.

3.6.2 Numerical integration

When a simulation includes modeling of oxygen or higher levels of analysis resolution, mathematically rigorous integration of the simultaneous differential equations representing a facility typically requires the use of numerical integration methods. Differential equations are used as finite difference equations to calculate finite difference terms (unit mass or energy per time). Related simulation objects are processed as a group, as determined by the existence of shared variables and simultaneous processes. State variables and finite difference terms of related simulation objects are collected into arrays at each simulation step and solved using simultaneous, fourth-order Runge-Kutta integration (RK4; Elliot, 1984). RK4 numerical integration is capable of accurate solutions for complex sets of simultaneous differential equations. However, RK4 integration may require small time-steps, on the order of minutes to hours, when high rates of energy or mass transfer characterized by first-order kinetics exist (e.g., high rates of water flow, active gas transfer, and

fixed-film bacterial processes). In addition, RK4 integration uses four iterations per time-step for the calculation of difference terms and updating of state variables, and thus all differential equations representing a facility must be processed four times per simulation step. These requirements may result in excessively long simulation processing times (e.g. 2 - 5 minutes, real time), depending on the number of state variables, number of simulation objects, length of the simulation period, and computer processing capacity.

3.6.3 Analytical integration

Analytical integration methods can accommodate high rate, first-order processes at larger time-steps and can be used to minimize calculation intensity and simulation execution times. However, aquaculture facilities are typically characterized by simultaneous processes within and between (i.e. advection) facility units, and achievement of analytical solutions requires the use of simplifying assumptions (Elliot, 1984). To explore tradeoffs between mathematical rigor and simulation processing times, simplified analytical integration methods were developed according to the CMR equation and solution given earlier. By this simplification, some simultaneous processes are unlinked and some first-order processes are represented as constants within a simulation time-step. Therefore, simulation objects and their variables are updated in order of their increasing dependence on other objects and variables. The simulation order used is facility climate, up to down stream facility units, and finally fish lots. In addition, variables within a facility unit are updated in order of increasing dependence on other variables, beginning with water temperature. Since simulations are processed in a stepwise manner, the use of simplified analytical integration is in effect Eulerian numerical integration (Elliot, 1984), for which the accuracy of finite difference terms is enhanced by the use of analytical integration where possible. Regarding fish process modeling (metabolism, feeding, and growth; see Chapter 7), for a given set of environmental conditions, differential equations can be solved by analytical integration except the most complex growth model (BIOE).

3.6.4 Combined analytical-numerical integration

To reduce computer processing time requirements for RK4 numerical integration, when high transfer rates characterized by first-order kinetics exist and small time-steps are required, difference terms for each of the four cycles of RK4 integration are calculated using simplified analytical integration. This approach supports rigorous consideration of simultaneous processes, as achieved

by normal RK4 numerical integration, while significantly reducing time-step constraints due to high rates of change of state variables.

3.6.5 Management and simulation time-steps

The size of the management time-step is based on the desired management intensity, i.e. the time interval between successive, periodic tasks of the facility and fish culture managers. Diurnal simulations (e.g., 1-hr time-step) are required to consider any process management performed within a 24-hour period, e.g., night time aeration for pond systems or diurnal control of oxygen injection rates for intensive systems.

The size of the simulation time-step is based on the nature of the aquaculture system and temporal resolution required to adequately capture system dynamics. Daily simulations (e.g., 1-day time-step) may require time-steps of less than one day, but variables and processes are still used as daily means. Daily simulations, for which diurnal variables and processes are expressed and used as daily means, always represent some level of simplification, at a degree depending on the type of facility and analysis resolution level. For example, all fish culture systems are at least characterized by diurnal fish process, resulting from day-versus-night activity levels and feeding rates of fish. However, diurnal simulations (e.g., 1-hr time-step) are required only when the variability of process rates and state variables within a day period, and the associated management responses, must be considered to adequately represent the system. For example, diurnal simulations may be used for solar-algae ponds for high-resolution modeling of heat transfer and primary productivity, and they may be used for intensive systems for high-resolution modeling of fish feeding and metabolism.

Use of diurnal simulations increases the number of calculations used in a simulation and lengthens simulation processing times considerably. A useful strategy is to begin design projects (see Chapter 2, AquaFarm design procedure) using a daily time-step for coarser, initial analyses, and then diurnal simulations are used as required for more refined analyses. In the development of AquaFarm, it was found that it was often not possible to achieve compatible results between diurnal and daily simulations for processes of passive heat transfer (see Chapter 5, Heat transfer), water stratification (above), and primary productivity (see Chapter 6, Phytoplankton processes). To avoid this incongruity, diurnal simulation sub-loops and hourly mean solar radiation values for temperature and phytoplankton modeling are used for daily simulations, within the daily time-step. This procedure is transparent to the user.

4. Methods of Aquatic Chemistry

Methods of aquatic chemistry used in AquaFarm mainly concern (1) physical properties of water, (2) dissolved gas concentrations, and (3) acid-base chemistry. These methods are based in the aquatic chemistry literature, and additional methods and solution procedures are developed to minimize calculation intensity. An integrated analytical framework is constructed for the application of aquatic chemistry to the simulation of aquaculture systems. These methods are used repeatedly over the course of a simulation to support the physical, chemical, and biological unit processes described in other chapters. In addition, these methods are directly accessible in the Aquatic Chemist Calculator provided within AquaFarm, which was used to generate data for the figures and analyses of this chapter.

Water quality variables considered include temperature and a host of dissolved and undissolved (particulate) compounds. The selection of the specific compounds considered is based on their potential (1) presence in source waters, (2) consumption, production, and accumulation through processes of aquaculture systems, and (3) importance with respect to aquaculture processes and fish performance. Representative compositions of naturally occurring freshwater and seawater are given in Tables 4.1 and 4.2. Additional constituents to be considered for aquaculture systems include nitrite, hydrogen sulfide, chlorine, ozone, and other treatment chemicals due either to their potential presence in source waters, production within facilities, and/or high toxicity to fish. Concentrations of compounds found in aquaculture systems are highly variable, both within and between different system types. Approximate maximum ranges are: pH (5–10), alkalinity (10–200 mg CaCO_3/L), DIC (2–40+ mg C/L), nitrate (0–100 mg N/L), nitrite (0–10 mg/L), and TAN (0–5 mg/L), DIP (0–1 mg/L), dissolved oxygen (1–15 mg/L), carbon dioxide (0.1–30 mg/L), dissolved organics (0–20+ mg/L, dry weight), and particulate solids (0–100+ mg/L, dry weight). Some compounds listed in Tables 4.1 and 4.2 can be ignored, based on their lack of involvement in aquaculture processes and fish performance. For aquaculture applications, maximum operational ranges can be assumed for water temperature (0 – 40 °C), salinity (0 – 40 ppt), and pH (5 – 10). Table 4.3 provides atomic weights of the elements used. Water quality variables, properties, and parameters used in AquaFarm are listed in Table 4.4. A subset of Table 4.4 was provided in Chapter 2 (Table 2.1) and lists the primary water quality variables used in AquaFarm.

Table 4.1. Representative composition of freshwater for major constituents (25 °C) *

Compound	Major species	Mass units	Concentration (mg/L)	Concentration (mmol/L)
Sodium	Na ⁺	Na	6.19	0.2692
Magnesium	Mg ²⁺	Mg	4.13	0.1698
Calcium ¹	Ca ²⁺	Ca	15.24	0.3802
Potassium	K ⁺	K	2.30	0.0589
Chloride	Cl ⁻	Cl	7.76	0.2188
Sulfate	SO ₄ ²⁻	S	3.86	0.1202
Bicarbonate ^{1, 2}	HCO ₃ ⁻	C	12.01	1.0000
Silicate ¹	Si(OH) ₄	Si	4.25	0.1514
Flouride	F ⁻	F	0.10	0.0050
Nitrate ¹	NO ₃ ⁻	N	0.24	0.0170
Phosphate ¹	HPO ₄ ²⁻	P	0.06	0.0020
Iron	Fe(III)	Fe	0.16	0.0029
Nitrogen gas	N ₂	N ₂	13.64	0.4871
Oxygen gas ¹	O ₂	O ₂	8.26	0.2582
Carbon dioxide gas ¹	CO ₂	CO ₂	0.50	0.0114
Argon gas	Ar	Ar	0.51	0.0126
Total dissolved solids (ppm)	Sum (no gases)	—	56.28	—

* Data from Stumm and Morgan (1981), Butler (1982), Colt (1984 and 1990 p.c.)

¹ Significantly impacted by biological uptake and release

² Total carbonate expressed as bicarbonate (includes CO₂ = 0.50 mg/L)

Table 4.2. Representative composition of seawater for major constituents (25 °C, 35 ppt salinity)*

Compound	Major species	Mass units	Concentration (mg/L)	Concentration (mmol/L)
Sodium	Na ⁺	Na	11020.94	479.3846
Magnesium	Mg ²⁺ , MgSO ₄	Mg	1320.06	54.3122
Calcium ¹	Ca ²⁺ , CaSO ₄	Ca	421.70	10.5215
Potassium	K ⁺	K	408.30	10.4429
Strontium	Sr ²⁺	Sr	8.08	0.0923
Chloride	Cl ⁻	Cl	19804.95	558.6255
Sulfate	SO ₄ ²⁻ , NaSO ₄ ⁻	S	926.43	28.8914
Bicarbonate ^{1, 2}	HCO ₃ ⁻	C	28.68	2.3882
Bromide	Br ⁻	Br	68.87	0.8619
Borate	H ₃ BO ₃ , B(OH) ₄ ⁻	B	4.40	0.4074
Silicate ¹	Si(OH) ₄ , MgH ₃ SiO ₄	Si	2.23	0.0794
Nitrate ¹	NO ₃ ⁻	N	0.12	0.0083
Phosphate ¹	HPO ₄ ²⁻ , MgPO ₄ ⁻	P	0.06	0.0020
Nitrogen gas	N ₂	N ₂	10.99	0.3925
Oxygen gas ¹	O ₂	O ₂	6.77	0.2116
Carbon dioxide gas ¹	CO ₂	CO ₂	0.41	0.0093
Argon gas	Ar	Ar	0.41	0.0103
Total dissolved solids (ppt)	Sum (no gases)	—	35.97	—

* Data from Stumm and Morgan (1981), Colt (1984 and 1990 p.c.)

¹ Significantly impacted by biological uptake and release

² Total carbonate expressed as bicarbonate (includes CO₂ = 0.41 mg/L).

Table 4.3. Atomic weights (Standard Methods, 1989; rounded to thousandths)

Element	Atomic Weight (g/mol)
Argon	39.948
Boron	10.811
Calcium	40.078
Carbon	12.011
Chloride	35.453
Hydrogen	1.008
Magnesium	24.312
Nitrogen	14.007
Oxygen	15.999
Phosphorus	30.974
Silicon	28.086
Sodium	22.990
Sulfur	32.066

Table 4.4. Names, units, and symbols of water quality variables

Variable (units)	Symbol
Physical Properties	
Temperature (°C)	T_C
Thermodynamic temperature ($T_C + 273.15$, °K)	T_K
Salinity (g/kg or ppt)	S
Chlorinity (g/kg or ppt)	CL
Ionic strength (molal, mol/kg)	I
Ionic strength (molar, mol/L)	I_M
Water density (kg/m^3)	ρ
Water specific weight (kN/m^3)	γ
Specific heat capacity ($\text{kJ/kg}\cdot^\circ\text{C}$)	HC
Latent heat of vaporization (kJ/kg)	LHV
Surface tension (N/m)	ST
Kinematic viscosity (m^2/s)	KV
Dynamic viscosity ($\text{N}\cdot\text{s}/\text{m}^2$)	DV
Mean depth of vapor-liquid phase interface, below water surface (m)	DP
Water vapor pressure (mm Hg)	P_W
Elevation above sea level (at water surface, m)	E
Barometric pressure (at water surface, mm Hg)	BP
Dissolved compounds (other than gases)	
Dissolved inorganic carbonates (mg C/L; mmol/L)	DIC; CO_3 , $\text{H}_2\text{CO}_3^{n-}$
Total ammonia nitrogen (mg N/L; mmol/L)	TAN; NH
Ionized ammonium (mg N/L; mmol/L)	$\text{NH}_4\text{-N}$; NH_4^+
Unionized ammonia (mg N/L; mmol/L)	$\text{NH}_3\text{-N}$; NH_3
Nitrite (mg N/L; mmol/L)	$\text{NO}_2\text{-N}$; NO_2^-
Nitrate (mg N/L; mmol/L)	$\text{NO}_3\text{-N}$; NO_3^-
Dissolved inorganic nitrogen (mg N/L)	DIN
Dissolved inorganic phosphorus (ortho-phosphate; mg P/L; mmol/L)	DIP; PO
Species of phosphoric acid (H_3PO_4 ; mmol/L)	$\text{H}_x\text{PO}_4^{n-}$
Total borate (mg B/L, mmol/L)	BO
Species of boric acid (H_3BO_3 or B(OH)_3 ; mmol/L)	$\text{H}_x\text{BO}_3^{n-}$, B(OH)_x^{n-}
Total silicate (ortho-silicate; mg Si/L, mmol/L)	SI
Species of silicic acid (H_4SiO_4 or Si(OH)_4 ; mmol/L)	$\text{H}_x\text{SiO}_4^{n-}$, $\text{SiO}_x(\text{OH})_y^{n-}$
Total sulfate (mg S/L, mmol/L)	SO
Species of sulfuric acid (H_2SO_4)	$\text{H}_x\text{SO}_4^{n-}$
Total sulfide (mg S/L, mmol/L)	HS
Species of hydrogen sulfide (H_xS^{n-})	H_xS^{n-}

Table 4.4. Continued

Variable (units)	Symbol
Dissolved Gases	
Dissolved oxygen (mg O ₂ /L)	DO, O ₂
Dissolved nitrogen (mg N ₂ /L)	DN, N ₂
Dissolved carbon dioxide (mg CO ₂ / L)	DC, CO ₂
Dissolved argon + trace (mg Ar/ L)	DA, Ar
Bunsen coefficient (L/L-atm)	B
Weight-volume constant (mg/ml)	K
Volume fraction	VF
Liquid phase	LP
Vapor phase	VP
Total pressure, LP (mm Hg)	P _t ^l
Partial pressure of individual gas, LP (mm Hg)	P _i ^l
Total pressure, dry VP (atm)	P _t ^{g dry}
Total pressure, wet VP (mm Hg)	P _t ^{g wet}
Partial pressure of individual gas i, wet VP (atm)	P _i ^{g wet}
Total saturometer (tensionometer) reading, LP (mm Hg wrt BP)	dP
Gas saturation, individual i or total gases (% or mm Hg)	GS _i , GS _t
Undissolved (particulate) compounds (dw = dry weight)	
Particulate inorganic solids (mg dw/ L)	PIS, PS
Particulate organic solids (mg dw/ L)	POS, PS
Settled inorganic and organic solids (g dw/ m ²)	PSS
Phytoplankton density (g C/ m ³ and mg chl-a/ m ³)	P
Secchi disk visibility depth (cm)	SDV

Table 4.4. Continued

Variable (units)	Symbol
pH Equilibria	
Hydronium	H^+
Hydroxide	OH^-
pH (active or free; NBS scale) = $-\log_{10}\{H^+\}$, with H^+ in mol/L	pH
Hardness (mg $CaCO_3$ /L)	HRD
Total alkalinity as mass (mg $CaCO_3$ /L)	ALK
Total alkalinity as equivalents (meq/L)	ALK_t
Carbonate alkalinity (meq/L)	ALK_c
Non-carbonate alkalinity (meq/L)	ALK_{nc}
Non-carbonate, non-water alkalinity (meq/L)	ALK_{ncw}
Alkalinity due to water hydroxide minus hydronium (meq/L)	ALK_w
Total acidity (meq/L)	ACD_t
Carbonate acidity (meq/L)	ACD_c
Non-carbonate acidity (meq/L)	ACD_{nc}
Active concentration of species i of compound (mmol/L)	$\{i\}$
Molar concentration of species i of compound (mmol/L)	$[i]$
Molar concentration of compound C (mmol/L)	mol_C or $[C]$
Equilibrium molar concentration of compound C (mmol/L)	$mol_{C_{eq}}$
Mass concentration of compound C (mg/L = g/m^3)	C
Equilibrium mass concentration of compound C (mg/L)	C_{eq}
Hybrid acid-base constant corrected for T_C and S	K'_{nj}
pK form of hybrid acid-base constant ($-\log_{10}$)	pK'_{nj}
Ionization fraction	α_{nj}
Activity coefficient	δ_I

4.1 Physical properties of water

Physical properties used in the modeling and analysis of aquaculture systems include: temperature, salinity, chlorinity, ionic strength, density, specific weight, hydrostatic head, heat capacity, vapor pressure, latent heat of vaporization, surface tension, dynamic viscosity, kinematic viscosity, Prandtl number, and barometric pressure.

4.1.1 Temperature

Temperature is input, maintained, and reported in degrees Celsius ($^{\circ}\text{C}$). Degrees Fahrenheit ($^{\circ}\text{F}$) may be optionally used in input data files for air and water temperatures. Thermodynamic (absolute) temperature, expressed in degrees Kelvin ($^{\circ}\text{K}$), is used in many calculations. $^{\circ}\text{C}$ and $^{\circ}\text{F}$, and $^{\circ}\text{C}$ and $^{\circ}\text{K}$, are related by:

$$^{\circ}\text{C} = (5 / 9) (^{\circ}\text{F} - 32)$$

$$^{\circ}\text{F} = (^{\circ}\text{C} \cdot 9 / 5) + 32$$

$$^{\circ}\text{K} = ^{\circ}\text{C} + 273.15$$

4.1.2 Salinity, chlorinity, and ionic strength

Salinity (S; g/kg or ppt) is a measure of the concentration of dissolved inorganic matter, not including dissolved gases. Rigorously, salinity is defined as the weight (g) of dissolved inorganic matter in 1 kg of seawater, after all Br^- and I^- have been replaced by the equivalent quantity of Cl^- and all HCO_3^- and CO_3^{2-} converted to oxide (Stumm and Morgan 1981). For modeling purposes, salinity values are converted to a per volume basis (g salts/ m^3) using water density.

Chlorinity (CL; g/kg or ppt) is used as a measure of salinity and is empirically determined by titration of seawater with AgNO_3 . Its use is possible due to the nearly constant composition of seawater for constituents $> 1 \text{ mg/kg}$, thus allowing characterization of all components given a value for chlorinity. The relationship between salinity and chlorinity is: $\text{CL} = \text{S} / 1.80655$ (Stumm and Morgan 1981). Riley and Skirrow (1975) provide a small correction term: $\text{CL} = (\text{S} - 0.03) / 1.805$, where if $\text{S} < 0.03$, then $\text{CL} = 0$.

Ionic strength, expressed in molal (I ; mol/kg) or molar (I_M ; mol/L) terms, is used to calculate activity coefficients and correct equilibrium constants for salinity. Ionic strength of water is defined by (Stumm and Morgan 1981):

$$I_M = 0.5 \sum (\text{mol} C_i Z_i^2) \text{ for all species } i$$

where $\text{mol} C_i$ = molar concentration of species i (mol/L)

Z_i = charge of species i

A simplified method is used to calculate ionic strength in saline solutions (Whitfield, 1974):

$$I = (19.9273 S) / (1000 - 1.005109 S)$$

and $I_M = I \rho / (1000 \text{ L/m}^3)$

Based on Whitfield (1974), example values of I_M at various salinities and a temperature of 25 °C are 0.10 ($S = 5$), 0.20 ($S = 10$), 0.41 ($S = 20$), and 0.74 ($S = 35$).

4.1.3 Water density, specific weight, and hydrostatic head

Water density (ρ , kg/m^3) is a function of water temperature (°C) and salinity (g/kg) (Figure 4.1). Water density decreases with increasing temperature above 4 °C (0 °C for seawater) and density increases with salinity. The following literature method is applicable to a temperature range of 0-40 °C and a salinity range of 0.5-43 g/kg (Millero and Poisson 1981):

$$\rho = \rho_0 + a S + b S^{3/2} + 4.8314 \times 10^{-4} S^2$$

where $\rho_0 = 999.842594 + 6.793952 \times 10^{-2} T_C - 9.095290 \times 10^{-3} T_C^2 + 1.001685 \times 10^{-4} T_C^3$
 $- 1.120083 \times 10^{-6} T_C^4 + 6.536336 \times 10^{-9} T_C^5$

$$a = 8.24493 \times 10^{-1} - 4.0899 \times 10^{-3} T_C + 7.6438 \times 10^{-5} T_C^2 - 8.2467 \times 10^{-7} T_C^3 + 5.3875 \times 10^{-9} T_C^4$$

$$b = -5.72466 \times 10^{-3} + 1.0227 \times 10^{-4} T_C - 1.6546 \times 10^{-6} T_C^2$$

The following simplified method was derived by regression, using values from Millero and Poisson (1981), and gives values within a maximum absolute error of < 1.0% for the temperature range 0-40 °C and salinity range 0-40 ppt:

$$\rho = 1001.361766 - (0.197208 T_C) + (0.79781 S) - (0.00172 T_C S)$$

The specific weight of water (γ ; kN/m^3 or kPa/m) is a function of water density and gravity:

$$\gamma = \rho g / (1000 \text{ N/kN})$$

where g = gravitational acceleration = 9.80665 m/s^2 and $1.0 \text{ kg}\cdot\text{m/s}^2$ is equivalent to 1.0 Newton (N). Hydrostatic head (ρ_h ; mm Hg/m) is calculated by (Millero and Poisson, 1981):

$$\rho_h = 760 / [101325 / (g \rho)]$$

4.1.4 Water heat capacity

The specific heat capacity of water (HC; J/g · °C, kJ/kg · °C, or kJ/kg · °K) is a function of water temperature and salinity (as chlorinity, CL; g/kg) (Figure 4.2). Maximum heat capacity occurs at 0 °C for freshwater and 40 °C for seawater, and heat capacity decreases with increasing salinity. The following literature method is applicable to a temperature range of 5-35 °C and a salinity range of 0.9-39.7 g/kg (Millero et al. 1973):

$$\begin{aligned} \text{HC} = & [4.2174 - 3.720283\text{e-}3 T_C + 1.412855\text{e-}4 T_C^2 - 2.654387\text{e-}6 T_C^3 \\ & + 2.093236\text{e-}8 T_C^4] + \text{CL} [-(13.81 - 0.1938 T_C + 0.0025 T_C^2) / 1000] \\ & + \text{CL}^{1.5} [(0.43 - 0.0099 T_C + 0.00013 T_C^2) / 1000] \end{aligned}$$

The following simplified method was derived by regression, using values from Millero et al. (1973), and gives values within a maximum absolute error of < 1.0% for the temperature range 0-40 °C and salinity range 0-40 ppt:

$$\text{HC} = 4.199578 - (0.00079 T_C) - (0.006234 S) + (0.000039 T_C S)$$

4.1.5 Water vapor pressure

The saturation vapor pressure of water (P_W , mm Hg) is a function of water temperature and salinity (Figure 4.3). Maximum vapor pressures for freshwater and seawater occur at 40 °C. The following literature method is applicable to a temperature range of 0-40 °C and salinity range 0 - 40 g/kg (Green and Carritt 1967):

$$\begin{aligned} P_W = & (760 \text{ mm Hg/atm}) (1.0 - 5.370\text{e-}4 S) \exp\{ 18.1973 (1.0 - 373.16 / T_K) \\ & + 3.1813\text{e-}7 (1.0 - \exp[26.1205 (1.0 - T_K / 373.16)]) \\ & - 1.8726\text{e-}2 (1.0 - \exp[8.03945 (1.0 - 373.16 / T_K)]) \\ & + 5.02802 \log_e(373.16 / T_K) \} \end{aligned}$$

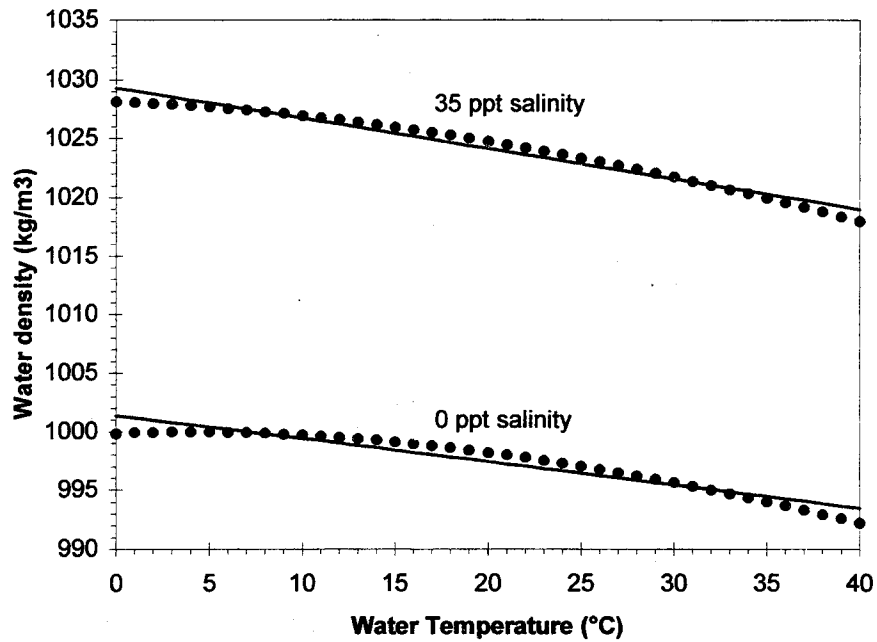


Figure 4.1. Water density as a function of water temperature (°C), for 0 and 35 ppt salinity levels, using rigorous (points) and simplified (lines) methods

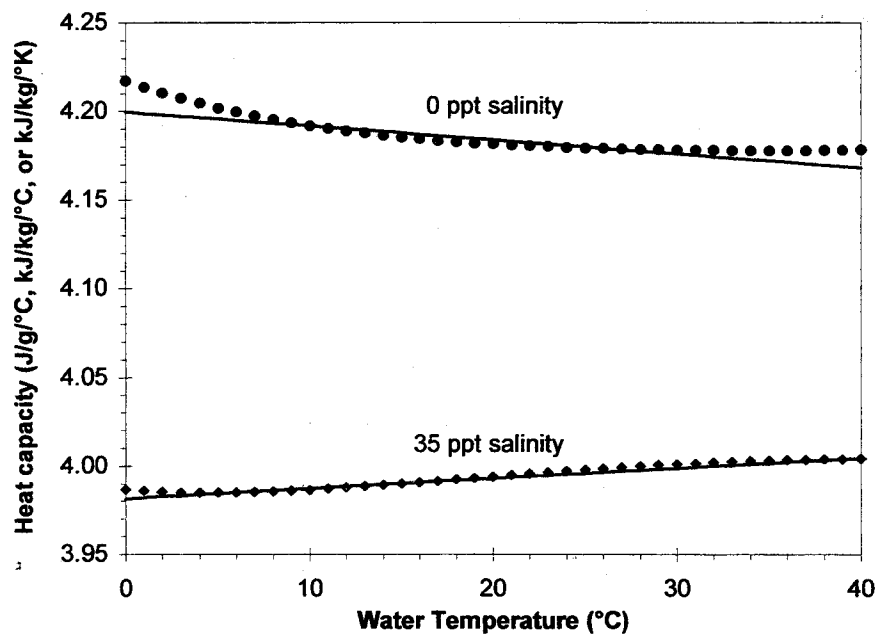


Figure 4.2. Water specific heat capacity as a function of water temperature (°C), for 0 and 35 ppt salinity levels, using rigorous (points) and simplified (lines) methods

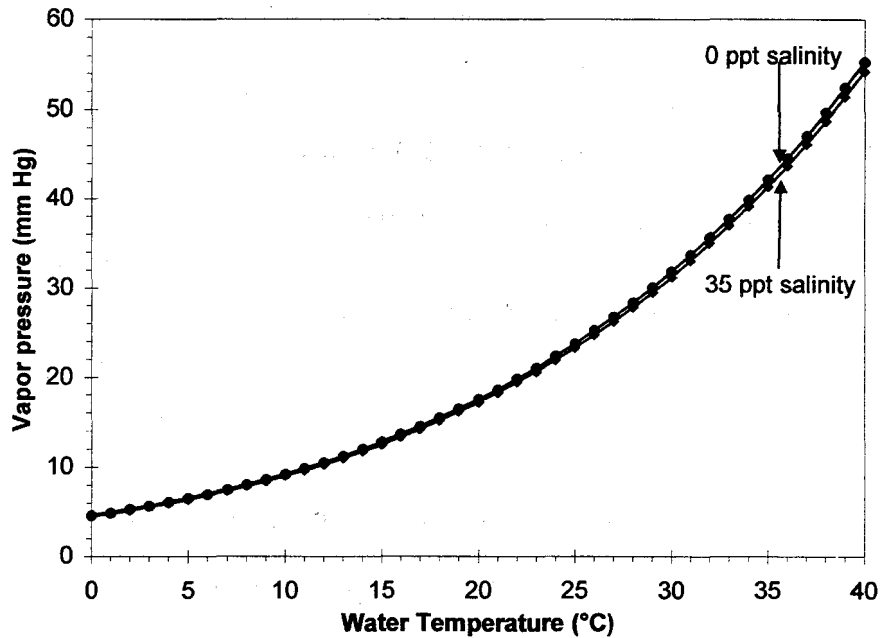


Figure 4.3. Water vapor pressure as a function of water temperature (°C), for 0 and 35 ppt salinity levels, using rigorous (points) and simplified (lines) methods

The following literature method is used as a simplified method and is applicable to a temperature range of 0-40 °C and salinity range 0 - 40 g/kg (Weiss and Price, 1980):

$$P_W = (760 \text{ mm Hg/atm}) \exp[24.4543 - 67.4509 (100 / T_K) - 4.8489 \log_e(T_K / 100) - 0.000544 S]$$

4.1.6 Additional methods

Latent heat of vaporization (LHV, kJ/kg) is calculated by (Brooker, 1967):

$$\text{LHV} = 2502.535259 - (2.38576424 T_C)$$

Surface tension (ST, N/m) is calculated by (Riley and Skirrow, 1975):

$$\text{ST} = (75.64 - 0.144 T_C + 0.0221 S)$$

Dynamic viscosity (DV, N-s/m²) is calculated by (Korson et al., 1969; Millero, 1974):

$$DV = 1.0020 \times 10^{-3} \left[1.1709 (20 - T_c) - 0.001827 (T_c - 20) (T_c - 20) / (T_c + 89.93) \right] \\ \{ 1.0 + [0.000366 + 5.185 \times 10^{-5} (T_c - 5.0)] (CL \rho / 1000)^{0.5} \\ + [0.002756 + 3.300 \times 10^{-5} (T_c - 5.0)] (CL \rho / 1000) \}$$

Kinematic viscosity (KV, m²/S) is calculated by (Korson et al., 1969; Millero, 1974; Millero and Poisson, 1981):

$$KV = DV / \rho$$

The following simplified method for kinematic viscosity (KV, m²/S) was derived by regression ($r^2 = 0.97$), using values from the method above:

$$KV = 0.000001 (1.613 - 0.02653 T_c + 0.001193 S)$$

Using linear regression on values listed in Welty et al. (1976) ($r^2 = 0.95$), the Prandtl number (PN; dimensionless) is calculated by:

$$PN = 12.928 - 0.244 T_c$$

4.1.7 Barometric pressure

Barometric pressure (BP; mm Hg) can be specified as an annual regime in the facility climate file along with other variables. However, use of a constant BP based on facility elevation is considered adequate and is calculated by (Colt, 1984):

$$BP = BP_0 / (10^{(E - E_0) / (67.4 T_{air})})$$

where BP_0 = BP at reference station (mm Hg), E = facility elevation above sea level (m), E_0 = reference station elevation above sea level (m), and T_a = average air temperature of facility and reference station (°K). If E_0 = zero (sea level), BP_0 = 760 mm Hg, and the air temperature is 20 °C ($T_a = 293.15$ °K), then the simplified form of this equation often used in the literature is derived:

$$BP = 760 / (10^{(ELV / 19758.31)})$$

4.2 General methods

Methods described in this section are applicable to dissolved gas and acid-base chemistry, for purposes of expressing and quantifying mass, molar, and active concentrations of compounds and correcting standard equilibrium constants of chemical reactions to temperature and salinity.

4.2.1 Mass, molar, molal, and normal concentrations

Concentrations as mass per unit volume (C ; mg/L or g/m^3) and as mass per unit weight (C_w ; mg/kg or ppm) are converted by (Snoeyink and Jenkins, 1980):

$$C_w = C / (\text{density kg/L})$$

Molality (m ; mmol/kg) and molarity (M ; mmol/L) of a dissolved compound are converted by (Stumm and Morgan, 1981; molarity of water = $55.56 \text{ mol/L} = 1000 \text{ g/L} / 18 \text{ g/mol}$):

$$m = M \times [\text{weight solution} / (\text{weight solution} - \text{weight solutes})] / (\text{density kg/L})$$

Mass (C ; mg/L) and molar concentrations are converted by molecular weight (mw ; mg/mmol), where $C = M \times mw$ and molar concentrations may be multiplied by ionization fractions to calculate species concentrations (e.g., unionized and ionized ammonia; not shown). A normal (equivalent) concentration (N ; eq/L) of a conjugate base is equal to its molar concentration multiplied by its level of hydrogen-ion dissociation according to the pH range in use and resulting compound species considered. For example at $5 \leq \text{pH} \leq 10$, HCO_3^- yields 1.0 eq/mol, CO_3^{2-} yields 2.0 eq/mol, and PO_4^{3-} yields 3.0 eq/mol. Additional terms for molar concentrations include (Stumm and Morgan, 1981):

$$\begin{aligned} \text{molC} &= \text{total molar concentration of compound C (mmol/L)} \\ &= \Sigma \text{ free (active) and associated species of compound} \end{aligned}$$

$$[i] = \text{total molar concentration of active-plus-associated species i (mmol/L)}$$

$$\{i\} = \text{active concentration (activity) of species i of compound (mmol/L)}$$

$$\delta_i = \text{activity coefficient of species i of compound (dimensionless), where } \delta_i \text{ approaches unity as concentrations of solutes approach zero}$$

$$\text{where } \delta_i = \{i\} / [i] \text{ or } \{i\} = \delta_i [i]$$

4.2.2 Concentration and activity

The activity coefficient of a given compound species i (δ_i ; dimensionless) accounts for both nonspecific interactions (ion electric fields) and specific interactions (solute-water interactions, ion pair association, and complex formation) in saline waters (Stumm and Morgan, 1981). Activity coefficients are a function of the ion charge of the species (z_i) and the ionic strength of the medium (I_M), using the Guntelberg relationship ($I_M < 0.1$ M) and Davies relationship (rigorous use 0.1 M $< I_M < 0.5$; use here 0.1 M $< I_M$) (Stumm and Morgan, 1981):

$$\text{If } I_M < 0.1 \text{ M, then: } \log_{10} \delta_i = -A B z_i^2 [I_M^{1/2} / (1.0 + I_M^{1/2})]$$

$$\text{If } I_M \geq 0.1 \text{ M, then: } \log_{10} \delta_i = -A B z_i^2 [I_M^{1/2} / (1.0 + I_M^{1/2}) - 0.2 I_M]$$

The influence of temperature on activity coefficients is accounted for by (Butler, 1982):

$$A = 0.5$$

$$B = (298.15 / T_K)^{2/3}$$

$$\text{giving } B = 1.0 \text{ at } T_K = 298.15 \text{ }^\circ\text{K (25 }^\circ\text{C)}$$

For water of any ionic strength I_M , δ_{H_2O} is set to 1.0, where $\{H_2O\}$ in freshwater and seawater is 1.00 and 0.98, respectively (Stumm and Morgan, 1981). If a species is uncharged ($z_i = 0.0$), then the following equation gives δ_i values that are greater than one (salting out effect), where a b_i value of 0.1 is used for CO_2 , NH_3 , H_3PO_4 , H_2S , $B(OH)_3$, and $Si(OH)_4$ (Butler, 1982):

$$\log_{10} \delta_i = b_i I$$

$$\text{and } \log_{10} \delta_i = b_i I_M (1000 \text{ L/m}^3) / \rho$$

4.2.3 Equilibrium constants

For the reversible reaction $aA + bB = cC + dD$, the equilibrium constant K is the ratio of the forward and reverse rate constants. Equilibrium equations for gases diffusing across a liquid-vapor boundary (Henry's Law) and for ionization of an acid ($HA = A^- + H^+$, or $HA + H_2O = A^- + H_3O^+$) are given below. Rigorously stated, species concentrations are expressed as active concentrations $\{\}$, as opposed to molar concentrations $[\]$. Equilibrium constants are a function of water temperature

and salinity. The generic, theoretical basis of this dependency is developed below, but empirically based methods given later are used when available.

$$K = k_f / k_r = [C]^c [D]^d / [A]^a [B]^b$$

$$K = [\text{gas}] / (\text{partial pressure gas})$$

$$K = [H^+] [A^-] / [HA]$$

4.2.4 Temperature dependence of equilibrium constants

Chemical equilibrium constants (K) are corrected for water temperature based on the simplifying assumption that change in heat capacity is close to zero and change in enthalpy is independent of temperature over the temperature range of interest (0 - 40 °C) (Table 4.5) (Stumm and Morgan, 1981).

$$K = {}^{\text{std}}K \exp \left(\frac{dH^\circ}{R} \left(\frac{1.0}{T_{K\text{std}}} - \frac{1.0}{TK} \right) \right)$$

where K = value of constant for freshwater at temperature T_K (°K), ${}^{\text{std}}K$ = value of constant for freshwater at standard temperature ($T_{K\text{std}} = 298.15$ °K (25 °C)), dH° = change in standard enthalpy of reaction (kJ/mol; $= \sum H^\circ \text{ products} - \sum H^\circ \text{ reactants}$; for acids, forward reaction is dissociation of hydrogen), R = gas constant (0.008314 kJ/(mol °K)).

4.2.5 Salinity dependence of equilibrium constants

Chemical equilibrium constants (K) are corrected for water salinity using ionic-strength dependant activity coefficients defined within the infinite dilution activity scale. Rigorous correction (interaction) terms based on additional equilibria related to the molality and composition of the solution are not used (Stumm and Morgan, 1981). In general, theoretical formulations for activity coefficients in saline mediums are not considered feasible (Stumm and Morgan 1981). For purposes here, a correction factor (F; dimensionless) is used based on reported, empirical determinations of mixed dissociation constants (K' ; see acid-base water chemistry below). If salinity is zero, then $\delta_i = 0$, $\{i\} = [i]$, and

$$K = \{H^+\} \{A^-\} / \{HA\} = [H^+] [A^-] / [HA]$$

$$K' = K$$

If salinity > 0 g/kg, then K is corrected for water salinity by:

$$\{i\} = \delta_i [i]$$

$$K' = K (\delta_{HA} / \delta_A) F$$

or $pK' = pK - \log_{10} \delta_{HA} + \log_{10} \delta_A - \log_{10} F$

where $K = \{H^+\} \{A^-\} / \{HA\}$

$$K' = \{H^+\} \delta_A [A^-] / \delta_{HA} [HA]$$

F is applied so that reported values for K' at 298.15 °K (25 °C) and 35 g/kg salinity are achieved (linear interpolation used, where if $I_M = 0$ then $F=1$, and if $I_M = I_{M-ref}$ then $F = f$):

$$F = 1.0 + [(f - 1.0) (I_M / I_{M-ref})]$$

$$f = (\text{reported } K') / (\text{calculated } K' \text{ @ } 25 \text{ C and } 35 \text{ g/kg})$$

$$I_{M-ref} = I_M \text{ at } 25 \text{ °C and } 35 \text{ g/kg salinity} = 0.740 \text{ M}$$

Table 4.5. Reported and derived constants for theoretically based temperature dependence of acid-base equilibrium constants¹

Species	$p^{std} K (25 \text{ °C})$	$dH^\circ (\text{kJ/mol})$	$dH^\circ/R (\text{°K})$	$dH^\circ/(R T K_{std})$	f
H2O	13.994	57.250	6886.02	23.0958	2.847
H2CO3*	6.352	11.107	1335.99	4.4809	1.325
HCO3-	10.329	16.432	1976.47	6.6291	5.535
CAC	8.480	-8.156	-981.02	-3.2904	9.408
H2PO4-	7.198	5.341	642.35	2.1545	4.426
HPO42-	12.380	68.846	8280.70	27.7736	1080
NH4 ⁺	9.246	52.261	6285.86	21.0829	0.924
H2S	6.919	21.670	2606.47	8.7421	1.135
H3BO3	9.237	15.200	1828.23	6.1319	1.879
H4SiO4	9.460	-69.211	-8324.69	-27.9211	1.879

¹ Based on values reported in Snoeyink and Jenkins (1980) and Stumm and Morgan (1981); also see Acid-base water chemistry later in this chapter

4.3 Dissolved gases

Dissolved gases are critical variables in aquaculture systems. Primary concerns are dissolved oxygen concentration, carbon dioxide concentration and its affect on pH, and total gas saturation. Equilibrium gas concentrations (100% saturation) are used to determine saturation levels of existing gas concentrations, for the interpretation and reporting of water quality, and to model gas diffusion. Gases considered in the equilibrium methods described below include oxygen, nitrogen, and carbon dioxide, since these gases may have significant partial pressures in the vapor phase interfacing facility waters. Argon and trace gases can be included with nitrogen, but this consideration is not likely to have a significant impact on water quality modeling. Gases including chlorine, ozone, hydrogen sulfide, and ammonia are considered by AquaFarm, but their vapor phase partial pressures (VF_{CL} , VF_{O_3} , VF_{HS} , and VF_{NH}) are considered to be zero, and thus the equilibrium concentrations of these gases are zero.

4.3.1 Equilibrium gas concentrations

Equilibrium concentrations of dissolved oxygen (DO_{eq}), nitrogen (DN_{eq} ; DN_{eq}^* if trace gases are included), and carbon dioxide (DC_{eq}) in the liquid phase (mol/L or mg/L) are proportional to their partial pressures in the vapor phase (atm) (Henry's Law; Snoeyink and Jenkins, 1980). Vapor phase partial pressures result from gas volume fractions and the total gas pressure. The proportionality constant (Henry's Law constant or coefficient of absorption; mol/L/atm) is a function of water temperature (gas dissolution is exothermic) and salinity (salting-out effect). Theoretically based temperature and salinity corrections described earlier in this chapter are not used in AquaFarm. Instead, as typically employed, practical methods based on Bunsen coefficients are used. A Bunsen coefficient (β ; L/L·atm) is defined as the volume of gas at STP (standard temperature 0 °C and pressure 760 mm Hg) absorbed per unit volume liquid at a given temperature and salinity when the gas partial pressure is one standard atmosphere (L/L·atm). Bunsen coefficients are proportional to Henry's constants for a given gas, water temperature, and water salinity.

4.3.2 Calculation of Bunsen coefficients

Regression equations used to compute Bunsen coefficients are the basis of the dissolved oxygen tables in the 15th Edition of the Standard Methods for the Examination of Water and Wastewater (Colt 1984). Alternative calculation methods for Bunsen coefficients from the literature are provided below, termed *short method* and *long method*. Simplified derivations of these Bunsen functions that yielded sufficient accuracy were not found. Calculated equilibrium concentrations for dissolved nitrogen, oxygen, and carbon dioxide are given in Figures 4.4, 4.5, and 4.6, respectively, as a function of water temperature (°C), for 0, 18, and 35 ppt salinity levels, using both short and long methods.

Using calculated Bunsen coefficients, equilibrium concentrations of nitrogen, oxygen, and carbon dioxide in water (C_{eq} , mg/L) are calculated as a function of water temperature, salinity, depth, total gas pressure at the water surface, and volume fraction of the gas in the vapor phase by (Colt 1984):

$$C_{eq} = (1000 \text{ ml/L}) W \beta P_t^{g \text{ wet}}$$

where W = molecular weight per molecular volume of gas (mg/ml; Table 4.3).

β = Bunsen coefficient of gas (L/L·atm)

$P_t^{g \text{ wet}}$ = partial pressure of gas in water-saturated (RH = 100%) vapor phase (atm)

$$P_t^{g \text{ wet}} = VF P_t^{g \text{ dry}}$$

where VF = volume (or mole) fraction of gas in dry vapor phase (RH = 0%) (Table 4.6)

$P_t^{g \text{ dry}}$ = total gas pressure of dry vapor phase (atm)

$$= (P_t^{g \text{ wet}} - P_W) / (760 \text{ mm Hg/atm})$$

where $P_t^{g \text{ wet}}$ = total gas pressure of water-saturated vapor phase (mm Hg)

$$= BP + (\sigma D (7.5006 \text{ mm Hg/kPa at } 0^\circ \text{C}))$$

P_W = saturation vapor pressure of water (mm Hg)

4.3.2.1 Calculation of Bunsen coefficients for oxygen

Short method: The Bunsen coefficient for oxygen (β_{O_2} , L/L·atm) is calculated by (constants a and b from Table 4.6; Weiss, 1970; Colt, 1984):

$$\beta_{O_2} = \exp[a_{1O_2} + a_{2O_2} (100 / T_K) + a_{3O_2} \log_e(T_K / 100) + S [b_{1O_2} + b_{2O_2} (T_K / 100) + b_{3O_2} (T_K / 100)^2]]$$

Long method: The Bunsen coefficient for oxygen (β_{O_2} , L/L·atm) is calculated by (Benson and Krause, 1980 and 1984; Colt, 1990 p.c.):

$$\beta_{O_2} = AV_{O_2} (\rho/1000) f [1.0 - t (1.0 + P_W / (760 \text{ mm Hg/atm})) / (k_{O_2} 18.0153)]$$

where AV_{O_2} = atomic volume (L/mol; Table 4.6)

$$f = 1000 - 0.716582 S$$

$$t = 0.000975 - 1.426e-5 T_C + 6.436e-8 T_C^2$$

k_{O_2} = Henry coefficient (atm)

$$= \exp[3.71814 + 5596.17 / T_K - 1049668 / T_K^2 + S (0.0225034 - 13.6083 / T_K + 2565.68 / T_K^2)]$$

4.3.2.2 Calculation of Bunsen coefficients for nitrogen

Short method: The Bunsen coefficient for nitrogen (β_{N_2} , L/L·atm), using VF_{N_2} or $VF_{N_2^*}$, is calculated by (constants a and b from Table 4.6; Weiss, 1970; Colt, 1984):

$$\beta_{N_2} = \exp[a_{1N_2} + a_{2N_2} (100 / T_K) + a_{3N_2} \log_e(T_K / 100) + S [b_{1N_2} + b_{2N_2} (T_K / 100) + b_{3N_2} (T_K / 100)^2]]$$

where K_{N_2} = K of pure N_2 (Table 4.6)

Long method: The Bunsen coefficient for nitrogen gas (β_{N_2} , L/L·atm), using $VF_{N_2^*}$, is expressed as a weighted mean of nitrogen and argon gases ($\beta_{N_2^*}$, L/L·atm) and is calculated by (constants a and b from Table 4.6; Benson and Krause, 1980 and 1984; Colt, 1990 p.c.):

β_{N2*} = weighted-mean β based on VF

$$= [(\beta_{N2} VF_{N2}) + (\beta_{Ar} VF_{Ar})] / (VF_{N2} + VF_{Ar})$$

where $\beta_{Ar} = \exp[a_{1Ar} + a_{2Ar} (100 / T_K) + a_{3Ar} \log_e(T_K / 100) + S [b_{1Ar} + b_{2Ar} (T_K / 100) + b_{3Ar} (T_K / 100)^2]]$

β_{N2} = as above

W_{N2*} = weighted-mean based on β and VF

$$= [(W_{N2} \beta_{N2} VF_{N2}) + (W_{Ar} \beta_{Ar} VF_{Ar})] / [(\beta_{N2} VF_{N2}) + (\beta_{Ar} VF_{Ar})]$$

4.3.2.3 Calculation of Bunsen coefficient for carbon dioxide

Short method: The Bunsen coefficient for carbon dioxide (β_{CO2} , L/L-atm) is calculated by (constants a and b from Table 4.6; k_{CO2} is expressed as mol/L/atm; Weiss, 1970 and 1974; Colt, 1984):

$$\beta_{CO2} = AV_{CO2} k_{CO2}$$

where AV_{CO2} = atomic volume (L/mol; Table 4.6)

$$k_{CO2} = \exp[a_{1CO2} + a_{2CO2} (100 / T_K) + a_{3CO2} \log_e(T_K / 100) + S [b_{1CO2} + b_{2CO2} (T_K / 100) + b_{3CO2} (T_K / 100)^2]]$$

Long method: The Bunsen coefficient for carbon dioxide (β_{CO2} , L/L-atm) is calculated by (Weiss, 1974; Colt, 1990 p.c.):

$$\beta_{CO2} = AV_{CO2} k_{CO2} f \exp[((1.0 - xp) 33.3e-03) / (0.08205601 T_K)]$$

where AV_{CO2} and k_{CO2} calculated as above

$$f = xp \exp[((xp - xb) / (0.08205601 T_K))]$$

$$xp = 1.0 + (P_W / (760 \text{ mm Hg/atm}))$$

$$xb = 0.001 (-1636.75 + 12.0408 T_K - 3.27957e-2 T_K^2 + 3.16528e-5 T_K^3)$$

Table 4.6. Constants used in the calculation of Bunsen coefficients and equilibrium concentrations for dissolved gases (data from Colt, 1984 and 1990 p.c.)

Parameter	Gas Species			
	DO	DN	DC	DA + trace
a_1	-58.3877	-59.6274	-58.0931	-55.6578
a_2	85.8079	85.7661	90.5069	82.0262
a_3	23.8439	24.3696	22.2940	22.5929
b_1	-0.0348920	-0.0515800	0.0277660	-0.0362670
b_2	0.0155680	0.0263290	-0.0258880	0.0162410
b_3	-0.0019387	-0.0037252	0.0050578	-0.0020114
W	1.42903	1.25043	1.97681	1.78419
AW	31.9988	28.0134	44.0098	39.948
AV	22.392	22.403	22.2626	22.390
VF	0.209460	0.780840	0.000345	0.009355
VF _{N2*}	—	0.790195	—	—

a_n, b_n : Constants of Bunsen equations

W: Molecular weight / molecular volume at STP of gas (mg/mL)
 = (MW mg/mol) / (mL/mol @ STP: 0 C, 760 mm Hg)

AW: Atomic weight (g/mol)

AV: Atomic volume (L/mol)

VF: Volume fraction of gas in dry air (RH = 0%). Volume fractions are equivalent to mole fractions and their sum equals one. The VF_{DC} value has been updated from an older value of 0.00032. For nitrogen, VF may be for nitrogen only (VF_{N2} = 0.780840) or include argon and other trace gases (VF_{Ar} = 0.009340 + 0.000015; VF_{N2*} = VF_{N2} + VF_{Ar} = 0.790195)

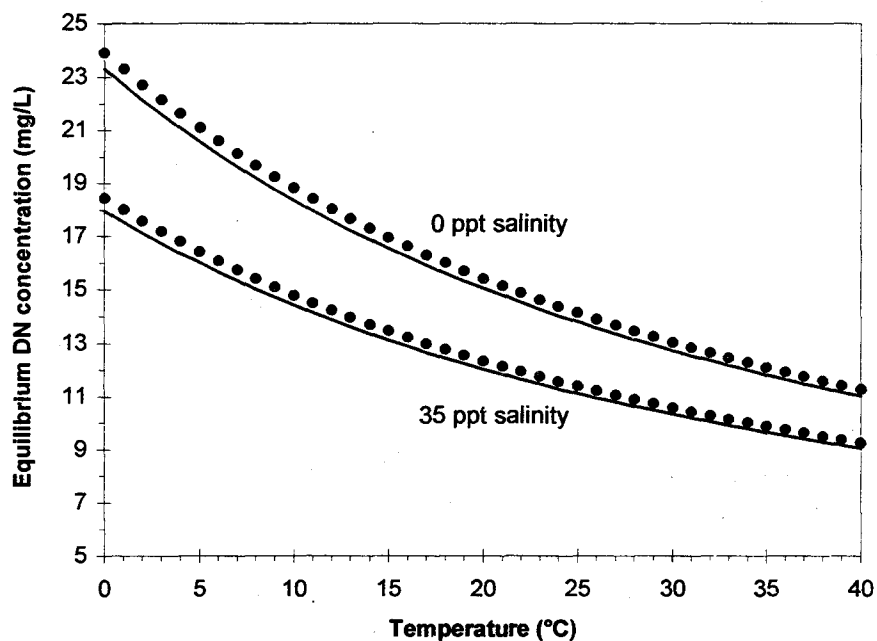


Figure 4.4. Equilibrium concentration of dissolved nitrogen (DN) as a function of water temperature (°C), for 0, 18, and 35 ppt salinities, using short (points) and long (lines) methods

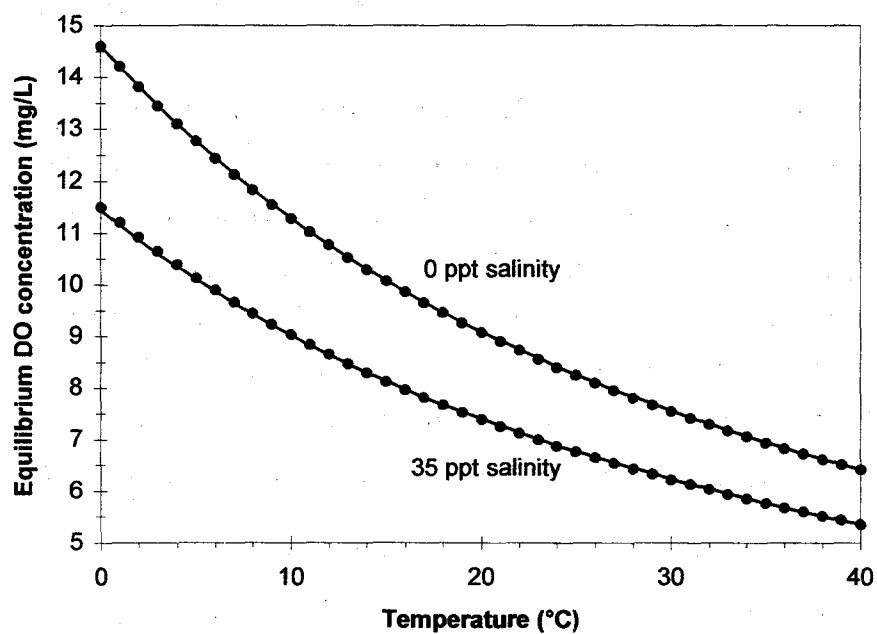


Figure 4.5. Equilibrium concentration of dissolved oxygen (DO) as a function of water temperature (°C), for 0, 18, and 35 ppt salinities, using short (points) and long (lines) methods

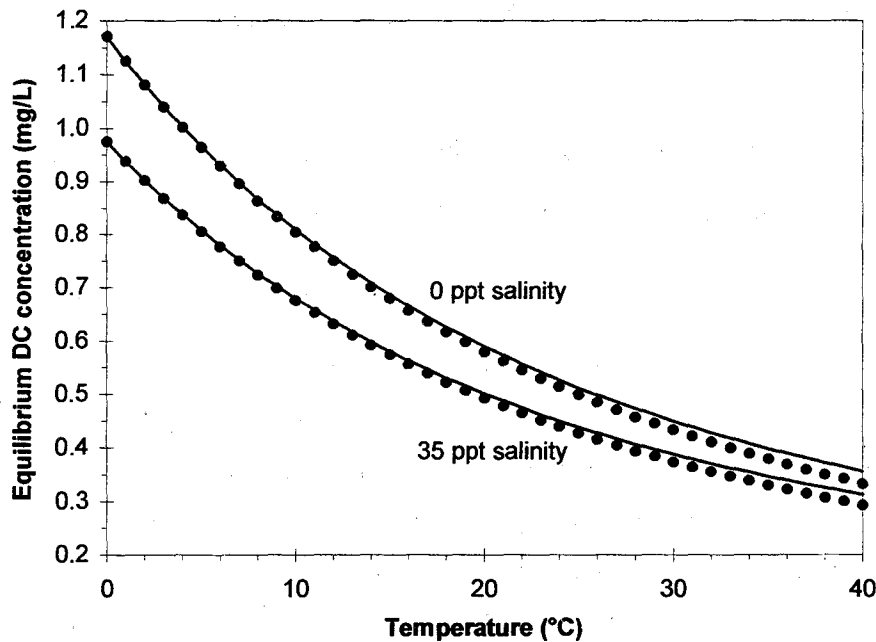


Figure 4.6. Equilibrium concentration of dissolved carbon dioxide (DC) as a function of water temperature (°C), for 0, 18, and 35 ppt salinities, using short (points) and long (lines) methods

4.3.3 Existing gas concentrations

For given water quality profiles, DN (mg N₂/L) and DC (mg CO₂/L) gas concentrations are not normally measured directly and are calculated from other measured variables. Calculations are based on Dalton's Law of Partial Pressures, which states that the total pressure exerted by a mixture of dissolved gases is equal to the sum of the partial pressures of the constituent gases. First, total carbonate concentration (DIC) is defined by the given pH, total alkalinity, and compound concentrations (e.g. ammonia, phosphates, silicates, and borates). Second, DC concentration is defined by temperature, salinity, pH, and DIC. Finally, DN or DN* is calculated (DN* includes argon and trace gases; see Table 4.6), depending on use of VF_{N2} or VF_{N2*}:

$$DN = DN_{eq1} (P_t^{g\text{ wet}} + dP - P_{O_2}^l - P_{CO_2}^l - P_w) / [VF_{N2*} (P_t^{g\text{ wet}} - P_w)]$$

where DN_{eq1} = equilibrium DN at given temperature, salinity, depth, BP, and VF nitrogen

$P_t^{g\text{ wet}}$ = total gas pressure of water-saturated vapor phase (mm Hg)

$P_{O_2}^l$ = partial pressure of oxygen in liquid phase (mm Hg)

$$= \left[\left[(760 \text{ mm Hg/atm}) / \left[(1000 \text{ ml/L}) (K_{O_2} \text{ mg/ml}) \right] \right] (DO_{eq} GS_{O_2} / 100) \right] / \beta_{O_2}$$

$$= P_{O_2}^{g \text{ wet}} (GS_{O_2} / 100)$$

$$P_{CO_2}^l = \text{partial pressure of carbon dioxide in liquid phase (mm Hg)}$$

$$= \left[\left[(760 \text{ mm Hg/atm}) / \left[(1000 \text{ ml/L}) (K_{CO_2} \text{ mg/ml}) \right] \right] ([H_2CO_3^*] \right.$$

$$\times (44.01 \text{ mg/mmol})) \right] / \beta_{CO_2}$$

Existing gas concentrations result from facility source water specifications (initial conditions) and subsequent facility processes (gas mass transfer). Ground waters are usually over saturated with carbon dioxide, may be deficient in oxygen, and may contain significant levels of ammonia and hydrogen sulfide. Potential sources of supersaturated gases are the supply water (e.g., ground water, river water below a fall, and pump-suction air leak) and the facility water systems (e.g., water heating, water blending, and water oxygenation). Gas super saturation may harm fish (see Chapter 7). Mass concentrations of gases vary with temperature and salinity but are often used to specify fish water quality criteria. Active concentrations of gases (liquid phase gas tension or partial pressure) are independent of temperature and salinity. Active gas concentrations can be used as fish water quality criteria, by specifying criteria as saturation levels instead of mass concentrations.

Total gas pressure in the liquid phase is defined by:

$$P_t^l = \text{liquid phase total dissolved gas pressure (mm Hg)}$$

$$= \sum P_i^l \text{ for DO, DN or DN}^*, \text{ DC, and water}$$

where $P_i^l = \text{partial pressure (tension) of gas } i \text{ in liquid phase (mm Hg; for water use } P_W)$

$$= \left[\left[(760 \text{ mm Hg/atm}) / \left[(1000 \text{ ml/L}) (K_i \text{ mg/ml}) \right] \right] C_i \right] / \beta_i$$

Total gas pressure in the vapor phase is defined by:

$$P_t^{g \text{ wet}} = \text{total gas pressure of water-saturated vapor phase (mm Hg)} = \sum P_i^{g \text{ wet}}$$

where $P_i^{g \text{ wet}} = \text{partial pressure of individual gas in water-saturated vapor phase (mm Hg)}$

Reporting and measurement of total gas saturation makes use of the following terms:

$$GS_t = \text{liquid phase total dissolved gas saturation (\%)} = 100 (P_t^l / P_t^{g \text{ wet}})$$

or $P_t^l = P_t^{g \text{ wet}} GS_t / 100$

and $dP = P_t^l - P_t^{g \text{ wet}}$

$$= 0 \text{ when } P_t^l = P_t^{g \text{ wet}}, \text{ i.e. when } GS_t = 100\%$$

$$\text{where } P_t^{g \text{ wet}} = BP + [\sigma D (7.5006 \text{ mm Hg/kPa})]$$

Existing (C) and equilibrium (C_{eq}) gas concentrations (mg/L) are related by

$$C = C_{eq} GS / 100$$

$$\text{where } GS = \text{liquid phase saturation of gas (percent)} = 100 (P^l / P^{g \text{ wet}})$$

4.4 Acid-base water chemistry

Many of the compounds present in aquaculture waters participate in acid-base chemistry, and the relative concentrations of their dissociation products (compound species) are a function of pH. In turn, pH is a function of temperature, salinity, and total compound concentrations. Many of these compound species, as well as pH, have direct impact on fish performance and/or are involved in the physical, chemical, and biological processes found in aquaculture systems. Unionized ammonia and carbon dioxide levels are particularly critical regarding fish performance and are primary excretory products of fish. Processes impacting pH levels in aquaculture systems include air-water diffusion of carbon dioxide (passive and active), fish-excretion of carbon dioxide, consumption of carbon dioxide by primary production, hydrogen-ion production and consumption by nitrification and denitrification, and pH and alkalinity control processes. The strategy used for pH modeling is to maintain compound and alkalinity concentrations by mass balances and calculate pH as needed. Also calculated are (1) ionization fractions of unionized species involved in gas transfer or toxic to fish (e.g. CO_2 , NH_3 , and H_2S), (2) carbonate levels given pH, alkalinity, and other variables, (3) pH and carbonate levels at equilibrium states for carbon dioxide diffusion and/or calcium carbonate precipitation-dissolution, and (5) required compound quantities for pH and alkalinity adjustment.

4.4.1 Scales for equilibrium constants and pH

Use of pH values and acid-base equilibrium constants is uncomplicated in freshwater. When salinity is present, additional effort is required to achieve compatible measurement scales for pH and equilibrium constants (Stumm and Morgan, 1981). In the methods developed here, the National Bureau of Standards (NBS) pH scale (pH_{NBS}) and mixed (hybrid) equilibrium constants (K') are used. These two methods are internally consistent (Stumm and Morgan, 1981) and endorsed by the

International Union of Pure and Applied Chemistry (IUPAC). pH_{NBS} is determined relative to that of a standard buffer and defined in terms of hydrogen ion activity ($-\log_{10} \{H^+\}$), based on the infinitely dilute aqueous reference state (Stumm and Morgan, 1981):

$$\text{pH}_{\text{NBS}} = -\log_{10} [\{H^+\} \text{ (mol/ 1000 mmol)}]$$

$$\{H^+\} = 10^{-\text{pH}_{\text{NBS}}} \text{ (1000 mmol/ mol)}$$

A mixed dissociation constant (K') is used with pH_{NBS} , where hydrogen ion activity is used in conjunction with molar concentrations for compounds (free plus associated ions, [i]).

$$K' = \{H^+\} [A] / [HA]$$

where $[A]$ = molar concentration of conjugate base

$[HA]$ = molar concentration of acid

If given pH values are based on $-\log_{10} [H^+]$, i.e. the total of free and associated H^+ (Hansson scale, pH_{HS}), then $\{H^+\}$ and $[H^+]$ are related by an estimated, empirically based, activity coefficient (δ_{H^+}). δ_{H^+} is a function of salinity. For seawater (Stumm and Morgan, 1981):

$$[H^+] = \{H^+\} / \delta_{H^+}$$

or $\text{pH}_{\text{HS}} = \text{pH}_{\text{NBS}} + \log_{10} \delta_{H^+}$

or $\text{pH}_{\text{NBS}} = \text{pH}_{\text{HS}} - \log_{10} \delta_{H^+}$

where δ_{H^+} = range 0 – 1 and $\log_{10} \delta_{H^+} < 0$

$$\text{pH}_{\text{HS}} \approx \text{pH}_{\text{NBS}} - 0.15 \quad (\text{e.g., seawater})$$

Similarly, if mixed dissociation constants are not available for a given acid, then the constant ionic medium (apparent) equilibrium constant used (cK) is converted to a mixed equilibrium constant by:

$$K' = {}^cK \delta_{H^+}$$

$$\text{p}K' = \text{p}{}^cK - \log_{10} \delta_{H^+}$$

$$\text{p}K' \approx \text{p}{}^cK + 0.15 \quad (\text{e.g., seawater})$$

4.4.2 Ionization fractions

The pH system model developed here includes only monoprotic acids and diprotic acids, where diprotic acids are considered to be monoprotic and triprotic acids are considered to be diprotic when one dissociation state is not considered (see below). Ionization fractions are used to determine species concentrations from total concentrations and are calculated by (Snoeyink and Jenkins, 1980; Stumm and Morgan, 1981):

α_{nj} = ionization fraction for dissociation n of monoprotic compound j

where $\alpha_{0j} = [\text{HA}] / {}^{\text{mol}}\text{HA} = \{\text{H}^+\} / D$

$\alpha_{1j} = [\text{A}^-] / {}^{\text{mol}}\text{HA} = K'_{1j} / D$

$D = \{\text{H}^+\} + K'_{1j}$

or ${}^{\text{mol}}\text{HA} / [\text{A}^-] = \{\text{H}^+\} / K'_{1j} = 10^{-\text{pH}} / 10^{-\text{p}K'_{1j}}$

$[\text{A}^-] = {}^{\text{mol}}\text{HA} / (1.0 + 10^{\text{p}K'_{1j} - \text{pH}})$

and α_{nj} = ionization fraction of dissociation n of diprotic compound j

where $\alpha_{0j} = [\text{H}_2\text{A}] / {}^{\text{mol}}\text{HA} = \{\text{H}^+\}^2 / D$

$\alpha_{1j} = [\text{HA}^-] / {}^{\text{mol}}\text{HA} = \{\text{H}^+\} K'_{1j} / D$

$\alpha_{2j} = [\text{A}^{2-}] / {}^{\text{mol}}\text{HA} = K'_{1j} K'_{2j} / D$

$D = \{\text{H}^+\}^2 + \{\text{H}^+\} K'_{1j} + K'_{1j} K'_{2j}$

4.4.3 Acid-base equilibrium constants

Acid-base equilibrium constants ($\text{p}K'$) are a function of temperature (0 - 40 °C) and salinity (0-40 ppt). Methods described below include (1) enthalpy and ionic-strength based functions introduced earlier, termed *derived methods*, and (2) functions available in the literature, termed *literature methods* (Figure 4.7). Derived methods are used when literature methods are not available or have limited application ranges for temperature and salinity. Derived methods were found to closely agree with literature methods, but they did not decrease calculation intensity (note that the derived methods contain terms that also must be calculated). $\text{p}K'$ values are converted to K' when they are used, expressed as mmol or mmol^2 , the latter units used for K'_w and K'_{CaCO_3} .

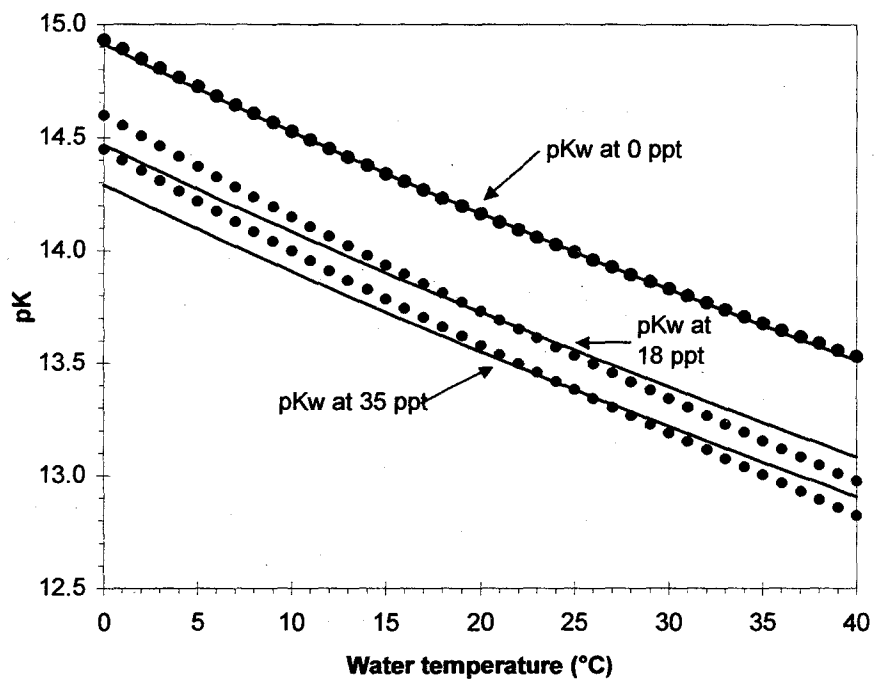


Figure 4.7A. pK' values for water as a function of water temperature ($^{\circ}\text{C}$), for 0, 18, and 35 ppt salinity levels, using literature (points) and derived (lines) methods

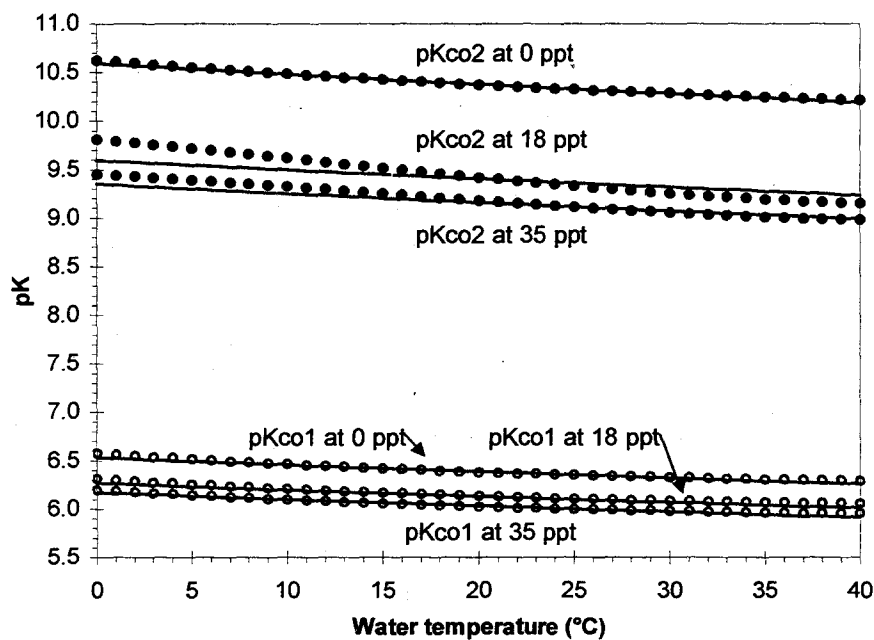


Figure 4.7B. pK' values for carbonates as a function of water temperature ($^{\circ}\text{C}$), for 0, 18, and 35 ppt salinity levels, using literature (points) and derived (lines) methods

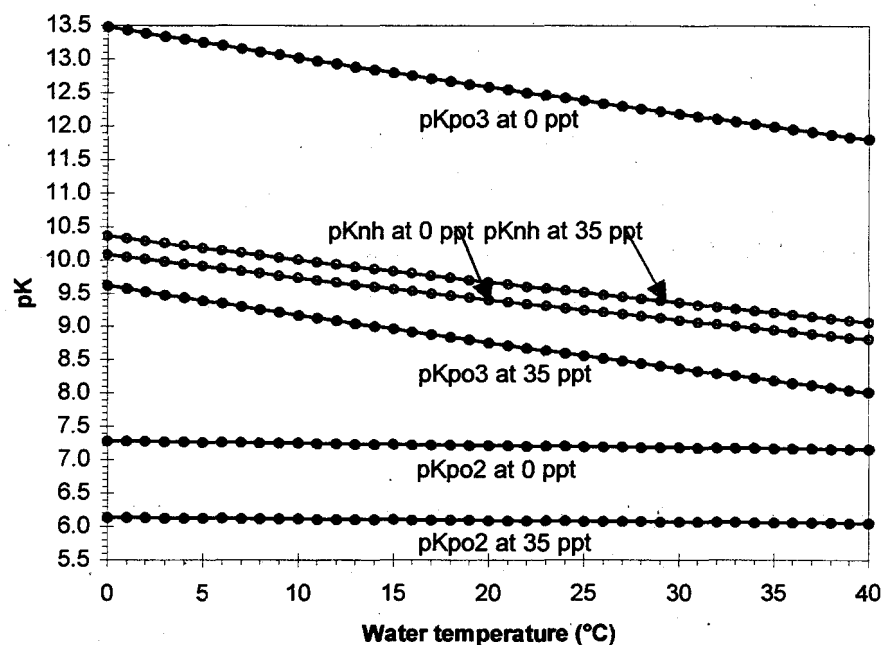


Figure 4.7C. pK' values for ammonia and ortho-phosphate as a function of water temperature (°C), for 0, 18, and 35 ppt salinity levels, using literature (points) and derived (lines) methods

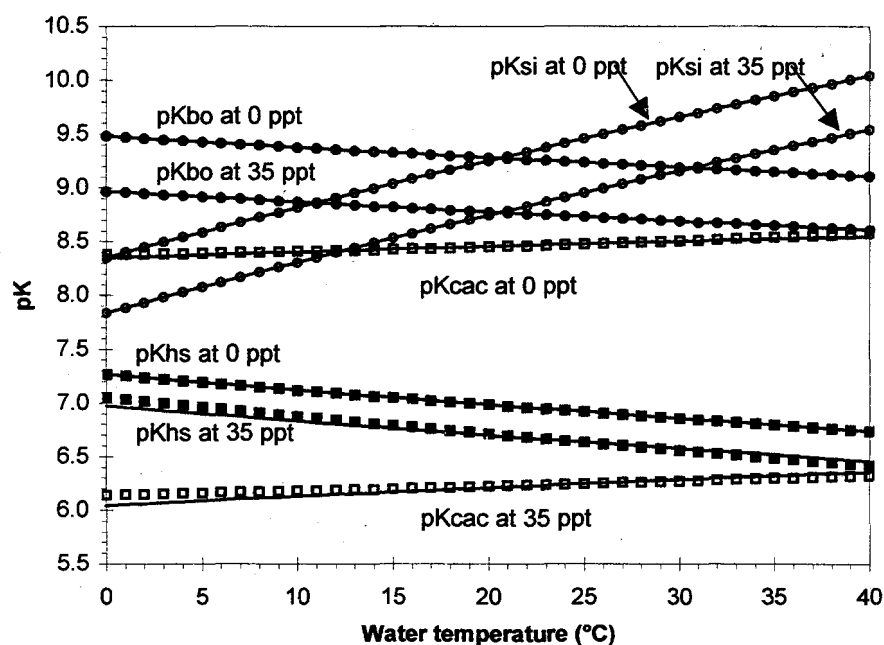


Figure 4.7D. pK' values for silicate, borate, sulfide, and calcite as a function of water temperature (°C), for 0, 18, and 35 ppt salinity levels, using literature (points) and derived (lines) methods

For the derived methods, values for $^{\text{std}}\text{pK}$ (25 °C, zero salinity), dH° (kJ/mol), combined terms, and f_i (dimensionless) (Table 4.5) are based on reported values. dH° values were calculated using reported pK and temperature (10 and 30 °C) data when possible, rather than heats of formation. This was done to minimize error due to the simplifying assumption that dH°_i is independent of temperature over the temperature range of interest (0 - 40 °C). For salinity corrections, ionic strength is computed by Whitfield (1974).

4.4.3.1 Water

Acid-base species of water include water, hydronium (hydrogen ions), and hydroxide. The equilibrium reaction is $\text{H}_2\text{O} = \text{H}^+ + \text{OH}^-$, where $\text{H}^+ \equiv \text{H}_3\text{O}^+$. The derived method for $S = 0 - 40$ g/kg and $T_C = 0 - 40$ °C is:

$$K'_W = 10^{-13.99} e^{(23.10 - 6886 / \text{TK})} (\delta_{\text{H}_2\text{O}} / \delta_{\text{OH}}) [1.0 + (2.847 - 1.0) (I_M / 0.740)]$$

The literature method for $S = 0$ g/kg and $T_C = 0 - 40$ °C (Loewenthal and Marais 1976) is:

$$\text{pK}'_W = 4787.3/\text{TK} + 7.1321 \log_{10}(\text{TK}) + 0.010365 \text{TK} - 22.801$$

The literature method for $S = 0 - 40$ g/kg and $T_C = 0 - 40$ °C (Dickson and Riley 1979) is:

$$\text{p}^c\text{K}_W = 3441.0/\text{TK} + 2.241 - 0.09415 (S^{0.50})$$

$$\text{pK}'_W = \text{p}^c\text{K}_W - \log_{10} \delta_{\text{H}^+}$$

$$\text{pK}'_W \approx \text{p}^c\text{K}_W + 0.15 \quad (\text{e.g., seawater})$$

4.4.3.2 Carbonic acid

Total carbonate ($^{\text{mol}}\text{C}_{\text{CO}}$) includes aqueous carbon dioxide, carbonic acid, bicarbonate, and carbonate, where $^{\text{mol}}\text{C}_{\text{CO}} = [\text{H}_2\text{CO}_3^*] + [\text{HCO}_3^-] + [\text{CO}_3^{2-}]$. Equilibrium reactions are $\text{H}_2\text{CO}_3 = \text{H}^+ + \text{HCO}_3^-$ and $\text{HCO}_3^- = \text{H}^+ + \text{CO}_3^{2-}$. The combined concentration of aqueous carbon dioxide ($\text{CO}_{2\text{aq}}$ or $^{\text{mol}}\text{DC}$) and carbonic acid (H_2CO_3) is represented as H_2CO_3^* , where the carbonic acid concentration is considered negligible (Stumm and Morgan, 1981):

$$[\text{H}_2\text{CO}_3^*] = [\text{H}_2\text{CO}_3] + [\text{CO}_{2\text{aq}}]$$

where $[\text{H}_2\text{CO}_3^*] \approx [\text{CO}_{2\text{aq}}]$

and $[\text{CO}_{2\text{aq}}] = {}^{\text{mol}}\text{DC} = \text{DC} / (44.009 \text{ mg/mmol for CO}_2)$

The derived method for $S = 0 - 40 \text{ g/kg}$ and $T_C = 0 - 40 \text{ }^\circ\text{C}$ is:

$$K'_{1\text{CO}} = 10^{-6.352} e^{(4.481 - 1336/\text{TK})} (\delta_{\text{H}_2\text{CO}_3^*} / \delta_{\text{HCO}_3}) [1.0 + (1.325 - 1.0) (I_M / 0.740)]$$

$$K'_{2\text{CO}} = 10^{-10.329} e^{(6.629 - 1976/\text{TK})} (\delta_{\text{HCO}_3} / \delta_{\text{CO}_3}) [1.0 + (5.535 - 1.0) (I_M / 0.740)]$$

The literature method for $S = 0 \text{ g/kg}$ and $T_C = 0 - 40 \text{ }^\circ\text{C}$ (Plummer and Busenberg 1982) is:

$$\text{p}K'_{1\text{CO}} = 356.3094 + 0.06091964 T_K - 21834.37/\text{TK} - 126.8339 \log_{10}(T_K) + 1684915.0/T_K^2$$

$$\text{p}K'_{2\text{CO}} = 107.8871 + 0.03252849 T_K - 5151.797/\text{TK} - 38.92561 \log_{10}(T_K) + 563713.9/T_K^2$$

The literature method for $S = 0 - 40 \text{ g/kg}$ and $T_C = 0 - 40 \text{ }^\circ\text{C}$ (Mehrbach et al. 1973) is:

$$\text{p}K'_{1\text{CO}} = -13.7201 + 0.031334 T_K + 3235.76 / T_K + (1.300\text{e-}5 S T_K) - 0.1032 S^{0.5}$$

$$\begin{aligned} \text{p}K'_{2\text{CO}} = & 5371.9645 + 1.671221 T_K + 0.22913 S + 18.3802 \log_{10}(S) - 128375.28/T_K \\ & - 2194.3055 \log_{10}(T_K) - (8.0944\text{e-}4 S T_K) - 5617.11 \log_{10}(S) / T_K + 2.136 S / T_K \end{aligned}$$

4.4.3.3 Ortho-phosphoric acid

Total ortho-phosphate (${}^{\text{mol}}\text{C}_{\text{PO}}$) includes dissociation products of ortho-phosphoric acid, where ${}^{\text{mol}}\text{C}_{\text{PO}} = [\text{H}_3\text{PO}_4] + [\text{H}_2\text{PO}_4^-] + [\text{HPO}_4^{2-}] + [\text{PO}_4^{3-}]$. Equilibrium reactions are $\text{H}_3\text{PO}_4 = \text{H}^+ +$

H_2PO_4^- (not considered), $\text{H}_2\text{PO}_4^- = \text{H}^+ + \text{HPO}_4^{2-}$, and $\text{HPO}_4^{2-} = \text{H}^+ + \text{PO}_4^{3-}$. Literature methods

were not found. The derived method for $S = 0 - 40 \text{ g/kg}$ and $T_C = 0 - 40 \text{ }^\circ\text{C}$ is:

$$K'_{1\text{PO}} = 10^{-7.198} e^{(2.155 - 642.4/\text{TK})} (\delta_{\text{H}_2\text{PO}_4} / \delta_{\text{HPO}_4}) [1.0 + (4.426 - 1.0) (I_M / 0.740)]$$

$$K'_{2\text{PO}} = 10^{-12.380} e^{(27.77 - 8281/\text{TK})} (\delta_{\text{HPO}_4} / \delta_{\text{PO}_4}) [1.0 + (1080 - 1.0) (I_M / 0.740)]$$

4.4.3.4 Hydrogen sulfide

Total sulfide ($^{\text{mol}}C_{\text{HS}}$) includes dissociation products of hydrogen sulfide, where $^{\text{mol}}C_{\text{HS}} = [\text{H}_2\text{S}] + [\text{HS}^-] + [\text{S}^{2-}]$. Equilibrium reactions are $\text{H}_2\text{S} = \text{H}^+ + \text{HS}^-$ and $\text{HS}^- = \text{H}^+ + \text{S}^{2-}$ (latter not considered). The derived method for $S = 0 - 40 \text{ g/kg}$ and $T_C = 0 - 40 \text{ }^\circ\text{C}$ is:

$$K'_{\text{HS}} = 10^{-6.919} e^{(8.742 - 2606/\text{TK})} (\delta_{\text{H}_2\text{S}} / \delta_{\text{HS}}) [1.0 + (1.135 - 1.0) (I_M / 0.740)]$$

The literature method for $S = 0 \text{ g/kg}$ and $T_C = 0 - 40 \text{ }^\circ\text{C}$ (Broderius and Smith 1977) is:

$$\text{p}K'_{\text{HS}} = 3.122 + 1132.0 / T_K$$

The literature method for $S = 0 - 40 \text{ g/kg}$ and $T_C = 0 - 40 \text{ }^\circ\text{C}$ (Goldhaber and Kaplan 1975) is:

$$\text{p}K'_{\text{HS}} = 2.527 - 0.169 (\text{CL}^{1/3}) + 1359.96 / T_K$$

4.4.3.5 Boric acid

Total borate ($^{\text{mol}}C_{\text{BO}}$) includes dissociation products of boric acid, where $^{\text{mol}}C_{\text{BO}} = [\text{B}(\text{OH})_3] + [\text{B}(\text{OH})_4^-] + [\text{B}(\text{OH})_5^{2-}]$. Equilibrium reactions are H_3BO_3 or $\text{B}(\text{OH})_3 = \text{H}^+ + \text{B}(\text{OH})_4^-$ and $\text{B}(\text{OH})_4^- = \text{H}^+ + \text{B}(\text{OH})_5^{2-}$ (latter not considered). The derived method for $S = 0 - 40 \text{ g/kg}$ and $T_C = 0 - 40 \text{ }^\circ\text{C}$ is:

$$K'_{\text{BO}} = 10^{-9.237} e^{(6.132 - 1828/\text{TK})} (\delta_{\text{B}(\text{OH})_4} / \delta_{\text{B}(\text{OH})_3}) [1.0 + (1.879 - 1.0) (I_M / 0.740)]$$

The literature method for $S = 35 \text{ g/kg}$ and $T_C = 0 - 40 \text{ }^\circ\text{C}$ (Stumm and Morgan 1981) is:

$$\text{p}K'_{\text{BO}} = 2291.9 / T_K + 0.01756 (T_K - 3.385) - 0.32051 (\text{CL}^{1/3})$$

4.4.3.6 Ammonium

Total ammonia ($^{\text{mol}}C_{\text{NH}}$) includes ammonium and ammonia, where $^{\text{mol}}C_{\text{NH}} = [\text{NH}_3] + [\text{NH}_4^+]$. The equilibrium reaction is $\text{NH}_4^+ = \text{H}^+ + \text{NH}_3$. The derived method for $S = 0 - 40 \text{ g/kg}$ and $T_C = 0 - 40 \text{ }^\circ\text{C}$ is:

$$K'_{\text{NH}} = 10^{-9.246} e^{(21.08 - 6286/\text{TK})} (\delta_{\text{NH}_4} / \delta_{\text{NH}_3}) [1.0 + (0.924 - 1.0) (I_M / 0.740)]$$

This method is similar to a literature method for $S = 0 - 40$ g/kg and $T_C = 0 - 40$ °C (Hampson, 1977; ionic strength (I) by Whitfield, 1974):

$$K'_{NH} = [10^{-9.246} e^{(21.0806 - 6285.17/T_K)}] [10^{-0.012 I}]$$

The literature method for $S = 0$ g/kg and $T_C = 0 - 40$ °C (Emerson et al. 1975) is:

$$pK'_{NH} = 0.09018 + 2729.92 / T_K$$

The literature method for $S = 0 - 40$ g/kg and $T_C = 0 - 40$ °C is based on methods for freshwater from Emerson et al. (1975), seawater data from Khoo et al. (1977), and ionic strength (I, mol/kg) computed by Whitfield (1974). Computed values compare well to Whitfield (1974) and Bower and Bidwell (1978). The method is:

$$p^C K_{NH} = 0.09018 + 2729.92 / T_K + (0.1552 - 0.0003142 T_C) I$$

$$pK'_{NH} = p^C K_{NH} - \log_{10} \delta_{H^+}$$

$$pK'_{NH} \approx p^C K_{NH} + 0.15 \quad (\text{e.g., seawater})$$

4.4.3.7 Silicates

Total ortho-silicate ($^{\text{mol}}C_{SI}$) includes dissociation products of ortho-silicic acid, where $^{\text{mol}}C_{SI} = [\text{Si}(\text{OH})_4] + [\text{SiO}(\text{OH})_3^-] + [\text{SiO}_2(\text{OH})_2^{2-}]$. Equilibrium reactions are $\text{Si}(\text{OH})_4 = \text{H}^+ + \text{SiO}(\text{OH})_3^-$ and $\text{SiO}(\text{OH})_3^- = \text{H}^+ + \text{SiO}_2(\text{OH})_2^{2-}$ (latter not considered). Literature methods were not found. The derived method for $S = 0 - 40$ g/kg and $T_C = 0 - 40$ °C is

$$K'_{SI} = 10^{-9.460} e^{(-27.92 + 8325/T_K)} (\delta_{\text{Si}(\text{OH})_3} / \delta_{\text{Si}(\text{OH})_4}) [1.0 + (1.879 - 1.0) (I_M / 0.740)]$$

4.4.4 Precipitation-dissolution chemistry

Precipitation-dissolution (PD) processes may act as sources and sinks of metals and alkalinity components (Snoeyink and Jenkins, 1980; Stumm and Morgan, 1981; Butler, 1982). PD chemistry is complex, regarding both equilibria states and rates, and includes compounds containing ortho-phosphates, magnesium and calcium hydroxides, and magnesium and calcium carbonates. Only calcium carbonate is considered here, in order to model the use of calcium carbonate compounds to maintain alkalinity levels (e.g., pond liming) and upper limitations to pH due to calcium carbonate

precipitation (e.g., solar algae ponds). Precipitation of calcium carbonate may also occur due to water heating. Of the five or more polymorphic forms of CaCO_3 that occur in nature, only calcite is considered here, and water hardness is considered to be calcium only (magnesium ignored). The equilibrium reaction is $\text{Ca}^{2+} + \text{CO}_3^{2-} = \text{CaCO}_3$. The solubility product is (K_{CaCO_3} , mmol^2):

$$\begin{aligned} K_{\text{CaCO}_3} &= \{\text{Ca}^{2+}\} \{\text{CO}_3^{2-}\} / \{\text{CaCO}_3(\text{s})\} = \{\text{Ca}^{2+}\} \{\text{CO}_3^{2-}\}, \text{ where } \{\text{CaCO}_3(\text{s})\} = 1 \\ &= [\text{Ca}^{2+}] [\text{CO}_3^{2-}] \delta_{\text{Ca}} \delta_{\text{CO}_3} \\ &= [\text{Ca}^{2+}] (^{\text{mol}}\text{CO} \alpha_{2\text{CO}}) \delta_{\text{Ca}} \delta_{\text{CO}_3} \end{aligned}$$

K_{CaCO_3} increases with decreasing temperature and increasing salinity. The derived method for calcite, $S = 0 - 40$ g/kg, and $T_C = 0 - 40$ °C is:

$$K_{\text{CaCO}_3\text{-C}} = 10^{-8.480} e^{(-3.290 + 981.0/\text{TK})} [1/(\delta_{\text{CO}_3} \delta_{\text{Ca}})] [1.0 + (9.408 - 1.0) (I_M/0.740)]$$

The literature method for calcite, $S = 0$ g/kg, and $T_C = 0 - 40$ °C is (if aragonite, replace 171.9065 with 171.9773 and 2839.319 with 2903.293; Plummer and Busenberg, 1982):

$$\text{p}K_{\text{CaCO}_3} = 171.9065 + 0.077993 T_K - 2839.319 / T_K - 71.595 \log_{10}(T_K)$$

The literature method for calcite, $S = 0 - 40$ g/kg, and $T_C = 0 - 40$ °C is (if aragonite, replace 0.1614 with 0.5115; Edmond and Gieskes, 1970)

$$\text{p}K_{\text{CaCO}_3\text{-C}} = -\log_{10} [0.000001 (0.1614 + 0.02892 \text{ CL} - 0.0063 T_C)]$$

The concentration product (CP) is compared to K_{CaCO_3} to determine if calcium carbonate will precipitate ($\text{CP} > K_{\text{CaCO}_3}$) or dissolve ($\text{CP} < K_{\text{CaCO}_3}$) under the current water quality, where:

$$\text{CP} = ^{\text{mol}}\text{CO} [\text{Ca}^{2+}] K'_{1\text{CO}} K'_{2\text{CO}} / (\{\text{H}^+\} \{\text{H}^+\} + \{\text{H}^+\} K'_{1\text{CO}} + K'_{1\text{CO}} K'_{2\text{CO}})$$

The status of calcium carbonate precipitation can be expressed by the Langelier index (LI; Snoeyink and Jenkins, 1980), where LI equals the current pH minus the pH at which calcium carbonate is at equilibrium (without carbon dioxide diffusion). LI is greater than zero for over saturated conditions (precipitation) and less than zero for under saturated conditions (precipitation).

4.4.5 Coordination chemistry

Coordination compounds consist of complexes of one or more central atoms (ions; e.g., Na^+ , K^+ , H^+ , Ca^{2+} , Mg^{2+} , Fe^{3+} , and Al^{3+}) surrounded by a number of ligands (ions or polar molecules; e.g., H_2O , OH^- , Cl^- , HCO_3^- , CO_3^{2-} , $\text{H}_x\text{PO}_4^{n-}$, $\text{H}_x\text{SO}_4^{n-}$, and dissolved and particulate organic compounds) (Snoeyink and Jenkins, 1980). Complexation reduces free (active) concentrations of participating species and impacts acid-base chemistry by reducing active concentrations of alkalinity components. Central ions (e.g., Ca^{2+} and Mg^{2+}) and ligands (e.g., HCO_3^-) in seawater are complexed to a significant extent (Snoeyink and Jenkins, 1980; Stumm and Morgan, 1981). For purposes here, the complexation of alkalinity components (conjugate bases) by coordination chemistry is accounted for by the salinity corrections used in acid-base equilibrium calculations.

The bulk of metal ions in natural waters and wastewaters are associated with particulates (e.g., clay and detritus) (Snoeyink and Jenkins, 1980) and dissolved organic compounds (e.g., humic substances) (Snoeyink and Jenkins 1980). Given that such compounds are common in aquaculture waters, metals remaining to complex with alkalinity components are reduced. Thus, for saline aquaculture waters, salinity corrections used in acid-base calculations may over compensate for metal interactions and therefore under estimate active concentrations. Reduction of free metal concentrations by complexation can impact fish through the reduction of water hardness (fish require Ca and Mg) and reduction of metal toxicity (Snoeyink and Jenkins, 1980).

4.4.6 Modeling acid-base systems

Acid-base systems are modeled as interdependent sets of variables and equations, where the specific variables and equations used depend on the compounds present and the pH range of interest. The methods described below are based on the conservative properties of total alkalinity and compound concentrations. For all of the presented models, the required number of equations equals the number of unknowns. The significance of individual species (conjugate bases) as components of total alkalinity dictates their inclusion in these models. Alkalinity is defined as a measure of the capacity of water to neutralize acid (hydronium ions) and is equal to the sum of all titratable bases for a given titration end-point. The alkalinity equation algebraically expresses the net deficiency of protons with respect to the reference proton level. For purposes here, this reference level (titration end-point) is approximately pH 4.5 (function of temperature, salinity, and total

alkalinity), at which $^{\text{mol}}\text{C}_{\text{CO}} \approx [\text{H}_2\text{CO}_3^*]$. Waters in equilibrium with atmospheric CO_2 and with $6.5 \leq \text{pH} \leq 9.0$ have alkalinities between 0.01 and 10.0 meq/L, e.g., freshwater at 0.6 meq/L (30 mg CaCO_3/L) and seawater at 2.3 meq/L (115 mg CaCO_3/L) (Stumm and Morgan, 1981). Total alkalinity expressed in terms of calcium carbonate (ALK ; mg CaCO_3/L) and in terms of equivalents (ALK_t ; meq/L) are related by:

$$\text{ALK}_t = \text{ALK} / (50.043 \text{ mg } \text{CaCO}_3/\text{meq})$$

where $\text{CaCO}_3 = 100.086 \text{ mg/mmol} @ 2.0 \text{ meq/mmol} = 50.043 \text{ mg/meq}$

If significant fractions of conjugate bases remain at the titration end-point pH, then corrections for all such compounds must be applied to the calculation of ALK_t (Snoeyink and Jenkins, 1980; Stumm and Morgan, 1981). Without this correction, the calculated alkalinity contribution of stronger acids (e.g., HNO_2 , H_2SO_4) is too high. The alkalinity contribution of a conjugate base (ALK_B) for a given compound (C) is:

$$\text{ALK}_B = [\text{C}] (\alpha_1 - \alpha_2)$$

α_1 = fraction of conjugate base present at current pH

α_2 = fraction of conjugate base present at endpoint pH of titration

However, for the methods developed below, using an operational pH range of 5 – 10 and a titration endpoint pH of approximately 4.5, it is assumed that $\alpha_2 \approx 0$ for all compounds considered and that this correction can be ignored.

4.4.6.1 Comprehensive alkalinity model

Compounds considered in the comprehensive alkalinity model are those that represent potentially significant components of total alkalinity. These compounds include naturally occurring compounds in aquaculture supply waters as well as products (metabolites) of fish and water treatment systems. Predominant natural compounds include carbonates and silicates in freshwater and carbonates, sulfates, and borates in seawater (Stumm and Morgan, 1981; Snoeyink and Jenkins, 1980). In addition to these compounds, fish and water system products include ammonia, nitrate, nitrite, and phosphate. Organic acids (e.g., humic compounds) may exist at significant concentrations, but they are ignored here. A rigorous pH system model for aquaculture waters in

terms of total alkalinity is given below, where equilibrium constants of conjugate bases (pK) range from -3 to 14 and compounds are listed in order of increasing pK value.

$$\begin{aligned} \text{ALK}_t = & -\{\text{H}^+\} + [\text{Cl}^-] + [\text{HSO}_4^-] + [\text{NO}_3^-] + 2[\text{SO}_4^{2-}] + [\text{H}_2\text{PO}_4^-] + [\text{NO}_2^-] + [\text{HCO}_3^-] \\ & + [\text{HS}^-] + 2[\text{HPO}_4^{2-}] + [\text{B}(\text{OH})_4^-] + [\text{NH}_3] + [\text{SiO}(\text{OH})_3^-] + 2[\text{CO}_3^{2-}] + \\ & 3[\text{PO}_4^{3-}] + 2[\text{B}(\text{OH})_5^{2-}] + 2[\text{SiO}_2(\text{OH})_2^{2-}] + 2[\text{S}_2^-] + [\text{OH}^-] \end{aligned}$$

4.4.6.2 Alkalinity Model 1

Simplified forms of the comprehensive alkalinity model are used, based on (1) the acid-base species that are present in the operational pH range ($5 \leq \text{pH} \leq 10$) and (2) the relative contribution of these species to total alkalinity. For the first task, if a conjugate base or its respective acid show negligible ionization fractions ($< 1.0\%$) over the 5 – 10 pH range, then the conjugate base is considered to be an insignificant component of alkalinity (Figure 4.8). Based on this simplification, acids considered to remain totally dissociated include (listed in order of increasing pK):

hydrochloric acid (HCl), sulfuric acid (H_2SO_4), nitric acid (HNO_3), bisulfate (HSO_4^-), phosphoric acid (H_3PO_4), and nitrous acid (HNO_2). Conjugate bases considered to not undergo further dissociation include those of boric acid ($\text{B}(\text{OH})_4^-$), silicic acid ($\text{SiO}(\text{OH})_3^-$), hydrogen sulfide (HS^-). Thus, triprotic acids are reduced to diprotic acids (e.g., phosphoric acid), and diprotic acids are reduced to monoprotic acids (e.g., boric acid, silicic acid, and hydrogen sulfide). The only listed compound violating the designated 1.0% limit is nitrous acid, which shows a maximum ionization fraction of about 2% HNO_2 and pH 5. However, total nitrite concentrations are typically very low in aquaculture systems (e.g. ≤ 0.3 mg N/L) and this exception is ignored.

The model resulting from these simplifications (below) is considered to be a rigorous model for aquaculture. Numerical procedures are used to solve for $\{\text{H}^+\}$ and $^{\text{mol}}\text{CO}_{\text{eq}}$.

$$\begin{aligned} \text{ALK}_t = & [\text{OH}^-] - \{\text{H}^+\} + [\text{HCO}_3^-] + 2[\text{CO}_3^{2-}] + [\text{HPO}_4^{2-}] + 2[\text{PO}_4^{3-}] + [\text{HS}^-] \\ & + [\text{B}(\text{OH})_4^-] + [\text{NH}_3] + [\text{SiO}(\text{OH})_3^-] \end{aligned}$$

$$\begin{aligned} \text{subst. } \text{ALK}_t = & K'_w / \{\text{H}^+\} - \{\text{H}^+\} + ^{\text{mol}}\text{CO} (\alpha_{1\text{CO}} + 2 \alpha_{2\text{CO}}) + ^{\text{mol}}\text{PO} (\alpha_{2\text{PO}} + 2 \alpha_{3\text{PO}}) \\ & + ^{\text{mol}}\text{HS} \alpha_{1\text{HS}} + ^{\text{mol}}\text{BO} \alpha_{1\text{BO}} + ^{\text{mol}}\text{NH} \alpha_{1\text{NH}} + ^{\text{mol}}\text{SI} \alpha_{1\text{SI}} \end{aligned}$$

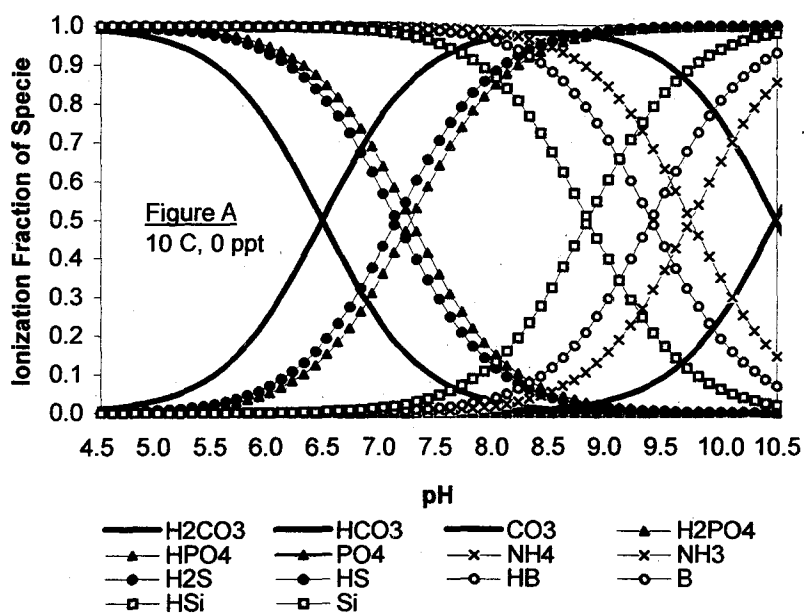


Figure 4.8A. Ionization fractions of compounds for which significant ionization exists over the pH range 5-10 (10 °C, 0 ppt)

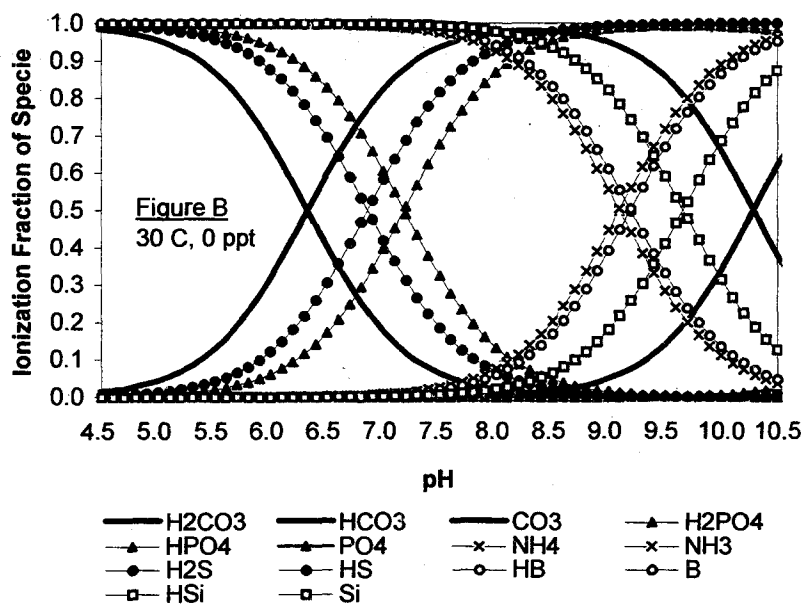


Figure 4.8B. Ionization fractions of compounds for which significant ionization exists over the pH range 5-10: (30 °C, 0 ppt)

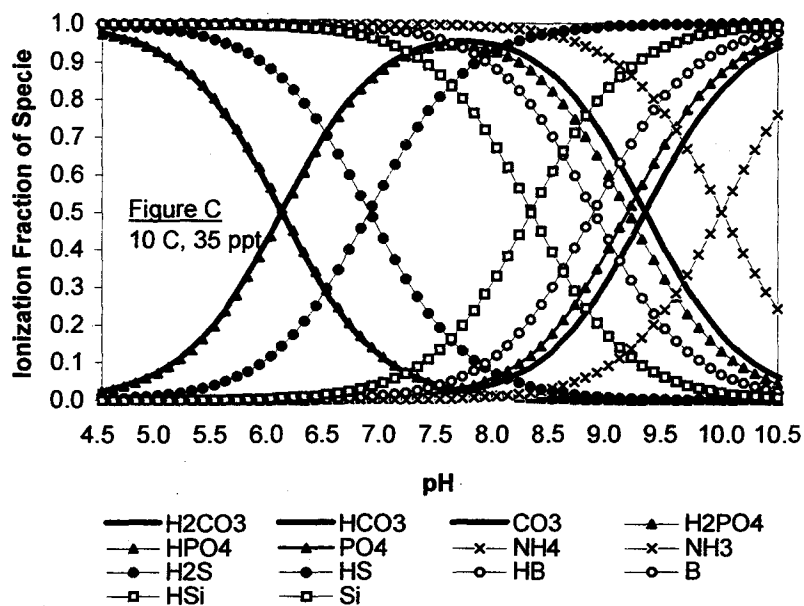


Figure 4.8C. Ionization fractions of compounds for which significant ionization exists over the pH range 5-10: C (10 °C, 35 ppt)

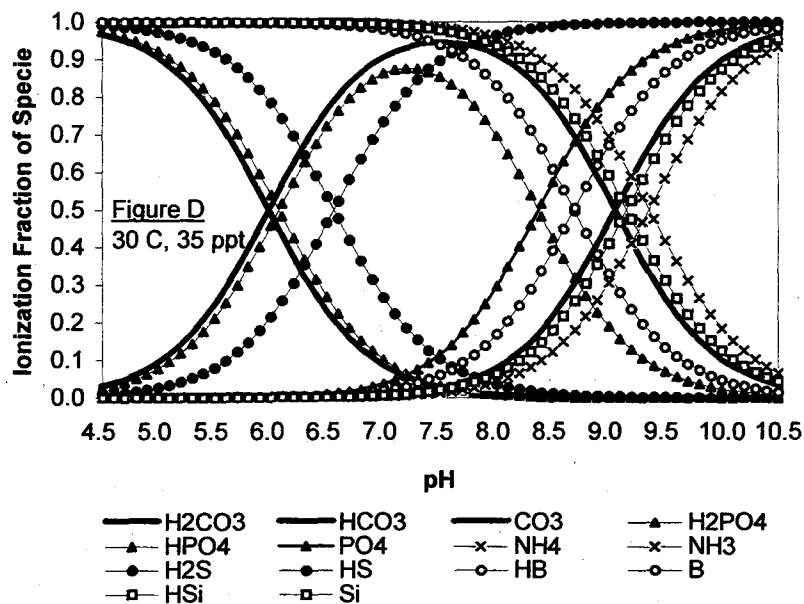


Figure 4.8D. Ionization fractions of compounds for which significant ionization exists over the pH range 5-10: D (30 °C, 35 ppt)

where $ALK_w = [OH^-] - \{H^+\}$

$$ALK_c = [HCO_3^-] + 2[CO_3^{2-}]$$

$$ALK_{ncw} = [HS^-] + [HPO_4^{2-}] + [B(OH)_4^-] + [NH_3] + [SiO(OH)_3^-] + 2[PO_4^{3-}]$$

$$ALK_{nc} = [OH^-] - \{H^+\} + [HS^-] + [HPO_4^{2-}] + [B(OH)_4^-] + [NH_3] + [SiO(OH)_3^-] + 2[PO_4^{3-}]$$

$$\text{and } ACD_t = \{H^+\} - [OH^-] + 2[H_2CO_3] + [HCO_3^-] + 2[H_2PO_4^{1-}] + [HPO_4^{2-}] + [H_2S] \\ + [H_3BO_3] + [NH_4^+] + [Si(OH)_4]$$

$$\text{substitute } = \{H^+\} - K'_w/\{H^+\} + {}^{mol}CO (2 \alpha_{CO} + \alpha_{ICO}) + {}^{mol}PO (2 \alpha_{1PO} + \alpha_{2PO}) \\ + {}^{mol}HS \alpha_{0HS} + {}^{mol}BO \alpha_{0BO} + {}^{mol}NH \alpha_{0NH} + {}^{mol}SI \alpha_{0SI}$$

$$\text{where } ACD_c = 2[H_2CO_3] + [HCO_3^-]$$

$$\text{and } ACD_{nc} = \{H^+\} - [OH^-] + 2[H_2PO_4^{1-}] + [HPO_4^{2-}] + [H_2S] + [H_3BO_3] + [NH_4^+] + [Si(OH)_4]$$

ALK_t , ALK_{nc} , ${}^{mol}CCO$, and pH are interrelated. An existing total carbonate concentration (${}^{mol}CO$) is defined by given values for pH and total concentrations of additional compounds, using the total alkalinity equation: ${}^{mol}CCO = (ALK_t - ALK_{nc}) / (\alpha_{1CO} + 2 \alpha_{2CO})$

4.4.6.3 Alkalinity Model 2

Alkalinity Model 1 may be simplified to include only carbonate and water species (ALK_c and ALK_w), depending on the alkalinity contributions of additional acid-base species (ALK_{ncw}) relative to $ALK_c + ALK_w$ over the 5 – 10 pH range. For natural waters, the literature indicates that alkalinity contributions from phosphates (PO), ammonia (NH), silicates (SI), and borates (BO) are often considered negligible and ignored (Snoeyink and Jenkins, 1980; Stumm and Morgan, 1981). For aquaculture waters, this simplification depends on water quality conditions, as demonstrated in Figures 4.9 and 4.10. In these figures, alkalinity contributions (relative to total alkalinity) including carbonates (ALK_c), non-carbonates and water (ALK_{ncw}), and water (ALK_w) are shown as a function of pH and as a function of carbon dioxide saturation, for various water quality conditions. Implications of these results regarding the appropriate use of Alkalinity Model 2 for aquaculture systems are discussed in Chapter 8.

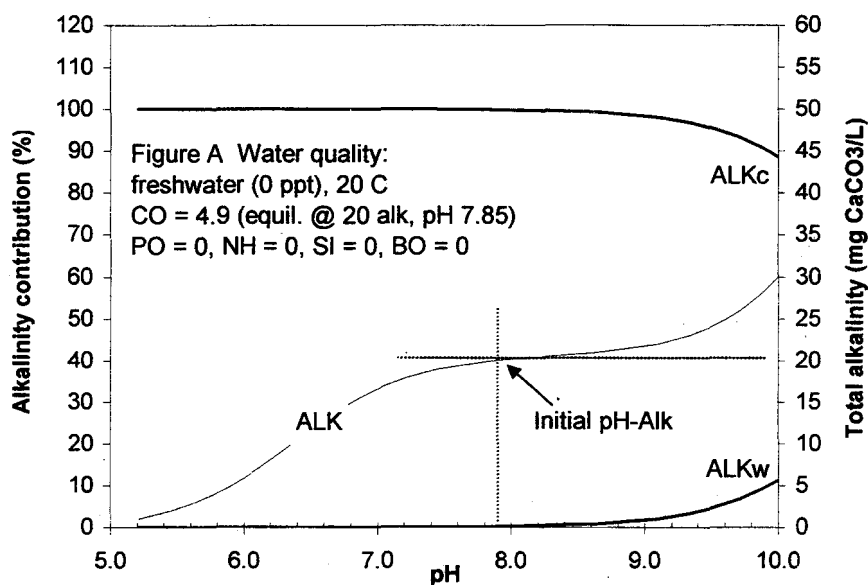


Figure 4.9A. Alkalinity contributions relative to total alkalinity as a function of pH for conditions: pure water, low alkalinity

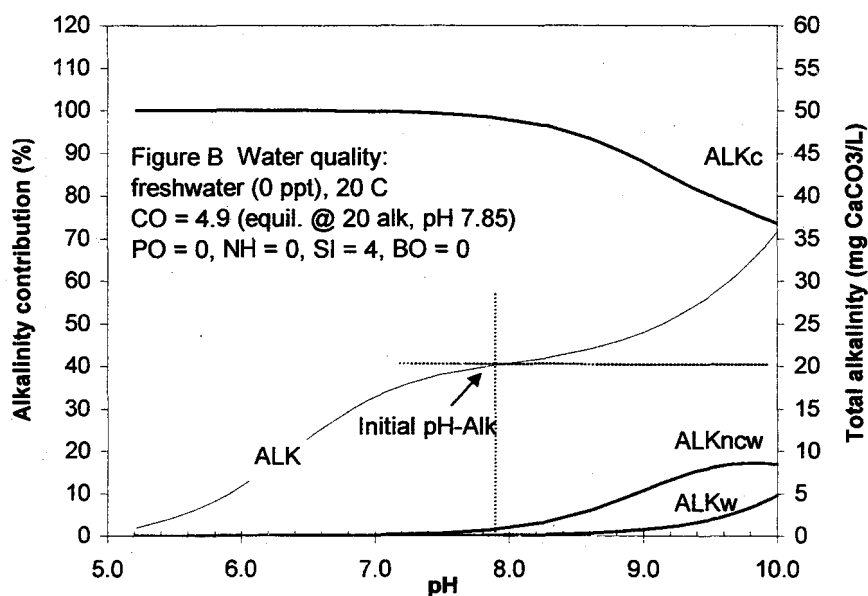


Figure 4.9B. Alkalinity contributions relative to total alkalinity as a function of pH for conditions: pure water except silicates present, low alkalinity

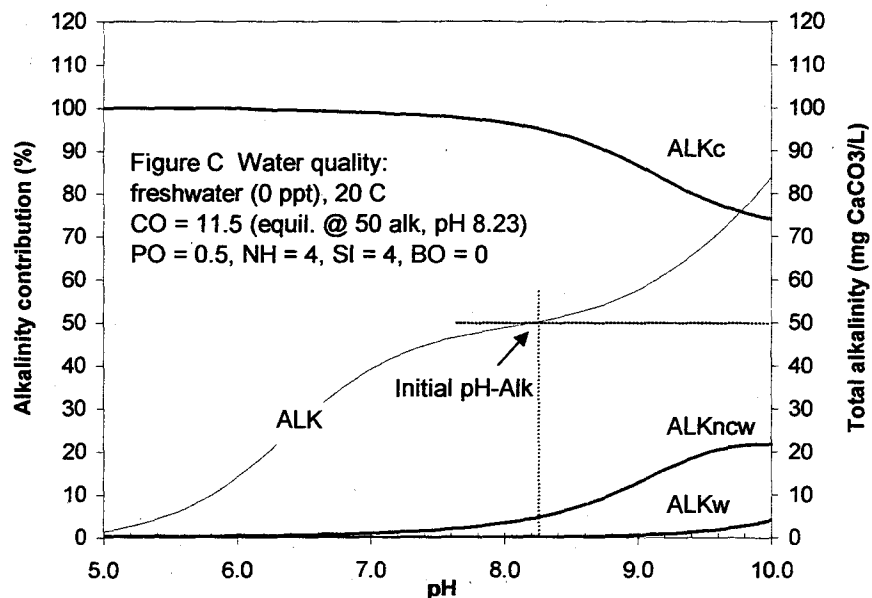


Figure 4.9C. Alkalinity contributions relative to total alkalinity as a function of pH for conditions: freshwater, high nutrient levels, moderate alkalinity

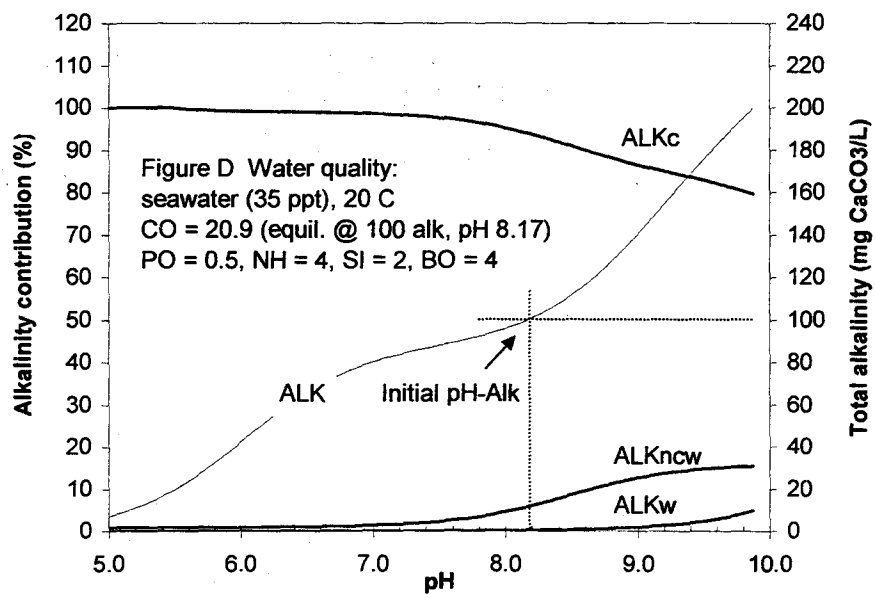


Figure 4.9D. Alkalinity contributions relative to total alkalinity as a function of pH for conditions: seawater, high nutrient levels, moderate alkalinity

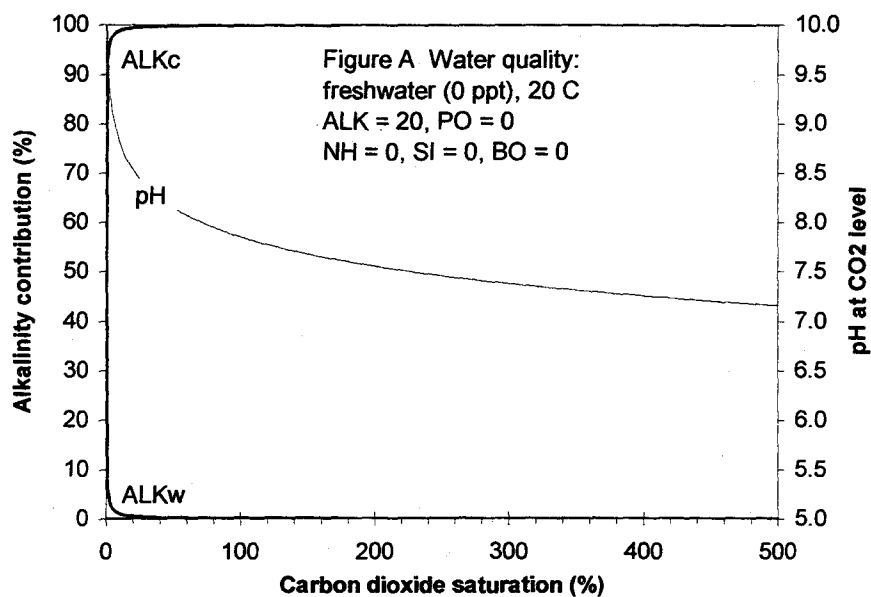


Figure 4.10A. Alkalinity contributions relative to total alkalinity as a function of carbon dioxide saturation for conditions: pure water, low alkalinity

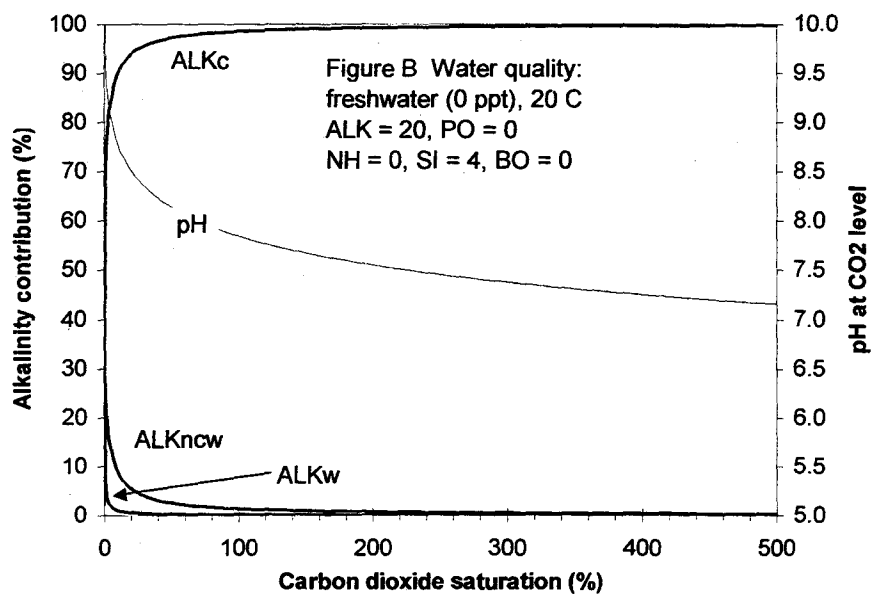


Figure 4.10B. Alkalinity contributions relative to total alkalinity as a function of carbon dioxide saturation for conditions: pure water except silicates present, low alkalinity

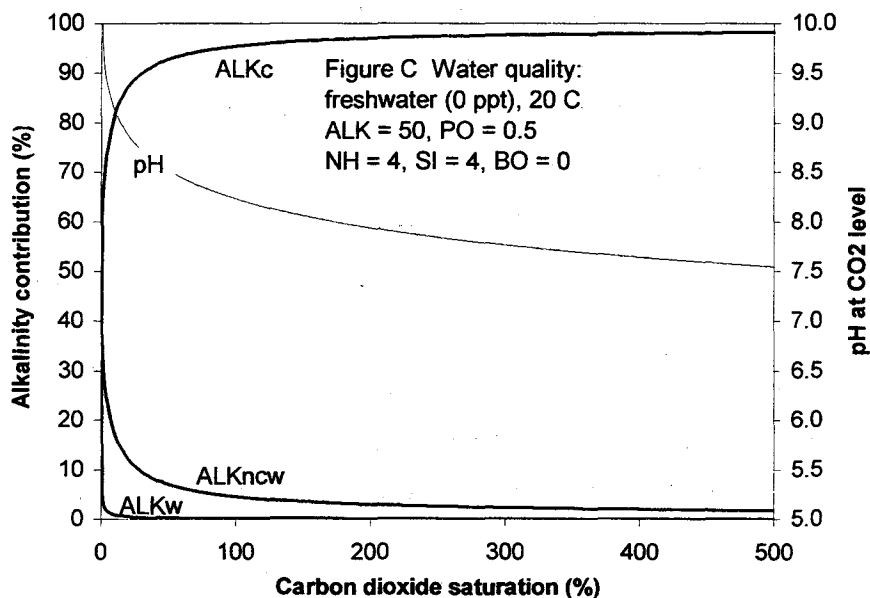


Figure 4.10C. Alkalinity contributions relative to total alkalinity as a function of carbon dioxide saturation for conditions: freshwater, high nutrient levels, moderate alkalinity

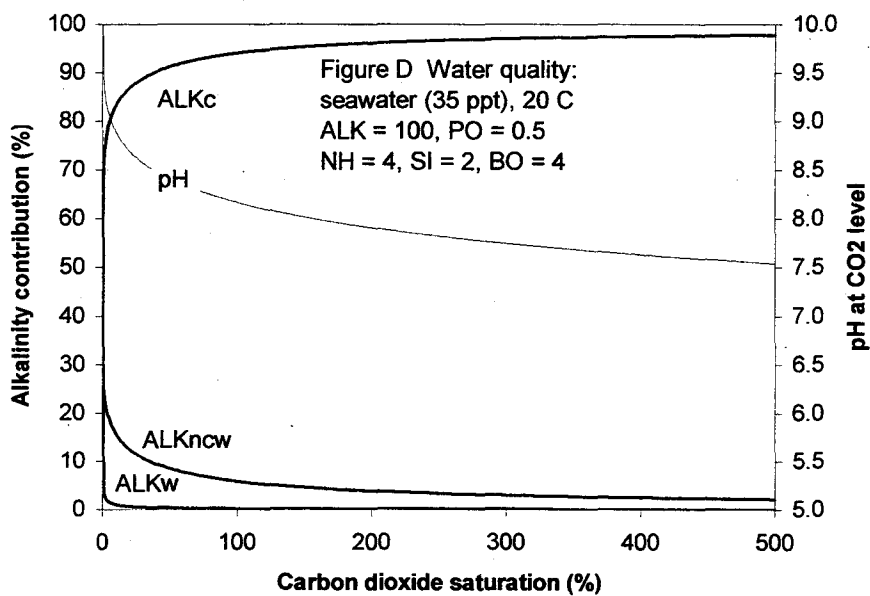


Figure 4.10D. Alkalinity contributions relative to total alkalinity as a function of carbon dioxide saturation for conditions: seawater, high nutrient levels, moderate alkalinity

In Figure 4.9, carbonates are held constant and pH and alkalinity are adjusted by a strong acid or base from initial levels, where at initial levels the given acid-base system is at equilibrium with atmospheric carbon dioxide. When pH levels are increased above initial levels, carbonates become under saturated and ALK_{ncw} increases in both absolute terms and relative to ALK_c . These results show that if an appreciable total concentration of PO, NH, SI, and BO exists, represented as ALK_{ncw} , then simplification of Alkalinity Model 1 is not appropriate at higher pH levels with carbonates held constant. Regarding the conditions used to generate Figure 4.9, addition of strong acids and bases to aquaculture waters may result from nitrification and denitrification, pH and alkalinity adjustment, and/or source water conditions. However, appreciable increases in pH without increases in carbonates are likely to occur only in solar algae ponds.

In Figure 4.10, total alkalinity levels and ALK_{ncw} compounds are held constant at given levels and total carbonates are a function carbon dioxide saturation. These analyses show that ALK_{ncw} becomes increasingly significant as carbon dioxide saturation is decreased. The range of carbon dioxide saturation levels used in Figure 4.10 can occur in aquaculture systems, due to the relatively high rates of carbon dioxide transfer by photosynthesis and respiration in conjunction with typically slow rates of carbon dioxide equilibration with the atmosphere. For example, intensive recirculation systems may show highly supersaturated carbon dioxide, and solar algae ponds in mid-afternoon may show highly under saturated carbon dioxide.

If total alkalinity can be assumed to consist of carbonates and water only, then the resulting acid-base system model is:

$$ACD_c = 2[H_2CO_3] + [HCO_3^-]$$

$$ACD_{nc} = \{H^+\} - [OH^-]$$

$$ALK_c = [HCO_3^-] + 2[CO_3^{2-}]$$

$$ALK_{nc} = [OH^-] - \{H^+\}$$

$$ALK_t = [OH^-] - \{H^+\} + [HCO_3^-] + 2[CO_3^{2-}]$$

$$= K'_w / \{H^+\} - \{H^+\} + {}^{mol}CO (\alpha_{1CO} + 2 \alpha_{2CO})$$

$$= K'_w / \{H^+\} - \{H^+\}$$

$$+ {}^{mol}CO (\{H^+\} K'_{1CO} + 2 K'_{1CO} K'_{2CO}) / (\{H^+\}^2 + \{H^+\} K'_{1CO} + K'_{1CO} K'_{2CO})$$

Alkalinity Model 2 consists of five unknowns, including $\{H^+\}$, $[OH^-]$, $[H_2CO_3^*]$, $[HCO_3^-]$, and $[CO_3^{2-}]$, and five equations: equilibria equations for K'_w , K'_{1CO} , and K'_{2CO} , and concentration conditions for ^{mol}CO and ALK_t . If DC diffusion is considered, then the equation $[H_2CO_3^*] = K_h P_{CO_2}$ is added, where P_{CO_2} is known. Numerical procedures are used to solve for $\{H^+\}$ and $^{mol}CO_{eq}$.

4.4.6.4 Alkalinity Model 3

Further simplification of Alkalinity Model 2 is possible when $[OH^-]$ and $\{H^+\}$ are approximated as zero, regarding their impact on total alkalinity, and the only significant components of alkalinity are carbonates. Analyses used to test this simplification are similar to those used for Alkalinity Model 2 and implications of this simplification are discussed in Chapter 8. In Figures 4.9 and 4.10, ALK_w is seen to be negligible except under extreme conditions. If this simplification is used, then the resulting alkalinity equation is sufficiently simple to be solved by the quadratic formula:

$$\begin{aligned} ^{mol}CO &= [H_2CO_3^*] + [HCO_3^-] + [CO_3^{2-}] \\ ALK_t &= [HCO_3^-] + 2[CO_3^{2-}] \\ &= ^{mol}CO (\alpha_{1CO} + 2 \alpha_{2CO}) \\ &= ^{mol}CO (\{H^+\} K'_{1CO} + 2 K'_{1CO} K'_{2CO}) / (\{H^+\}^2 + \{H^+\} K'_{1CO} + K'_{1CO} K'_{2CO}) \end{aligned}$$

giving $\{H^+\} = (a + b^{1/2}) / (2 ALK_t)$

where $a = ^{mol}CO K'_{1CO} - ALK_t K'_{1CO}$

$$b = a^2 - [4 ALK_t (ALK_t K'_{1CO} K'_{2CO} - 2 ^{mol}CO K'_{1CO} K'_{2CO})]$$

and $\{H^+\}_{eq} = (a + b^{1/2}) / (2 ALK_t)$

where $a = [H_2CO_3^*_{eq}] K'_{1CO}$

$$b = a^2 + (4 ALK_t [H_2CO_3^*_{eq}] K'_{1CO} K'_{2CO})$$

and $^{mol}CO_{eq} = [H_2CO_3^*_{eq}] / [\{H^+\}^2 / (\{H^+\}^2 + \{H^+\} K'_{1CO} + K'_{1CO} K'_{2CO})]$

4.4.7 Solution procedures for acid-base systems

In the use of Alkalinity Models 1 – 3, equilibrium constants are calculated at the existing temperature and salinity, total compound concentrations are substituted into equations, and system equations are solved for $\{H^+\}_{eq}$, $^{mol}CO_{eq}$, and other variables. Direct solutions are attainable for Alkalinity Model 3. For Alkalinity Models 1 and 2, solutions for $\{H^+\}_{eq}$ and $^{mol}CO_{eq}$ are lengthy, multiple-root functions, and the Newton-Raphson (NR) numerical method is used to solve system equations. Geometrically, the NR method consists of extending the tangent at point x_i to where it crosses zero and setting the next guess, x_{i+1} , to the abscissa at the zero crossing (Figure 4.11). Solutions (convergence) are not achieved when unrealistic water quality conditions exist, which is handled in the computer programming of this method by a maximum allowed number of iteration cycles (e.g. 30) and error messages. For realistic water quality conditions, solutions are normally attained in ≤ 5 iterations when the initial pH used in the NR procedure is within a few units of the equilibrium pH. A template of the NR procedure is given below, where a solution for $\{H^+\}$ is achieved when $f(\{H^+\}) \approx 0$, or $|pH_i - pH_{i+1}| \leq \text{error tolerance (e.g. 0.0001)}$:

$$H_{i+1} = H_i - f(H_i) / [df(H_i) / d(H_i)]$$

or
$$H_{i+1} = H_i - f(H_i) / f'(H_i)$$

where H_{i+1} = newly calculated H ($\{H^+\}$ is represented simply as H)

H_i = current H, where first iteration uses original H and succeeding iterations use previously calculated value

$f(H_i) = 0$, where all terms of master equation are grouped on one side of equation

$df(H_i) / d(H_i)$ = derivative of function with respect to H_i

To implement NR solution procedures for H and $^{mol}CO_{eq}$, $f(H_i)$ and $f'(H_i)$ functions are derived below, including optional carbon dioxide and calcium carbonate equilibria. The number of terms in the ALK_{nc} and ACD_{nc} functions and function derivatives depends on the compounds present. Functions used include total compound concentrations, total alkalinity, total acidity, compound speciation, acid-base equilibria, and carbon dioxide and calcium carbonate solubility. In processing NR iterations, K' values are calculated once prior to the first iteration and ionization fractions (α_i) are calculated at the new H_i for each iteration.

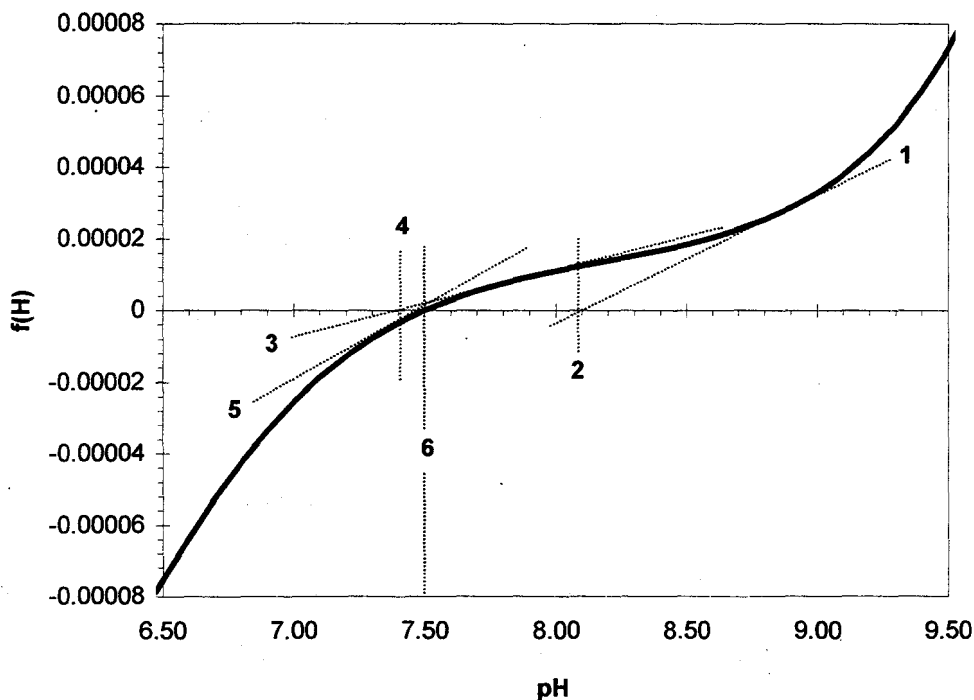


Figure 4.11. Geometric illustration of the Newton-Raphson (NR) numerical method, applied to Alkalinity Models 1 and 2, showing $f(H^+)$ vs. $\{H^+\}$ for 25 °C temperature, 0 ppt salinity, 10 mg CaCO_3/L alkalinity, and 7.5 equilibrium pH

For all models, total compound concentrations other than carbonates are constant and ALK_{nc} is calculated depending on the compounds present:

$$\begin{aligned}
 \text{ALK}_{\text{nc}} &= K'_{\text{W}/\text{H}} - \text{H} + {}^{\text{mol}}\text{PO} (\alpha_{2\text{PO}} + 2 \alpha_{3\text{PO}}) + {}^{\text{mol}}\text{HS} \alpha_{1\text{HS}} + {}^{\text{mol}}\text{BO} \alpha_{1\text{BO}} \\
 &\quad + {}^{\text{mol}}\text{NH} \alpha_{1\text{NH}} + {}^{\text{mol}}\text{SI} \alpha_{1\text{SI}} \\
 &= K'_{\text{W}/\text{H}} - \text{H} \\
 &\quad + {}^{\text{mol}}\text{PO} (\text{H} K'_{2\text{PO}} + K'_{2\text{PO}} K'_{3\text{PO}}) / (\text{H}^2 + \text{H} K'_{2\text{PO}} + K'_{2\text{PO}} K'_{3\text{PO}}) \\
 &\quad + {}^{\text{mol}}\text{HS} K'_{1\text{HS}} / (\text{H} + K'_{1\text{HS}}) + {}^{\text{mol}}\text{BO} K'_{1\text{BO}} / (\text{H} + K'_{1\text{BO}}) \\
 &\quad + {}^{\text{mol}}\text{NH} K'_{1\text{NH}} / (\text{H} + K'_{1\text{NH}}) + {}^{\text{mol}}\text{SI} K'_{1\text{SI}} / (\text{H} + K'_{1\text{SI}})
 \end{aligned}$$

4.4.7.1 Closed system

For closed systems, carbon dioxide and calcium carbonate equilibria are not considered and $^{\text{mol}}\text{CO}$ is constant:

$$f(H) = \text{ALK}_c + \text{ALK}_{nc} - \text{ALK}_t$$

$$\begin{aligned} \text{where } \text{ALK}_c &= ^{\text{mol}}\text{CO} (\alpha_{1\text{CO}} + 2 \alpha_{2\text{CO}}) \\ &= ^{\text{mol}}\text{CO} (H K'_{1\text{CO}} + K'_{1\text{CO}} K'_{2\text{CO}}) / (H^2 + H K'_{1\text{CO}} + K'_{1\text{CO}} K'_{2\text{CO}}) \end{aligned}$$

4.4.7.2 Carbon dioxide equilibrium

Direct solutions for equilibrium carbonate concentrations ($^{\text{mol}}\text{CO}_{\text{eq}}$) due to carbon dioxide diffusion are attainable for Alkalinity Model 3. For Alkalinity Models 1 and 2, $^{\text{mol}}\text{CO}_{\text{eq}}$ and the corresponding $\{H^+\}_{\text{eq}}$ are determined by using a calculated equilibrium H_2CO_3^* value (independent of pH), where $^{\text{mol}}\text{CO}$ is controlled by carbon dioxide diffusion (i.e. H_2CO_3^*) and both pH and $^{\text{mol}}\text{CO}$ are subject to change. The total quantity of carbon dioxide diffusing to equilibrium is equal to the new total carbonate ($^{\text{mol}}\text{CO}_{\text{eq}}$) minus the original total carbonate ($^{\text{mol}}\text{CO}$).

$$\begin{aligned} f(H) &= ^{\text{mol}}\text{CO}_{\text{eq}} (\alpha_{1\text{CO}} + 2 \alpha_{2\text{CO}}) + \text{ALK}_{nc} - \text{ALK}_t \\ &= (^{\text{mol}}\text{DC}_{\text{eq}} / \alpha_{0\text{CO}}) (\alpha_{1\text{CO}} + 2 \alpha_{2\text{CO}}) + \text{ALK}_{nc} - \text{ALK}_t \\ &= ^{\text{mol}}\text{DC}_{\text{eq}} (\alpha_{1\text{CO}} / \alpha_{0\text{CO}} + 2 \alpha_{2\text{CO}} / \alpha_{0\text{CO}}) + \text{ALK}_{nc} - \text{ALK}_t \\ &= ^{\text{mol}}\text{DC}_{\text{eq}} (K'_{1\text{CO}} / H + 2 K'_{1\text{CO}} K'_{2\text{CO}} / H^2) + \text{ALK}_{nc} - \text{ALK}_t \end{aligned}$$

$$\text{where } ^{\text{mol}}\text{DC}_{\text{eq}} = \text{DC}_{\text{eq}} / (\text{mw CO}_2)$$

$$^{\text{mol}}\text{CO}_{\text{eq}} = ^{\text{mol}}\text{DC}_{\text{eq}} / \alpha_{0\text{CO}}$$

4.4.7.3 Calcium carbonate equilibrium

If calcium carbonate equilibrium exists, $^{\text{mol}}\text{CO}$ is controlled by calcium carbonate precipitation and dissolution. ALK_t , ALK_{nc} , ACD_{nc} , pH, and $^{\text{mol}}\text{CO}$ are all subject to change. ACD_t and

$(\text{ALK}_t - 2[\text{Ca}^{2+}])$ are constant, conservative properties (Snoeyink and Jenkins, 1980) and are used in solution procedures.

$$\begin{aligned}
 \text{ALK}_t - 2[\text{Ca}^{2+}] &= (\text{ALK}_t - \text{eqvCa}^{2+}) = \text{ALK}_t - 2 K_{\text{CaCO}_3} / (^{\text{mol}}\text{CO}_{\text{eq}} \alpha_{2\text{CO}}) \\
 \text{ACD}_t &= \text{ACD}_{\text{nc}} + \text{ACD}_c \\
 ^{\text{mol}}\text{CO}_{\text{eq}} &= (\text{ACD}_t - \text{ACD}_{\text{nc}}) / (\alpha_{1\text{CO}} + 2 \alpha_{0\text{CO}}) \\
 f(\text{H}) &= [^{\text{mol}}\text{CO}_{\text{eq}} (\alpha_{1\text{CO}} + 2 \alpha_{2\text{CO}})] + \text{ALK}_{\text{nc}} - (2 K_{\text{CaCO}_3} / (^{\text{mol}}\text{CO}_{\text{eq}} \alpha_{2\text{CO}})) \\
 &\quad - (\text{ALK}_t - 2 \text{Ca}^{2+}) \\
 &= [(\text{ACD}_t - \text{ACD}_{\text{nc}}) (\alpha_{1\text{CO}} + 2 \alpha_{2\text{CO}}) / (\alpha_{1\text{CO}} + 2 \alpha_{0\text{CO}})] + \text{ALK}_{\text{nc}} \\
 &\quad - (2 K_{\text{CaCO}_3} / \alpha_{2\text{CO}}) [(\alpha_{1\text{CO}} + 2 \alpha_{2\text{CO}}) / (\text{ACD}_t - \text{ACD}_{\text{nc}})] \\
 &\quad - (\text{ALK}_t - 2 \text{Ca}^{2+}) \\
 &= [(\text{ACD}_t - \text{ACD}_{\text{nc}}) (\text{H} K'_{1\text{CO}} + 2 K'_{1\text{CO}} K'_{2\text{CO}}) / (\text{H} K'_{1\text{CO}} + 2 \text{H}^2)] \\
 &\quad + \text{ALK}_{\text{nc}} - (2 K_{\text{CaCO}_3} / (\text{ACD}_t - \text{ACD}_{\text{nc}})) (\text{H} K'_{1\text{CO}} + 2 \text{H}^2) / (K'_{1\text{CO}} K'_{2\text{CO}}) \\
 &\quad - (\text{ALK}_t - 2 \text{Ca}^{2+})
 \end{aligned}$$

The quantity of calcium carbonate precipitating or dissolving ($[\text{Ca}^{2+}]_{\text{pd}}$) is proportional to the new total carbonate ($^{\text{mol}}\text{CO}_{\text{eq}}$) minus the original total carbonate ($^{\text{mol}}\text{CO}$) and equal to the new total calcium ($[\text{Ca}^{2+}]_{\text{eq}}$) minus the original total calcium ($[\text{Ca}^{2+}]$).

$$\begin{aligned}
 [\text{Ca}^{2+}]_{\text{eq}} &= K_{\text{CaCO}_3} / (^{\text{mol}}\text{CO}_{\text{eq}} \alpha_{2\text{CO}}) \\
 [\text{Ca}^{2+}]_{\text{pd}} &= [\text{Ca}^{2+}]_{\text{eq}} - [\text{Ca}^{2+}] \\
 \text{eqvCa}^{2+}_{\text{pd}} &= [\text{Ca}^{2+}]_{\text{pd}} (2 \text{ meq/mmol}) \\
 \text{Ca}^{2+}_{\text{pd}} &= [\text{Ca}^{2+}]_{\text{pd}} (100 \text{ mg CaCO}_3 / \text{mmol})
 \end{aligned}$$

4.4.7.4 Carbon dioxide and calcium carbonate equilibria

For carbon dioxide and calcium carbonate equilibria, $^{\text{mol}}\text{CO}$ is controlled by carbon dioxide diffusion, not by calcium carbonate precipitation/dissolution, where the term $(\text{ALK}_t - 2[\text{Ca}^{2+}])$ is again constant.

$$f(\text{H}) = ^{\text{mol}}\text{CO}_{\text{eq}} (\alpha_{1\text{CO}} + 2 \alpha_{2\text{CO}}) + \text{ALK}_{\text{nc}} - 2 K_{\text{CaCO}_3} / (^{\text{mol}}\text{CO} \alpha_{2\text{CO}}) - (\text{ALK}_t - 2 \text{Ca}^{2+})$$

$$\begin{aligned}
&= \text{newALK}_c + \text{ALK}_{nc} - 2 K_{\text{CaCO}_3} / (\text{molCO} \alpha_{2\text{CO}}) - (\text{ALK}_t - 2 \text{Ca}^{2+}) \\
&= (\text{molDC}_{\text{eq}} / \alpha_{0\text{CO}}) (\alpha_{1\text{CO}} + 2 \alpha_{2\text{CO}}) + \text{ALK}_{nc} - 2 K_{\text{CaCO}_3} / (\text{molCO} \alpha_{2\text{CO}}) \\
&\quad - (\text{ALK}_t - 2 \text{Ca}^{2+}) \\
&= \text{molDC}_{\text{eq}} (\alpha_{1\text{CO}} / \alpha_{0\text{CO}} + 2 \alpha_{2\text{CO}} / \alpha_{0\text{CO}}) + \text{ALK}_{nc} \\
&\quad - (2 K_{\text{CaCO}_3} / \text{molDC}_{\text{eq}}) (\alpha_{0\text{CO}} / \alpha_{2\text{CO}}) - (\text{ALK}_t - 2 \text{Ca}^{2+}) \\
&= \text{molDC}_{\text{eq}} (K'_{1\text{CO}} / H + 2 K'_{1\text{CO}} K'_{2\text{CO}} / H^2) + \text{ALK}_{nc} \\
&\quad - (2 K_{\text{CaCO}_3} / \text{molDC}_{\text{eq}}) (H^2 / (K'_{1\text{CO}} K'_{2\text{CO}})) - (\text{ALK}_t - 2 \text{Ca}^{2+})
\end{aligned}$$

The quantity of carbon dioxide diffusing and the quantity of calcium carbonate precipitating or dissolving are given below, where changes in ACD_t are due to carbon dioxide diffusion and changes in $[\text{Ca}^{2+}]$ are due to calcium carbonate precipitation/dissolution.

$$\begin{aligned}
\text{delta molDC} &= (\text{ACD}_{t\text{-eq}} - \text{ACD}_{t\text{-init}}) / 2 \\
\text{delta molCO} &= \text{molCO}_{\text{eq}} - \text{molCO}_{\text{init}} \\
\text{delta molCO}_{\text{pd}} &= \text{delta molCO} - \text{delta molDC} \\
\text{delta } [\text{Ca}^{2+}]_{\text{pd}} &= [\text{Ca}^{2+}]_{\text{eq}} - [\text{Ca}^{2+}] \\
\text{delta } \text{Ca}^{2+}_{\text{pd}} &= [\text{Ca}^{2+}]_{\text{pd}} (100 \text{ mg CaCO}_3 / \text{mmol})
\end{aligned}$$

4.4.7.5 Derivation of first derivative terms

The NR methods requires derivatives, $f'(H_i)$, of the functions described above. The following derivative terms (DT) are based on the rules of differential calculus, where these terms are additive to achieve the full derivative of the master equation.

Water:

$$\begin{aligned}
\text{DT} &= d(K'_w / H - H) / dH \\
&= -k_w / H^2 - 1.0
\end{aligned}$$

Monoprotic acids:

$$\text{DT} = d(\text{molC } K'_{1\text{C}} / (H + K'_{1\text{C}})) / dH$$

$$= -^{\text{mol}}\text{C} (K'_{1\text{C}} / (H + K'_{1\text{C}})^2)$$

Diprotic acids (including carbonate when carbon dioxide and calcium carbonate equilibria are not considered):

$$\begin{aligned} \text{DT} &= d(^{\text{mol}}\text{C} (H K'_{1\text{C}} + K'_{1\text{C}} K'_{2\text{C}}) / (H^2 + H K'_{1\text{C}} + K'_{1\text{C}} K'_{2\text{C}})) / dH \\ &= ^{\text{mol}}\text{C} ((K'_{1\text{C}}/a^2) (K'_{1\text{C}} K'_{2\text{C}} - H^2) - (2 K'_{1\text{C}} K'_{2\text{C}}/a^2) (K'_{1\text{C}} + 2 H)) \end{aligned}$$

where $a = H^2 + H K'_{1\text{C}} + K'_{1\text{C}} K'_{2\text{C}}$

Carbon dioxide equilibrium:

$$\begin{aligned} \text{DT} &= d(^{\text{mol}}\text{DC}_{\text{eq1}} (K'_{1\text{CO}}/H + 2 K'_{1\text{CO}} K'_{2\text{CO}}/H^2) + \text{ALK}_{\text{nc}} - \text{ALK}_{\text{t}}) / dH \\ &= ^{\text{mol}}\text{DC}_{\text{eq1}} (-K'_{1\text{CO}}/H^2 - 4 K'_{1\text{CO}} K'_{2\text{CO}}/H^3) \end{aligned}$$

Calcium carbonate equilibrium:

$$\begin{aligned} \text{DT} &= d(((\text{ACD}_{\text{t}} - \text{ACD}_{\text{nc}}) (H K'_{1\text{CO}} + 2 K'_{1\text{CO}} K'_{2\text{CO}}) / (H K'_{1\text{CO}} + 2 H^2)) \\ &\quad + \text{ALK}_{\text{nc}} - (2 K_{\text{CaCO}_3} / (\text{ACD}_{\text{t}} - \text{ACD}_{\text{nc}})) (H K'_{1\text{CO}} + 2 H^2) / (K'_{1\text{CO}} K'_{2\text{CO}}) \\ &\quad - (\text{ALK}_{\text{t}} - 2 \text{Ca}^{2+})) / dH \\ &= (-1 - k_{\text{w}}/H^2) t_3/t_2 + K'_{1\text{CO}} t_1/t_2 - (K'_{1\text{CO}} + 4 H) t_3 t_1 / (t_2 t_2) \\ &\quad + 2 K_{\text{CaCO}_3} (-1 - k_{\text{w}}/H^2) t_2 / (K'_{1\text{CO}} K'_{2\text{CO}} t_1 t_1) \\ &\quad - 2 K_{\text{CaCO}_3} (4 H + K'_{1\text{CO}}) / (K'_{1\text{CO}} K'_{2\text{CO}} t_1) \end{aligned}$$

where $t_1 = |\text{ACD}_{\text{t}} - (H - k_{\text{w}}/H)|$

$$t_2 = H K'_{1\text{CO}} + 2 H^2$$

$$t_3 = H K'_{1\text{CO}} + 2 K'_{1\text{CO}} K'_{2\text{CO}}$$

Carbon dioxide and calcium carbonate equilibria:

$$\begin{aligned} \text{DT} &= d(^{\text{mol}}\text{DC}_{\text{eq1}} (K'_{1\text{CO}}/H + 2 K'_{1\text{CO}} K'_{2\text{CO}}/H^2) + \text{ALK}_{\text{nc}} \\ &\quad - (2 K_{\text{CaCO}_3} / ^{\text{mol}}\text{DC}_{\text{eq1}}) (H^2 / (K'_{1\text{CO}} K'_{2\text{CO}})) - (\text{ALK}_{\text{t}} - 2 \text{Ca}^{2+})) / dH \\ &= ^{\text{mol}}\text{DC}_{\text{eq1}} (-K'_{1\text{CO}}/H^2 - 4 K'_{1\text{CO}} K'_{2\text{CO}}/H^3) \\ &\quad + (-4 H K_{\text{CaCO}_3}) / (^{\text{mol}}\text{DC}_{\text{eq1}} K'_{1\text{CO}} K'_{2\text{CO}}) \end{aligned}$$

4.4.8 pH and Alkalinity Adjustment

Adjustment of pH and alkalinity is used in all types of aquaculture systems. Typical objectives are (1) to maintain minimum pH and alkalinity levels, e.g., to neutralize the acidification impacts of nitrification and pond soils, (2) to minimize the downward pH impact of carbon dioxide addition, or (3) to provide minimum alkalinity levels for solar algae ponds for pH buffering and maintenance of DIC for primary productivity. High pH levels may also be problem, with respect to fish water quality criteria, either directly or due to the high associated proportion of TAN as unionized ammonia. Occurrence of high, afternoon pH levels in solar algae ponds due to low carbon dioxide levels is rarely controlled directly, but highly alkaline source waters used for intensive systems may be conditioned with acids and some aquarium fish species require low pH levels. The methods described below are used to perform pH and alkalinity adjustments, by calculating the required quantity of a selected compound (Table 4.7) based on initial conditions and the desired pH or alkalinity level. Related process application and control methods for static and flowing waters are discussed in Chapter 3 (Process management).

Alkalinity adjustments can be calculated directly from ALKinit, ALKnew, and CMPalk. Alkalinity adjustments are similar to the addition of any type of compound to achieve a desired set point. In contrast, pH adjustments require various manipulations of the master alkalinity equation. For the pH adjustment methods described below, the following terms are used:

Xinit = initial level of variable X (mg X/L: alkalinity and hardness as mg CaCO₃/L)

Xadj = adjusted level variable X (units as above)

CMPalk = alkalinity content of compound (g CaCO₃ /g compound)

CMPhrd = hardness content of compound (g CaCO₃ /g compound)

CMPco = carbonate content of compound (g CO₃-C /g compound)

CMPpo = phosphate content of compound (g PO₄-P /g compound)

CMPadd = required amount of compound added (mg compound/L)

Table 4.7. pH and alkalinity adjustment compounds

Adjustment	Compound
Decrease pH	Carbon dioxide (CO ₂ , gas)
Decrease pH	Nitric acid (HNO ₃ , liquid)
Decrease pH	Hydrochloric acid (HCl, liquid)
Decrease pH	Sulfuric acid (H ₂ SO ₄ , liquid)
Decrease pH	Phosphoric acid (H ₃ PO ₄ , liquid)
Increase pH or alkalinity	Sodium hydroxide (NaOH, liquid)
Increase pH or alkalinity	Sodium bicarbonate (NaHCO ₃ , solid)
Increase pH or alkalinity	Sodium carbonate (Na ₂ CO ₃ , solid)
Increase pH or alkalinity	Agricultural limestone (CaCO ₃ , solid)
Increase pH or alkalinity	Hydrated lime (Ca(OH) ₂ , solid)
Increase pH or alkalinity	Burnt lime (CaO, solid)

4.4.8.1 Strong acids and bases

Strong acid and base compounds include nitric, hydrochloric, and sulfuric acids for decreasing pH and sodium hydroxide, hydrated lime, and burnt lime for increasing pH. Addition of these compounds is equivalent to the addition of H⁺ or OH⁻, which results in changes to total alkalinity, where the conjugate bases and acids of these compounds are not considered. Procedure:

- 1) Calculate total alkalinity at the adjusted pH (ALK_{adj}) using current levels for all compounds
- 2) $CMP_{add} = (ALK_{adj} - ALK_{init}) / CMP_{alk}$
- 3) $HRD_{adj} \text{ (mg CaCO}_3\text{/L)} = HRD_{init} + (CMP_{add} * CMP_{hrd})$

4.4.8.2 Carbon dioxide

Addition of carbon dioxide to decrease pH results in changes to CO but ALK remains constant. Procedure:

- 1) Calculate ALK_{nc} at the adjusted pH
- 2) Calculate the proportion of ALK_c at the adjusted pH (factor f)
- 3) $CO_{adj} \text{ (mg C/L)} = (12.011 \text{ mg/mmol}) (ALK_{init} - ALK_{nc}) / [f (50.043 \text{ mg/meq})]$
- 4) $CMP_{add} \text{ (mg/L)} = (CO_{adj} - CO_{init}) / CMP_{co}$

4.4.8.3 Phosphoric acid

Addition of phosphoric acid to decrease pH results in changes to PO but ALK remains constant. Procedure:

- 1) Calculate alkalinity at the adjusted pH with no PO present (ALK_{np})
- 2) Calculated the proportion of alkalinity due PO at the adjusted pH (factor f)
- 3) $PO_{adj} \text{ (mg P/L)} = (30.974 \text{ mg/mmol}) (ALK_{init} - ALK_{np}) / [f (50.043 \text{ mg/meq})]$
- 4) $CMP_{add} \text{ (mg/L)} = (PO_{adj} - PO_{init}) / CMP_{po}$

4.4.8.4 Sodium bicarbonate

Addition of sodium bicarbonate results in changes to ALK and CO. Sodium bicarbonate can decrease or increase pH to a limiting level defined by the mean of pK'_{1C} and pK'_{2C} (pH_{limit} , e.g. 8.3) but is normally used to increase pH. As pH_{limit} is approached, the required quantity of sodium bicarbonate to achieve an incremental change in pH increases exponentially. Therefore, pH can be increased to a limit of $pH_{min} = (pH_{limit} - 0.1)$ or decreased to a limit of $pH_{max} = (pH_{limit} + 0.1)$. Additional logic includes: (1) if pH is $pH_{min} \leq pH \leq pH_{max}$, then no adjustment is attempted, (2) pH can be adjusted down to pH_{max} and up to pH_{min} , (3) if $pH < pH_{min}$, then pH cannot be decreased, and (4) if $pH > pH_{max}$, then pH cannot be increased. Procedure:

- 1) Calculate ALK_{nc} at the adjusted pH
- 2) Calculate the proportion of ALK_{nc} at the adjusted pH (factor f)
- 3) $CMP_{add} \text{ (mg/L)} = [((12.011 \text{ mg/mmol}) [(-ALK_{init}/(50.043 \text{ mg/meq})) + (CO_{init}/(12.011 \text{ mg/mmol})) + (ALK_{nc}/(50.043 \text{ mg/meq}))] / f) - CO_{init}] / CMP_{co}$
- 4) $CO_{adj} \text{ (mg C/L)} = CO_{init} + (CMP_{add} \text{ } CMP_{co})$
- 5) $ALK_{adj} \text{ (mg CaCO}_3\text{/L)} = ALK_{init} + (CMP_{add} \text{ } CMP_{alk})$

4.4.8.5 Calcium carbonate and sodium carbonate

Addition of calcium carbonate and sodium carbonate results in changes to ALK, CO, and HRD. Addition of these compounds can increase pH to a level where CaCO_3 is at equilibrium (pH_{limit} , e.g. 8.2), but only if CaCO_3 is initially under saturated and can therefore dissolve when added. As pH_{limit} is approached, the required quantity of these compounds to achieve an incremental change in pH increases exponentially. Therefore, pH can be increased to a limit of $\text{pH}_{\text{max}} = \text{pH}_{\text{limit}} - 0.1$. Procedure:

If $\text{pH}_{\text{adjusted}} \geq \text{pH}_{\text{limit}}$, then:

- 1) $\text{pH}_{\text{adjusted}} = \text{pH}_{\text{limit}}$
- 2) $\text{CMPadd (mg/L)} = (\text{ALKeql} - \text{ALKinit}) / \text{CMPalk}$
- 3) $\text{COadj (mg C/L)} = \text{COinit} + (\text{CMPadd} \text{ CMPco})$
- $\text{ALKadj (mg CaCO}_3\text{/L)} = \text{ALKeql}$
- $\text{HRDadj (mg CaCO}_3\text{/L)} = (\text{CMPadd} \text{ CMPhrd})$

Else if $\text{pH}_{\text{adjusted}} < \text{pH}_{\text{limit}}$, then:

- 1) ALK_{nc} (meq/L) is calculated at $\text{pH}_{\text{adjusted}}$
- 2) The proportion of ALK_{c} is calculated at $\text{pH}_{\text{adjusted}}$ (factor f)
- 3) $\text{CMPadd (mg/L)} = [((12.011 \text{ mg/mmol}) (\text{ALK}_{\text{nc}} - [\text{ALKinit} / (50.043 \text{ mg CaCO}_3\text{/meq}) - (2 \text{ COinit} / (12.011 \text{ mg/mmol}))]) / (2 - f) - \text{COinit}) / \text{CMPco}]$
- 4) $\text{COadj (mg C/L)} = \text{Cinit} + (\text{CMPadd} \text{ CMPco})$
- $\text{ALKadj (mg CaCO}_3\text{/L)} = \text{ALKinit} + (\text{CMPadd} \text{ CMPalk})$
- $\text{HRDadj (mg CaCO}_3\text{/L)} = \text{HRDinit} + (\text{CMPadd} \text{ CMPhrd})$

5. Methods of Aquacultural Engineering

Methods of aquacultural engineering used in AquaFarm represent a wide range of physical processes. These include facility climate, heat and gas transfer, water flow mechanics and budgets, solid sedimentation and filtration, chemical filtration, and compound addition. All of these methods have a basis in the engineering literature, with some additional development provided here. While all of the methods presented in this dissertation can be considered to fall under aquacultural engineering, the methods described below are those remaining after the grouping of other methods under aquatic chemistry, aquatic biology, and fish biology.

5.1 Facility climate

Climate variables are used in many of the methods in AquaFarm, including passive heat and gas transfer, water stratification, water mass balances (water budgets), primary productivity, and fish culture day length (photoperiod). Climate variables include (1) annual regimes of daily mean air temperature, solar radiation, time of sunrise and sunset, day length, cloud cover, precipitation, wind speed, and relative humidity and (2) diurnal regimes of solar radiation and air temperature. Predicted, annual and diurnal regimes of facility climate variables can be:

- 1) Interpolated from user-supplied historical datasets: Datasets may include annual regimes of daily mean values and diurnal minimum-maximum values for air temperature. Intermediate data between given values (at any given periodicity) are calculated by linear interpolation. Local climate data collection at facility sites is rare, and is mainly accomplished at aquaculture research stations. However, local or regional climate data is available for most regions of the world, both in printed and electronic forms.
- 2) Defined by controlled climates: An entire facility, sub-system, or individual facility unit can be housed in an opaque (no solar radiation) or greenhouse (ambient solar radiation) structure, in which photoperiod, air temperature, and humidity are ambient or controlled (see Chapter 2, Facility unit specifications).
- 3) Estimated as a function of facility latitude and altitude, seasonal and diurnal parameters, and time of year and day: These methods are described below and are used to approximate climatic conditions and to avoid the need for facility climate data files.

5.1.1 Solar radiation

Calculation methods for short-wave solar radiation (ϕ_s ; wavelength $0.14 \mu\text{m} - 4.0 \mu\text{m}$; Fritz et al., 1980) are largely adapted from Nath (1996), with some additional development here. In turn, methods described by Nath (1996) are principally based on procedures and calculations described by Fritz et al. (1980) and Hsieh (1986). Method variables are listed in Table 5.1 and method equations are listed in Table 5.2. During a simulation, for each simulation step, the equations in Table 5.2 are used in the reverse order of their listing, where values are progressively substituted and finally ϕ_s is calculated. Short-wave solar radiation incident on a water surface (ϕ_s) and penetrating a water surface (ϕ_{sn}) at a given time (calendar date and time of day) is a function of site altitude, latitude, longitude, and cloud cover (Table 5.3).

Daily mean ϕ_s is obtained by numerically integrating hourly mean ϕ_s from sunrise to sunset. Hourly mean ϕ_s values are calculated by completing the solar radiation algorithm (Table 5.1) for each daylight hour from sunrise to sunset (i.e., $h_r \leq h_a \leq h_s$). For hours that span sunrise and sunset, hourly mean values are adjusted for the portion of the hour within the daylight period. Alternatively, to minimize calculation intensity, hourly mean ϕ_s for daylight hours can be calculated from $\phi_{s,max}$ by (Monteith, 1973):

$$\phi_s = \phi_{s,max} \sin(\pi t / p)$$

where t = elapsed time (day) since sunrise over the photoperiod and a sine function is assumed to sufficiently approximate diurnal radiation regimes. Use of this method is assessed in Chapter 8. To achieve ϕ_s values for higher elevations cited in Kreider and Kreith (1981; e.g. Albuquerque, New Mexico), it was found necessary to apply a small, elevation correction factor (ϕ_{ECF}) to ϕ_s .

Solar radiation values used in passive heat transfer and primary productivity calculations are corrected for reflectivity of the water surface (A_s), which is a function of the solar altitude angle and atmospheric conditions (water surface conditions and surrounding topography are not considered). In addition, for primary productivity, the index of refraction for light going from air to water is used to correct the light extinction coefficient for angle of incidence, based on the relative change in length of light travel due to refraction (Piedrahita, 1989):

Table 5.1. Method variables for short-wave solar radiation

Symbol	Definition
a	α expressed in degrees
A_{ct}	Astronomical correction term (hr): accounts for variations in daylength caused by changes in the velocity of the earth as it revolves around the sun (dimensionless)
AOR	Angle of refraction of light traveling from air to water (radians)
AOR_L	Relative change in length of light travel due to refraction (dimensionless)
A_s	Short-wave reflectivity of water surface (e.g., daily mean 0.06; Henderson-Sellers, 1984)
A_t	Atmospheric transmission coefficient: function of the geographic location of a site and time of the year (empirically based; reported range 0.7 – 0.97)
CC	Fraction of the sky that is covered by clouds (0 – 1; in tenths)
h_a	Hour angle (radians; range $-\pi$ to $+\pi$): angular distance through which the earth must rotate to bring the meridian of a given point on the earth's surface directly below the sun (<0 morning, $=0$ noon, >0 afternoon)
h_r	Local sunrise hour angle (radians)
h_s	Local sunset hour angle (radians; positive by convention, where $h_s = -h_r$)
I_{SC}	Solar constant ($2880 \text{ cal/cm}^2\text{-day}$ or $120580 \text{ kJ/m}^2\text{-day}$): solar radiation intensity outside the atmosphere
JD	Julian day of the year (1 – 365 or 366; may include fraction of day depending on use)
L_{ct}	Longitude correction term (hr): based on the time taken by the sun to traverse 1° of longitude (4 minutes)
L_g	Site longitude ($^\circ$)
L_s	Standard meridian for the time zone ($^\circ$)
L_t	Site latitude (radians)
m	Optical air mass (dimensionless): empirically based and a function of barometric pressure (and thus of altitude)
p	Photoperiod (hours or fraction of day): time between sunrise and sunset
R_{es}	Relative distance between the earth and sun (dimensionless): normalized radius of the earth's orbit
t_L	Local clock time (hr)
t_{rise}	Local time of sunrise (hr)
t_s	Solar time (hr) with respect to the angular movement of the sun across the sky, where local solar noon occurs when the sun is immediately above the site meridian
t_{set}	Local time of sunset (hr)
x	Cloud cover variable (Table 5.3)
y	Cloud cover variable (Table 5.3)
Z	Site altitude relative to sea level (m)
ZA	Zenith angle (radians): angle of incidence measured from solar noon (0 at solar noon)

Table 5.1. Continued

Symbol	Definition
α	Solar altitude (radians): angle between the earth-sun line and the earth's surface; expressed in degrees (0 – 90) for calculation equation for ϕ_{sn}
β	Calculation variable
δ	Solar declination (radians): angle between the earth-sun line and the earth's equatorial plane (varies daily); N. hemisphere (+); S hemisphere (-); spring and fall (zero)
ϕ_{ECF}	Elevation correction factor for ϕ_s (dimensionless; default 3.0)
ϕ_s	Incident short-wave solar radiation on a horizontal surface on earth ($\text{kJ/m}^2\text{-day}$)
ϕ_{smax}	Daily maximum ϕ_s , assumed to occur at the local solar noon ($\text{kJ/m}^2\text{-day}$)
ϕ_{sn}	ϕ_s that penetrates the water surface ($\text{kJ/m}^2\text{-day}$)

Table 5.2. Method equations for short-wave solar radiation

Variable	Function
ϕ_s	$= (I_{SC} / R_{es}^2) (\sin \alpha) (A_t^m) (1.0 - 0.65 C_c^2) + \phi_{ECF} Z$
R_{es}	$= 1.0 + 0.017 \cos (2 \pi (186 - JD) / 365)$
$\sin \alpha$	$= (\sin L_t) (\sin \delta) + (\cos \delta) (\cos L_t) (\cos h_a)$
P	$= -h_r * 24 / \pi$
t_{rise}	$= 24 * [0.5 * (PI + h_r) / PI]$
t_{set}	$= 24 * [0.5 - 0.5 * h_r / PI]$
h_r	$= -\cos^{-1} (-\tan L_t \tan \delta)$
δ	$= 0.4028 \sin [2 \pi (JD - 79.75) / 365]$
h_a	$= \pi (t_s - 12) / 12$, or for fractional from of t_s , h_a is $(t_s 2 \pi) - \pi$
t_s	$= t_L + A_{ct} + L_{ct}$
A_{ct}	$= (9.87 \sin 2 \beta - 7.53 \cos \beta - 1.5 \sin \beta) / 60$
β	$= (\pi/180) (360/364) (JD - 81)$
L_{ct}	$= (L_s - L_g) / (360 / 24)$
L_s	If $L_g \geq 0$, then $L_s = L_g - \text{remainder of } L_g / 15$. If $L_g \leq 0$, then $L_s = L_g - 15 - \text{remainder of } L_g / 15$.
A_t	$= 0.0685 \cos [2 \pi (JD + 10) / 365] + 0.80$
m	$= [(288 - 0.0065 Z) / 288]^{5.256} / [\sin \alpha + 0.15 (a + 3.885)]^{-1.253}$
ϕ_{sn}	$= \phi_s (1 - A_s)$
A_s	$= x \alpha^y$

Table 5.3. Cloud cover type, cloud cover values (CC), and empirically based parameters x and y (Fritz et al., 1980)

Cloud cover type	CC	x	y
Clear	0.0	1.18	- 0.77
Scattered	0.1-0.5 (0.5)	2.20	- 0.97
Broken	0.6-0.9 (0.75)	0.95	- 0.75
Overcast	1.0	0.35	- 1.45

If $(-1.4 \leq h_a \leq 1.4)$, then $ZA = \arccos(\sin \alpha)$, else $ZA = 1.4$

$AOR = \arcsin(\sin(ZA) / 1.33)$

$AOR_L = \cos(AOR)$

5.1.2 Air temperature

Method equations used to calculate diurnal and annual air temperature values are listed below and method variables are listed in Table 5.4. It is assumed that sinusoid functions sufficiently approximate annual and diurnal air temperature regimes. Site specific, empirically based parameters are used to adjust the magnitude, amplitude, and shape of these sinusoids to local conditions. T_{am} , T_{aamp} , and T_{dm} are calculated by (Straskraba and Gnauck, 1985):

$$T_{am} = 25.92 + 0.4893 L'_t - 0.02739 L'^2_t + 0.0001782 L'^3_t$$

$$T_{aamp} = 2.0 (1.536 + 0.05735 L'_t - 0.01296 L'^2_t + 0.0001312 L'^3_t)$$

$$T_{dm} = T_{am} + (T_{aa} / 2.0) \sin[\pi (JD + P_{amax}) / 180] - (T_{acf} Z)$$

$$T_{am} = (T_{amin} + T_{amax}) / 2.0$$

$$T_{aamp} = T_{amax} - T_{amin}$$

$$P_{amax} = 451 - JD_{amax}$$

Table 5.4. Method variables for air temperature, cloud cover, precipitation, wind speed, and relative humidity

Symbol	Definition
af	Angular frequency (radians/hr)
CC	Fraction of sky covered by clouds (in tenths; 0-1): e.g., clear (0.0), scattered (0.5), broken (0.75), overcast (1.0), dry season (0.375), and wet season (0.625).
JD _{amax}	Julian day of the year when T _{amax} occurs
L _t	Site latitude calculation term (degrees) = $ L_t - 3.4 $ where L _t is in degrees
pa	Phase angle (radians)
P _{amax}	Phase angle corresponding to JD _{amax} : e.g., N hemisphere (220°), S hemisphere (100°)
PCP	Precipitation (mm/day)
RH	Relative humidity (%)
T _{aamp}	Amplitude of annual temperature regime (°C)
T _{acf}	Temperature change for each 100m altitude above mean sea level (range 0.5 - 0.8)
T _{am}	Mean temperature of annual temperature regime (°C)
T _{amax}	Maximum daily mean temperature of annual temperature regime (°C)
T _{amin}	Minimum daily mean temperature of annual temperature regime (°C)
T _{damp}	Amplitude of diurnal temperature regime (°C) = T _{dmax} - T _{dmin}
T _{din}	Daily mean air temperature (°C)
T _{dmax}	Diurnal maximum air temperature (°C)
T _{dmin}	Diurnal minimum air temperature (°C)
t _h	Time of day (hr; 0-24)
T _{hm}	Hourly mean air temperature (°C)
t _{hmax}	Time of diurnal maximum temperature (hr)
t _{hmaxo}	Time of diurnal maximum temperature relative to sunset (hr; +/-)
t _{hmid}	Mid point time between times of diurnal minimum and maximum temperatures (hr)
t _{hmin}	Time of diurnal minimum temperature (hr)
t _{hmino}	Time of diurnal minimum temperature relative to sunrise (hr; +/-)
WS	Wind speed (m s^{-1} ; at a height of 2m above the water surface)

T_{am} and T_{aamp} calculations are rough approximations, given the lack of consideration of additional variables such as the proximity to large water bodies. It is preferable to specify T_{amin} and T_{amax} based on the site-specific climate history and calculate T_{am} and T_{aamp} based on these values. For similar reasons, P_{amax} can be based on a specified JD_{amax}. The default P_{amax} of 220° for the northern hemisphere corresponds to a JD_{amax} of 231 or August 19.

For diurnal simulation, T_{hm} is calculated as a function of T_{dmin} , T_{dmax} , t_{hmin} , t_{hmax} , and t_h , using a sinusoid equation (Card et al., 1976; see Chapter 8):

$$T_{hm} = T_{dm} + (T_{dmax} - T_{dmin}) a \{ \sin(\pi t_h/12 - c) + b \sin[2(\pi t_h/12 - c)] \}$$

T_{dmin} and T_{dmax} can be specified in a weather data file or calculated from a given T_{damp} :

$$T_{dmax} = T_{dm} + (T_{damp} / 2)$$

$$T_{dmin} = T_{dm} - (T_{damp} / 2)$$

where T_{damp} is specified as a set of four, quarterly mean values for the year. Parameters a , b , and c are calculated by:

$$af = 2\pi / 24$$

$$x = af(t_{hmid} - t_{hmin})$$

$$a = 0.5 / [\sin(x) + b \sin(2x)]$$

$$b = -\cos(x) / [2 \cos(2x)]$$

$$c = t_{hmid} af$$

$$t_{hmid} = (t_{hmin} + t_{hmax}) / 2$$

Times t_{hmin} and t_{hmax} are calculated based on given offsets from sunrise (e.g. 0.0 hr) and sunset (e.g. -3.0 hr), respectively, where given offsets are used as constant values for the year. If t_{hmin} and t_{hmax} occur at 0600h and 1500h respectively, then $a = 0.4483$, $b = 0.2706$, and $c = 2.7489$, as used by Culberson and Piedrahita (1992) and Nath (1997). If the time from t_{hmin} to t_{hmax} or from t_{hmax} to t_{hmin} is less than eight hours, then the method of Card et al. (1976) becomes unsuitable (multiple highs and lows) and linear interpolation is used to calculate T_{hm} .

5.1.3 Cloud cover, precipitation, wind speed, and relative humidity

Annual regimes for cloud cover, precipitation, wind speed, and relative humidity (Table 5.4) are based on given seasonal mean values. Each variable is specified as a set of four, quarterly mean values (similar to T_{damp}). Annual quarters are Jan-Mar, Apr-Jun, Jul-Sep, and Oct-Dec. Specified values for each quarter are maintained for about 80% of the quarter, and transitions between

quarters are smoothed with a sinusoid scalar (see Chapter 8). Values are used as daily means and diurnal regimes are not considered. Values (V) are calculated by:

$$V = V_2 + 0.5 \{ 1 + \sin[\text{PI} (SS - 0.5)] \} (V_1 - V_2)$$

where V_1 = value for current quarter

V_2 = value for next quarter

SS = season transition scalar (0-1)

5.1.4 Interpolation of periodic data

Annual regimes of facility climate and source water quality variables can be specified as regularly and/or irregularly spaced periodic data. Interpolation is used to determine values for days not specified. Interpolation may be accomplished by either linear or quadratic methods. Linear interpolation requires at least two, and quadratic interpolation requires at least three, day-variable data pairs over the period of interest. For variables with high day-to-day variability, the more frequently data is specified, the better an interpolated regime will match existing conditions. If the quadratic method is used, data should be evenly spaced and without extreme variations within short time periods, or peculiar numbers may result (very large or negative numbers) as the interpolation attempts to fit parabolas to irregular points.

Linear: $V = [V_1(d-d_2)/(d_1-d_2)] + [V_2(d-d_1)/(d_2-d_1)]$

Quadratic: $V = V_1(d-d_2)(d-d_3)/(d_1-d_2)(d_1-d_3) + V_2(d-d_1)(d-d_3)/(d_2-d_1)(d_2-d_3) + V_3(d-d_1)(d-d_2)/(d_3-d_1)(d_3-d_2)$

where V = variable value

d = Julian day (1 - 365), where subscripts 1-3 for contiguous data pairs

5.2 Heat transfer

Heat transfer processes that influence water temperatures in aquaculture systems include passive (natural) heat transfer between facility waters and the environment and active (managed) transfer using water heaters and chillers. The overall heat-energy transfer rate of a facility unit is a function of its climate (ambient or controlled), water stratification, water volume, water flow rate, water temperature, air-water and air-wall-water surface areas, position with respect to soil grade,

wall dimensions and materials, and heat transfer rates of heaters and chillers. Passive heat transfer may result in desirable or undesirable temperatures.

Heat transfer rates of facility units are used in heat balances for prediction of water temperatures and calculation of energy requirements for heaters and chillers. Heat transfer rates of each mode considered are individually quantified and compiled into heat transfer budgets. Heat transfer modes include (1) influent and effluent water flow, (2) heating and chilling, (3) surface radiation (combined short and long wave), (4) surface evaporation, (5) open surface convection-conduction, and (6) air-wall-water convection-conduction. Heat transfer budgets generated by simulation can be used to identify and correct heat transfer problems and improve resulting water temperatures. Corrective options include partial or complete burying in soil, use of insulation, use of greenhouses and controlled environments, covering exposed water surfaces, use of shade tarps, and use of heaters and chillers. If a facility unit is housed, constant values for air temperature and humidity can be specified, wind speed and precipitation are assumed to be occluded, and solar radiation may be ambient or blocked.

5.2.1 Heat transfer model

For open water bodies such as fish ponds, a variety of predictive models for water temperature have been developed. These include empirically based models (e.g., Wax et al., 1987) and mechanistic models, the latter including applications to plug flow reactors (salmon raceways; Geiselman, 1984), completely mixed reactors (described below), and thermally stratified water bodies (e.g., Culberson and Piedrahita, 1992). The heat transfer model described here is similar to the approach used by Nath (1997), which is mainly based on Ryan et al. (1974), Fritz et al. (1980), and Henderson-Sellers (1984). Added here are heat conduction at air-wall-water interfaces, active heat transfer by heater and chillers, consideration of facility unit materials and housing, special cases impacting heat transfer rates (e.g., use of aeration), and thermal stratification. Method variables are listed in Table 5.5.

The heat energy transfer modes considered include (1) advective water flow (ϕ_{qi} , ϕ_{qe}), (2) net short-wave solar radiation penetrating the water surface (ϕ_{sn}), (3) net atmospheric long-wave radiation (ϕ_{an}), (4) water surface long-wave radiation (ϕ_{ws}), (5) evaporative heat transfer (ϕ_e), (6) air-water conductive heat transfer (ϕ_{aw}), (7) air-wall-water conductive heat transfer (ϕ_{aww}),

Table 5.5. Method variables for heat energy transfer

Symbol	Definition
b	Calculation variable ($\text{kJ}/(\text{m}^2 \text{ day mmHg (m/s)})$)
DEF	Diffusion enhancement factor (dimensionless)
DEF ₀	Diffusion enhancement factor parameter (dimensionless; default value 1.0)
DIA	Conduit diameter for tubular shapes or equivalent diameter for other shapes (m)
e	Efficiency of heater or chiller (%; includes fuel conversion and heat energy losses)
K	Thermal conductivity of wall material ($\text{J}/\text{s-m-}^\circ\text{C}$)
K _a	Convective coefficient for air-wall ($\text{J}/\text{s-m}^2\text{-}^\circ\text{C}$)
KV	Kinematic viscosity (m^2/s)
K _w	Convective coefficient for water-wall ($\text{J}/\text{s-m}^2\text{-}^\circ\text{C}$)
K _{wm}	Modified value for K _w , used in place of K _w for stated conditions ($\text{J}/\text{s-m}^2\text{-}^\circ\text{C}$)
L	Length of conduit or channel (m)
P _a	Water vapor pressure above the water surface (mm Hg)
PN	Prandtl number (dimensionless)
P _w	Water vapor pressure (saturated) at the current water temperature (mm Hg)
Q _e	Effluent water flow rate (m^3/day)
r	Water surface reflectance to long-wave radiation (dimensionless; 0.03 used)
Rn	Radius of wall (m), tubular facility units
RN	Reynolds number (dimensionless)
SA	Surface area, context specific used (m^2)
SA _{aw}	Air-water surface area (m^2)
SA _{aww}	Air-wall-water surface area (m^2), for a single wall or all walls of a facility unit, inside and outside assumed equal
T _{ac}	Air temperature ($^\circ\text{C}$)
T _{ak}	Absolute air temperature ($^\circ\text{K}$)
T _{av}	Virtual air temperature ($^\circ\text{K}$)
TC	Thermal conductance of a wall, single layer or composite ($\text{J}/\text{s-m}^2\text{-}^\circ\text{C}$)
TCC	Overall thermal conductance of a facility units ($\text{J}/\text{s-m-}^\circ\text{C}$)
T _{wc}	Water temperature ($^\circ\text{C}$)
T _{wc, sp}	Set point water temperature for water heating and chilling ($^\circ\text{C}$)
T _{wk}	Absolute water temperature ($^\circ\text{K}$)
T _{wv}	Virtual water temperature ($^\circ\text{K}$)
U	Water velocity (m/s)
W	Total wall width (thickness; m), tubular facility units
WP	Wetted perimeter (m)
WS	Wind speed (m/s; reference height of 2.0 m above the pond water surface)
X	Thickness of wall material (m)
CSA	Cross sectional flow area (m^2)
ε _a	Atmospheric emissivity (dimensionless)
ε _w	Emissivity of water (dimensionless; 0.97 used)
φ _{an}	Heat transfer – net atmospheric long-wave radiation ($\text{kJ}/\text{m}^2\text{-day}$)

Table 5.5. Continued

Symbol	Definition
ϕ_{aw}	Heat transfer – air-water conductive heat transfer ($\text{kJ/m}^2\text{-day}$)
ϕ_{aww}	Heat transfer – air-wall-water conductive heat transfer ($\text{kWhr/m}^3\text{-day}$)
ϕ_e	heat transfer – evaporative heat transfer ($\text{kJ/m}^2\text{-day}$)
ϕ_{hc}	Heat transfer – active heat transfer by heaters and chillers ($\text{kWhr/m}^3\text{-day}$)
ϕ_{net}	Heat transfer – sum of all modes except water advection ($\text{kWhr/m}^3\text{-day}$)
ϕ_q	Heat transfer – advective water flow ($\text{kWhr/m}^3\text{-day}$)
ϕ_{sn}	Heat transfer – net short-wave solar radiation penetrating water surface ($\text{kJ/m}^2\text{-day}$)
ϕ_{ws}	Heat transfer – water surface long-wave radiation ($\text{kJ/m}^2\text{-day}$)
λ	Calculation variable ($\text{kJ}/(\text{m}^2\text{ day mmHg } ^\circ\text{K}^{1/3})$)
σ	Stefan-Boltzmann constant ($4.896\text{e-}6\text{ kJ/m}^2\text{-day-K}^4$)

and (8) active heat transfer by heaters and chillers (ϕ_{hc}). Heat transfer modes that are assumed to be negligible include water-soil and water-wall-soil heat conduction (Losordo and Piedrahita, 1991), solar radiation on exterior surfaces of facility unit walls (Geiselman, 1984), precipitation (Henderson-Sellers, 1984), and water seepage. Water thermal stratification tends to decrease passive heat transfer for the water body as a whole, as the surface layer insulates lower layers from heat transfer. Stratification methods are described in Chapter 3 and applied in Chapter 8.

Specifications regarding facility unit dimensions, materials, and housing are described in Chapter 2. For purposes of passive heat transfer, these specifications are used to establish the environmental exposure and heat transfer modes of a given facility unit. An entire facility, fish rearing system, or individual facility unit can be housed, where solar radiation, wind, and precipitation may be occluded and air temperature and humidity may be controlled. If a facility unit is housed in an opaque building, input and output radiation terms are all zero. If shade cloth is used, radiation values are scaled according to the specified shade cloth rating. If an attached top wall is used, air flow is zero, evaporative heat transfer is not considered, and the layer of trapped air over the water surface is equal in thickness to the existing free board. Side and bottom walls may be soil, or soil may be against the outside of the wall, but heat transfer of water-soil and water-wall-soil is assumed to be negligible. For example, heat transfer of buried pipes other than advective flow is completely ignored.

Over the course of a simulation, at each simulation step, heat transfer rates of each mode are calculated for each facility unit. Heat transfer rates are compiled into heat budgets for tabular and

graphical display (see Chapter 8) and combined into heat-balance differential equations for predicting water temperatures. The formulation of the heat-energy differential equation is similar to that used for mass-balance differential equations for completely mixed or thermally-stratified reactors (see Chapter 3, Facility unit modeling), where heat energy content and transfer rate are analogous to compound concentration and transfer rate. The rate of change of water heat-energy content (dH/dt ; kWhr/m³-day) is given by ($WJ = \text{kWhr}/3600 \text{ kJ}$):

$$dH/dt = Q_i \rho_i HC_i T_i WJ / V - (Q_e + dV/dt) \rho_e HC_e T_e WJ / V + \phi_{\text{net}}$$

where $\phi_{\text{net}} = (SA_{\text{aw}} / V) (\text{hr} / 3600 \text{ s}) (\phi_{\text{sn}} + \phi_{\text{an}} - \phi_{\text{ws}} - \phi_e \pm \phi_{\text{aw}}) \pm \phi_{\text{aww}} \pm \phi_{\text{hc}}$

All heat transfer rates other than that due to water advection are combined to a single term (ϕ_{net}).

The heat energy content of water (H ; kWhr/m³) is a function of water density (kg/m³), heat capacity (kJ/kg-°C), and temperature, which in turn are a function of temperature and salinity:

$$H = \rho HC T (\text{kWhr}/3600 \text{ kJ})$$

$$\phi_q = Q H / V$$

Based on heat energy content, temperature is calculated by:

$$T = H / \rho HC (\text{kWhr}/3600 \text{ kJ})$$

5.2.2 Radiation

Short-wave solar radiation penetrating the water surface (ϕ_{sn} ; see Facility climate) is a heat source. Atmospheric long-wave radiation (ϕ_{an}) is a heat source and consists of solar energy absorbed by atmospheric water vapor and carbon dioxide that is re-radiated to the earth's surface. The net amount of long-wave radiation absorbed by a water surface is equivalent to the incident minus reflected amounts and is a function of air temperature and cloud cover (Henderson-Sellers, 1984), where atmospheric emissivity is calculated by (Wunderlich, 1972):

$$\phi_{\text{an}} = (1 - r) \epsilon_a \sigma T_{\text{ak}}^4$$

$$\epsilon_a = 0.937e-5 T_{\text{ak}}^2 (1.0 + 0.17 C_c^2)$$

Water surface long-wave radiation is a heat loss, consists of re-radiated heat energy, and is calculated by (Henderson-Sellers, 1984):

$$\phi_{\text{ws}} = \epsilon_w \sigma T_{\text{wk}}^4$$

5.2.3 Evaporation

Heat energy lost from a water body through water evaporation due to the latent heat of vaporization (evaporative heat loss) is a function of water temperature, air temperature, atmospheric pressure, humidity, and wind speed. Evaporative heat loss is calculated by (Ryan et al., 1974; Henderson-Sellers, 1984):

$$\phi_e = (P_w - P_a) [\lambda (T_{wv} - T_{av})^{1/3} + (b \text{ WS})] \text{ DEF}$$

$$b = b_0 (1000 / \text{BP}) (86400 \text{ s/day}) (\text{kJ}/1000 \text{ J})$$

$$\lambda = \lambda_0 (1000 / \text{BP}) (86400 \text{ s/day}) (\text{kJ}/1000 \text{ J})$$

where $\lambda_0 = 2.7 \text{ W/m}^2 \cdot ^\circ\text{K}^{1/3}$ and $b_0 = 3.2 \text{ W/(m}^2 \text{ (m/s))}$ (Ryan et al., 1974), and where P_w must be greater than P_a (evaporation occurs only if there is a vapor pressure deficit). If T_{wv} is not greater than T_{av} , then the associated term is set to zero. Vapor pressures P_w and P_a are calculated by methods given under Water properties (Chapter 4) and Air properties (this chapter). Virtual water and air temperatures, T_{wv} and T_{av} , are calculated by (Ryan et al., 1974):

$$T_{wv} = T_{wk} / [1.0 - (0.378 P_w / \text{BP})]$$

$$T_{av} = T_{ak} / [1.0 - (0.378 P_a / \text{BP})]$$

As shown, values for b and λ are a function of BP. Reported methods also show the use of constants for these terms (e.g., Nath, 1996), where it is assumed that BP = 750.06 mmHg:

$$b = 3.2 \text{ W/(m (m/s))} (1000 / 750.06 \text{ mmHg}) (86400 \text{ s/day}) (\text{kJ}/1000 \text{ J})$$

$$= 368.61 \text{ kJ/(m day mmHg (m/s))}$$

$$\lambda = 2.7 \text{ W/m}^2 \cdot ^\circ\text{K}^{1/3} (1000 / 750.06 \text{ mmHg}) (86400 \text{ s/day}) (\text{kJ}/1000 \text{ J})$$

$$= 311.02 \text{ kJ/(m}^2 \text{ day mmHg } ^\circ\text{K}^{1/3})$$

For use in facility unit water budgets, water lost by evaporation (Q_{evp} , m^3/day ; $Q_{evp,mm}$, mm/day) is calculated as a function of ρ and LHV, where ρ and LHV are calculated by methods described in Chapter 4:

$$Q_{evp} = \phi_e SA_{aw} / (\rho \text{ LHV})$$

$$Q_{evp,mm} = (1000 \text{ mm/m}) \phi_e / (\rho \text{ LHV})$$

5.2.4 Air-water conduction

Heat energy transfer at the air-water interface due to air-water heat conduction is calculated from its relationship to evaporative transfer using the Bowen ratio. The Bowen ratio is the ratio between the virtual temperature difference and the vapor pressure difference of the water and air (Ryan et al., 1974):

$$\phi_{aw} = \phi_e 0.61 (BP / 1000) (T_{wk} - T_{ak}) / (e_s - e_a)$$

If evaporative heat loss is zero, then conductive heat loss or gain is calculated by (Fritz, 1980; converted to kJ/m²-day):

$$\begin{aligned}\phi_{aw} &= 0.9 \text{ WS (km/1000 m)(3600 s/hr) } (T_{ac} - T_{wc}) [41.868 \text{ (kJ/m}^2) / (\text{cal/cm}^2)] \text{ DEF} \\ &= 35.65 \text{ WS } (T_{ac} - T_{wc}) \text{ DEF}\end{aligned}$$

5.2.5 Heat transfer enhancement

Components such as in-tank aeration, gas exchangers, and trickling biofilters, as typically found in intensive aquaculture systems, complicate heat transfer modeling. Such components greatly enhance air-water interface areas and contact (mixing) conditions. To consider such conditions, a diffusion enhancement factor (DEF; dimensionless) is applied to evaporative and air-water conductive heat transfer when a facility unit contains aeration (surface, sub-surface, or gravity), airlift pumping, foam fractionation, or trickling filtration. This method is based on the assumption that the increase in PHT is proportional to the increase of the overall air-water diffusion coefficient for oxygen (K_{O_2} ; see Gas transfer, this chapter):

$$\text{DEF} = 1.0 + \text{DEF}_0 [((K_{O_2, \text{passive}} + K_{O_2, \text{active}}) / K_{O_2, \text{passive}}) - 1]$$

5.2.6 Air-wall-water conduction

Heat energy transfer at air-wall-water interfaces is a function of air and water convection against the wall, wall thermal conductivity, and the air-water temperature difference (Welty, et al, 1976):

$$\phi_{aww} = TC \text{ SA}_{aww} (T_{ac} - T_{wc}) (24 \text{ hr/day}) (\text{kW/ } 1000 \text{ W})$$

The convective heat transfer coefficient for air at the air-wall interface (K_a ; $\text{J/s-m}^2\text{-}^\circ\text{C}$), under conditions of free convection, varies from about 5 to 50 $\text{J/s-m}^2\text{-}^\circ\text{C}$ (Welty et al., 1976). K_a is applied to all exposed wall surfaces, such as exposed pipe and tank walls. Due to a number of complicating factors and required specifications, K_a is used as a constant value and is applied uniformly to all exposed walls over the course of a simulation (default value 25 $\text{J/s-m}^2\text{-}^\circ\text{C}$). The convective heat transfer coefficient for water at the water-wall interface (K_w ; $\text{J/s-m}^2\text{-}^\circ\text{C}$), under conditions of forced convection (turbulent flow), varies from about 100 to 10000+ $\text{J/s-m}^2\text{-}^\circ\text{C}$ (Welty, et al, 1976) and is calculated by (Geiselman, 1984):

$$K_w = 23.0 \text{ RN}^{-0.2} \text{ PN}^{-2/3} \text{ U HC (1000 J/kJ) } \rho \text{ (1000 g/kg) (m}^3\text{/10e6 cm}^3\text{)}$$

$$K_w = 23.0 \text{ RN}^{-0.2} \text{ PN}^{-2/3} \text{ U HC } \rho$$

$$\text{RN} = \text{DIA U / KV}$$

$$\text{DIA} = 4.0 \text{ CSA / WP}$$

Calculations for the Prandtl number (PN) and kinematic viscosity (KV) are described in Chapter 4. A minimum water velocity (U) of 0.01 m/s is used for all facility units. The conduit diameter (DIA) is calculated as an equivalent diameter for shapes other than tubular. If the ratio $L/\text{DIA} > 60.0$, K_w is used as calculated above. Otherwise, a modified value is used (K_{wm}):

$$\text{If } 2.0 \leq L/\text{DIA} \leq 20.0, \text{ then: } K_{wm} = K_w [1.0 + (\text{DIA}/L)^{0.7}]$$

$$\text{If } 20.0 \leq L/\text{DIA} \leq 60.0, \text{ then: } K_{wm} = K_w [1.0 + 6.0 * (\text{DIA}/L)]$$

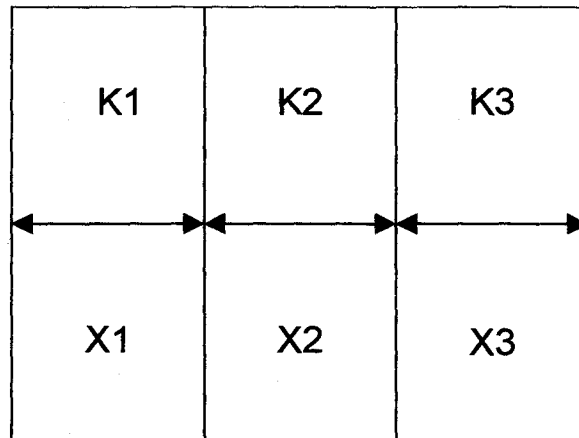
A wall may consist of multiple layers, for which materials are combined to determine the thermal conductance of the wall and walls are combined to determine the overall thermal conductance of a facility unit (Table 5.6; Welty et al., 1976). The thermal conductance ($\text{J/s-m}^2\text{-}^\circ\text{C}$) of a single wall with n layers of material is (Figure 5.1A):

$$\text{TC} = 1.0 / (X_1/K_1 + X_2/K_2 + X_n/K_n + 1.0/K_a + 1.0/K_w)$$

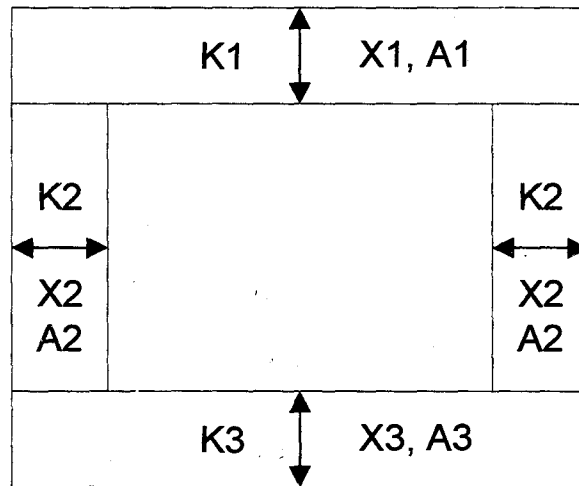
The overall thermal conductance ($\text{J/s-m}^2\text{-}^\circ\text{C}$) of a facility unit with n walls, including bottom (if elevated above ground), sides and ends, and top is (Figure 5.1B):

$$\text{TC} = (\text{SA}_1 \text{ TC}_1 + \text{SA}_2 \text{ TC}_2 + \text{SA}_n \text{ TC}_n) / (\text{SA}_1 + \text{SA}_2 + \text{SA}_n)$$

A: Single wall



B: Combined walls - rectangular shape



C: Combined walls - tubular shape

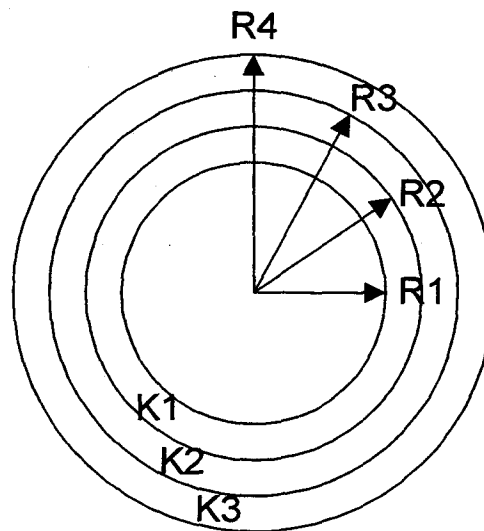


Figure 5.1. Thermal conductance terms for walls of facility units

Table 5.6. Thermal conductivity of materials (TC; W/m-°K, W/m-°C, or J/s-m-°C) ¹

Material	W/m-°C or J/s-m-°C
Earth (average)	1.6745
Sand (dry)	0.345
Sandy loam (4 % water)	0.94
Sandy loam (10 % water)	1.87
Loose fill (rock)	0.062
Asphalt	0.74
Cement, plaster, sand aggregate	0.72
Concrete	1.0877
Concrete block, 2 hole, 8 in.	1.0396
Concrete block, 2 hole, 8 in., aggregate fill	0.5770
Concrete block, 2 hole, 8 in., insulation fill	0.2294
Ice	1.9413
Glass, single pane	1.0212
Glass, double pane	0.5490
Glass, triple pane	0.3636
Rubber	0.1674
Polyvinyl chloride (PVC)	0.1673
Epoxy resin	0.1882
Polyester resin	0.2164
Acrylic resin	0.2077
Fiberglass (polyester resin)	0.2308
Polyethylene (high density)	0.3289
Aluminum	206.5986
Steel, mild	47.2211
Steel, stainless	21.4622
Soft woods	0.1423
Wood composite	0.0563
Plywood	0.12
Air space (<= 4 in)	0.0252
Cellular glass insulation	0.058
Blanket fiber glass insulation	0.0435
Expanded polystyrene	0.0326
Expanded polyurethane	0.0296

¹ Values represent averages of reported values (Henderson and Perry, 1976; Midwest Plan Service, 1987; Creswell, 1993; Adey and Loveland, 1991)

For tubular facility units (e.g. pipes), the thermal conductance of a wall with n layers of material is (Figure 5.1C):

$$TC = 1.0 / \{ (R_n - R_1) [\ln(R_2/R_1)/K_1 + \ln(R_3/R_2)/K_2 + \ln(R_n/R_3)/K_3] + 1.0/K_a + 1.0/K_w \}$$

Water heat exchangers or elements used for heating and/or chilling can be installed in a facility unit and are managed by specified control variables (see Chapter 3, Process management). The rate of energy consumption (ϕ_{hc} ; kWhr/m³-day) required for a heater/chiller is calculated by:

$$\phi_{hc} = Q_e \rho_e HC_e (T_{wc,sp} - T_{wc}) (\text{day}/86400 \text{ s}) (24 \text{ hr/day}) / (e / 100)$$

Q_e is the influent-effluent water flow rate (m³/day), or for static facility units, the water volume divided by the desired time to set point. As needed for resource budgets, energy requirements of heating/chilling are converted from terms of kWhr/day to the type of energy (fuel) used.

5.3 Energy and power

Energy is consumed by air and water pumps, aerators, and water heaters and chillers. Power (PW) is expressed as kilowatts (kW; 1.0 kW = 1.341 HP) or kilowatt-hours (kWhr/day = kW x 24 hr/day). Conversion of joules (J), watts (W), and work (N-m/s) is based on the equivalency: $W = J/s = N\text{-m/s}$. Energy is expressed as kWhr, where kWhr = kW x time (hr), or kWhr = kWhr/day x time (days). Energy can be provided as electrical or fuel energy, where kilowatt-hours are used as internal calculation units and are converted to equivalent fuel volumes when energy resources are reported. The conversion is based on reported heats of combustion (Jensen, 1983): diesel (10.8 kWhr/L), gasoline (9.6 kWhr/L), methanol (5.2 kWhr/L), propane (7.1 kWhr/L), and methane (natural gas, 10.3 kWhr/m³).

For electrical power, current (I , amperes), voltage (V , volts), motor power factor (PF, 0-1, e.g. 0.9), and electrical power consumption (PW, kW) of single and three phase (ϕ) motors are related by (Jensen, 1983):

$$PW = PF I V / (1000 \text{ W/kW})$$

$$PW = PF I V 3^{0.5} / (1000 \text{ W/kW})$$

These relationships hold for other uses of electrical power (e.g. resistive heaters), where PF is dropped from the equations. Power and amperage values are calculated over the course of facility simulations and used in resource accounting and sizing of electrical supplies, thermal protection, and motors. Voltage and phase values are user specified and default values are based on power levels (1 ϕ 120VAC for ≤ 1.0 kW; 1 ϕ 220VAC for 1.0 - 4.0 kW; 3 ϕ 220VAC for ≥ 4.0 kW). Motor power input (PW; electrical or fuel energy) and output power (PW_{bp}; brake power, mechanical energy) are related by the motor efficiency rating (e; e.g., 0.8), where PW_{bp} = e PW.

5.4 Air properties and compression

The mass density of wet air (ρ_{air} ; kg/m³) is a function of barometric pressure (BP; mm Hg), vapor pressure of water (VP; mm Hg; based on air temperature), relative humidity (RH; %), and air temperature (T_{ak} ; °K) (Lapina, 1982):

$$\rho_{\text{air}} = [(BP - VP \text{ RH} / 100) / (2.153 T_{\text{ak}})] + [(VP \text{ RH} / 100) / (3.461 T_{\text{ak}})]$$

The water vapor pressure of air (VP_{air}; mm Hg) at a given temperature and relative humidity is a function of the water vapor pressure at the air temperature:

$$VP_{\text{air}} = VP \text{ RH} / 100$$

Mass air flow rate (M_{air} ; kg/hr) and volumetric air flow rate (V_{air} ; m³/hr) are related by:

$$V_{\text{air}} = M_{\text{air}} / \rho_{\text{air}}$$

Compressed air is used by facility units such as packed column aerators, air diffusers, foam fractionators, and airlift pumps. Power used by air compressors such as centrifugal (regenerative) blowers is based on the adiabatic compression formula (Hackney, 1981):

$$PW_a = [M_{\text{air}} (\text{hr}/3600 \text{ s}) R T_{\text{ak}} / (n e)] [(P_o / P_i)^n - 1.0]$$

where PW_a = power applied for air pumping (kW), M_{air} = mass air flow rate (kg/hr), R = gas constant (0.287), T_{ak} = air inlet temperature (°K), n = 0.283 (for air only), e = combined efficiency of compressor and motor (e.g. 0.7), P_i = inlet absolute pressure (kPa, based on BP), and P_o = outlet absolute pressure (kPa). For example, when P_i is BP and P_o is equivalent to BP plus 2.0 m water

head, pumping air at $170 \text{ m}^3/\text{hr}$ (100 cfm) at $e = 0.7$ demands approximately 1.25 kW (1.68 HP) of power. For use in aeration, the adiabatic compression formula can be rearranged to calculate M_{air} (and then V_{air}) from a known PW value:

$$M_{\text{air}} = PW_a n e / \{(\text{hr}/3600 \text{ s}) R T_{\text{ak}} [(P_o / P_i)^n - 1.0]\}$$

5.5 Water mechanics

Water flow mechanics include water pumping, pressurized flow in pipe and vessel systems, and gravity flow in basins, open and closed channels, and cascades and packed columns. The mechanics considered in a particular simulation depend on facility specifications and mechanics may be ignored. Simulation objectives are to (1) test user-specified water systems with respect to their hydraulic integrity and capacity to supply required water flow rates, (2) establish water volumes, hydraulic retention times, flow rates, and velocities for facility units, and (3) generate energy requirements and other operation conditions for water pumping that can be used for selecting specific water pumps. All of the methods described here are based on constant water flow rates. While water flow rates typically vary over the course of a simulation, adjustments to water flowrate are accomplished between simulation steps and flow rates are constant within a simulation step. Method variables are listed in Table 5.7.

5.5.1 Water volumes, flow rates, velocities, and retention times

A number of terms are used in mass and heat balances and water mechanics. These include facility unit total volume ($V_{\text{fu}}; \text{m}^3$), water volume ($V_{\text{w}}; \text{m}^3$), water velocity ($U; \text{m/s}$), water flow rate ($Q; \text{m}^3/\text{day}$), hydraulic loading rate (HLR; $\text{m}^3/\text{m}^2\text{-hr}$), and mean hydraulic retention time (θ ; day). As described in Chapter 2, a number of dimensional and hydraulic specifications for facility units are involved in these calculated variables. Calculation of areas and volumes are accomplished by standard geometrical methods (Heisler, 1984) which are not repeated here.

Table 5.7. Method variables for water flow mechanics

Symbol	Definition
AL_D	Airlift pump depth (water surface to pump input; cm)
AL_{ID}	Airlift pump inside pipe diameter (cm)
AL_L	Airlift pump lift (water surface to pump output; cm)
AL_{SR}	Airlift pump submergence ratio (cm/cm)
AL_{TL}	Airlift pump total length (cm)
BP	Barometric pressure at a water surface (mm Hg)
CSA	Cross-sectional flow area (m^2)
e	Combined motor and pump efficiency (%)
e_m	Motor efficiency (%): conversion of electrical or fuel energy to mechanical energy (brake power)
e_p	Pump efficiency (%): conversion of mechanical energy (brake power) to water flow energy (water power)
g	Gravitational acceleration (9.81 m/s^2)
H	Height of packed columns (m)
HA	Water head added by a water pump (m; equivalent to TDH)
HG	Hydraulic gradient (slope; m/m)
HL_f	Head loss of pipe fitting(s) (m)
HL_{fp}	Head loss proportion of fittings relative to pipe or vessel wall friction (%)
HL_m	Head loss of media and accumulated solids (m)
HL_{mc}	Head loss of clean media (m)
HL_{ml}	Head loss of media at PS_{max} loading (m)
HL_p	Head loss of pipe (m)
HLR	Hydraulic loading rate ($m^3/m^2\text{-hr}$)
HL_t	Total water head loss of pressurized facility unit (m)
HWC	Hazen-Williams coefficient of pipe material (dimensionless)
ID	Inside diameter of pipe (m)
L	Pipe length (m)
MC	Manning coefficient (dimensionless)
$NPSH_A$	Available net positive suction head (m; absolute pressure)
$NPSH_R$	Required net positive suction head (m; absolute pressure)
P	Water pressure (kPa, gage; $kPa = kN/m^2$)
P_s	Static pressure head at surface of intake water for pump (m; absolute)
PS	Particulate solids held by media (kg, dry weight)
PS_{max}	Maximum particulate solids held by media (kg, dry weight)
P_w	Vapor pressure of water at temperature and salinity (mm Hg)
PW	Power consumption rate of a water pump motor (kW)
Q	Water flow rate through facility unit (m^3/day)
Q_{max}	Maximum water flowrate capacity (m^3/day)
TDH	Total dynamic head at water pump (m; equivalent to HA)

Table 5.7. Continued

Symbol	Definition
U	Water velocity (m/s)
U_{ef}	Velocity enhancement factor (≥ 1.0 ; dimensionless)
V_{fu}	Facility unit volume (m^3)
VV	Void volume of packing media (%)
V_w	Facility unit water volume (m^3)
WP	Water flow wetted perimeter (m)
Z	Water elevation (m)
γ	Specific weight of water (kN/m^3 , kPa/m)
θ	Mean hydraulic retention time (day)

Maximum water flow rates for facility units may be based on U, HLR, or θ . For pipe flow, a reasonable water velocity is about 3.0 m/s generally and 1.0 m/s for pump inlets (Mott, 1979). Water hammer (especially when $U > 1.5$ m/s), pressure drop, and pump power use increase with decreasing pipe diameter, and thus a tradeoff exists between construction and operation costs. For fish rearing units, desired ranges in water velocity can be based on fish swimming speed or so that particulate solids do not settle. Rearing unit water flow rates are often specified in terms of water exchange rate ($1/\theta$). For water treatment units, HLR values ($m^3/m^2\text{-hr}$) are typically used to limit water flowrates. Example minimum-maximum HLR values are 1.5 – 3.5 for solid settling basins (Chen et al., 1994), 100 – 250 for packed column aerators (Grace and Piedrahita, 1994; Hackney, 1981), 30 – 250 for trickling biofilters (Wheaton et al., 1994), and 15 – 50 for upflow sand filters and 80 – 250 for fluidized bed filters (Malone and Burden, 1988).

The water volume of a flooded facility unit is based on internal dimensions, minus the volume of any freeboard, internal media, settled solids, and fish biomass (approximately 1.0 L/kg), where the latter two are typically negligible. The water displacement of media is based on the portion of the total volume occupied by media and the void volume of the media. Void volumes are typically 85 – 95% depending on media size. The water volume of an open cascade is approximated as a flooded facility unit. The water velocity of a flooded facility unit is a function of its water flow rate and cross-sectional flow area, the latter depending on water flow pattern (i.e., longitudinal, lateral, circular, or torroidal). For longitudinal and lateral flow, the cross-sectional flow area is the cross-sectional plane perpendicular to the flow, minus any area occluded by media. Circular and torroidal flow patterns can be induced in circular tanks, rectangular tanks with rounded ends, and lateral flow

units, by the force and direction of the influent water stream and aeration techniques. Under these conditions, water velocity is calculated using a given velocity enhancement factor (U_{ef}). U_{ef} values can also be used for longitudinal flow when flow baffles are used to move settled solids. U , HLR, and θ of a flooded facility unit are related by:

$$HLR = Q (\text{day}/24 \text{ hr}) / CSA$$

$$U = Q U_{ef} (\text{day}/86400 \text{ s}) / CSA$$

$$\theta = V_w / Q$$

For a non-flooded facility unit, such as packed column aerators and trickling biofilters, some portion of the total volume in addition to the freeboard volume is occupied by air. Thus, determination of V_w , U (vertical, downward flow), and θ for a given flow rate is more complex. Reported methods calculate θ values for packed columns as a function of column height, hydraulic loading, water properties, and media characteristics and fouling level (Hackney, 1981). However, required parameters for other than a few specialized media types are lacking in the literature. Thus, θ values are simply based on a given, constant water velocity for fully wetted, non-flooded media. Velocity values for various media types and HLR levels are only sparsely reported in the literature, but a value of about 0.18 m/s appears to be reasonable (Grace and Piedrahita, 1994). HLR, Q , θ , and V_w of a non-flooded facility unit are calculated by:

$$HLR = Q (\text{day}/24 \text{ hr}) / CSA$$

$$Q = U (86400 \text{ s/day}) CSA VV / 100$$

$$\theta = H / [U (86400 \text{ s/day})]$$

$$V_w = Q \theta$$

5.5.2 Gravity flow for cascades, basins, and channels

Maximum gravity flow rates are not calculated for open-water cascades (e.g. aeration cascades) and water basins. For cascades, it is assumed that any given flow is possible. For basins, it is assumed that the available freeboard is adequate to provide the internal hydraulic gradient required for a given flow rate. Maximum gravity flow rates for open and closed (with respect to atmosphere) channels are based on hydraulic slope (< 0.0 required), cross sectional dimensions, and materials (Manning equation; Jensen, 1983). Manning coefficients range from 0.025 for rough

surfaces (e.g. soil) to 0.010 for smooth surfaces (e.g. plastic) (Table 5.8). Weighted mean coefficients based on surface areas are used when the channel sides and bottom are different materials. Maximum water flow rate is inversely proportional to the Manning coefficient and is calculated by:

$$Q_{\max} = (2446.85 \text{ m}^3/\text{day} / \text{ft}^3/\text{s}) 1.49 \text{ CSA } (10.76 \text{ ft}^2/\text{m}^2) \\ [\text{CSA } (3.281 \text{ ft/m}) / \text{WP}]^{0.667} (-\text{HG})^{0.50} / \text{MC}$$

5.5.3 Airlift water pumps

Airlift pumps provide a simple method to move water at low elevation heads (Spotte, 1979; Castro and Zielinski, 1980; Loyless and Malone, 1998). Maximum water flow rates for airlift pumps are based on given specifications, assuming that the optimum air-water flowrate ratio (G/L; lpm/lpm; range 1 – 30) with respect to pumping rate is used. A general expression for calculating optimum G/L values is not available (tabular and graphical approaches are used in the listed references), and a given, constant G/L value (default 3.0) is used to determine required air supply rates (Q_{air} ; m^3/day) as a function of water flow rate. The air flow supplied to the pump is used to calculate pump power consumption, using the adiabatic air compression formula and including the required air-release pressure and static water head of the pump diffuser or sparger, friction losses in the air supply plumbing, and the efficiency of the air pump and motor. Facility units up and down stream of an airlift pump must be non-pressurized. Q_{\max} is calculated by (Spotte, 1979):

$$AL_{\text{TL}} = AL_{\text{D}} + AL_{\text{L}}$$

$$AL_{\text{SR}} = AL_{\text{D}} / AL_{\text{L}}$$

$$Q_{\max} = [(0.758 AL_{\text{SR}}^{3/2} AL_{\text{TL}}^{1/3}) + 0.01196] AL_{\text{ID}}^{2.2} (1440 \text{ min/day}) (\text{m}^3 / 1000 \text{ L})$$

$$Q_{\text{air}} = Q \text{ G/L}$$

5.5.4 Pressurized flow and pump systems

Pressurized flow is used for pressurized pipes and vessels (e.g., mechanical filters) supplied by water pumps. Water flow rates of a pressurized flow stream can be limited by the constraints described earlier as well as the capacities of water pumps. Pump power requirements are based on the given facility unit configuration, elevations and hydraulic gradients, dimensions and materials,

Table 5.8. Hazen-Williams and Manning coefficients¹

Pipe material and condition	Hazen-Williams coefficient (fouled – new)	Manning coefficient for closed conduit (new - fouled)	Manning coefficient for open channel (new - fouled)
Glass, polyvinyl chloride (PVC), HD polyethylene (PE), ABS, rubber, fiberglass, and resins (epoxy, polyester, acrylic)	100 – 140	0.008 – 0.012	0.010 – 0.014
Steel, aluminum, welded	80 – 120	0.010 – 0.014	0.012 – 0.016
Concrete	60 – 100	0.012 – 0.016	0.014 – 0.018
Corrugated metal	40 – 80	0.018 – 0.022	0.020 – 0.030
Earth			0.025 – 0.040

¹ Values represent approximate averages of reported ranges for clean and fouled conditions (Hammer, 1977; Grant, 1981; Huguenin and Colt, 1989)

and water pump efficiency. Simulations are performed for each pressurized flow stream in a facility. Each flow stream consists of at least one water pump and discharge pipe plus one or more, up and down stream, pipes or pressurized facility units in serial and/or parallel configurations. For parallel water flow configurations, where two or more branches diverge from and re-converge to a common flow stream, water mechanics are not modeled by rigorous, iterative methods such as the Hardy Cross technique (Mott, 1979). As described in Chapter 3 (Facility hydraulics), flow control devices (e.g. valves) used to allocate flow rates to parallel branches are assumed to exist. By principles of water mechanics, head losses in each of the parallel branches are equal, and water flow rates at the divergent and convergent junctions are equal. Thus, the branch with the highest head loss is used as the head loss between the junctions and the head loss of parallel branches are assumed to be equalized by flow control valves.

5.5.5 Energy balance

For water flow in pressurized systems, where the available volume is completely filled by water (non compressible fluid) and flow rate is constant, an energy balance is used to model the pressurized flow path from its influent (point 1) to effluent (point 2) locations (Mott, 1979):

$$P_1/\gamma + U_1^2/2g + Z_1 + HA - HL_t = P_2/\gamma + U_2^2/2g + Z_2$$

$$HA = (P_2/\gamma - P_1/\gamma) + (U_1^2/2g - U_2^2/2g) + (Z_2 - Z_1) + HL_t$$

Energy terms (expressed as water head, m) include pressure energy (P/γ ; all pressures are expressed as gage pressures), kinetic energy ($U^2/2g$), potential energy (Z), total energy losses (HL_t ; head loss), and energy added by pumps (HA ; head added). For use in AquaFarm, this energy balance is simplified by assuming that kinetic head terms are equivalent or are zero. Pressure head terms can be similarly ignored or P_1 and/or P_2 can be set to given values when point 1 and/or point 2 is not at atmospheric pressure (zero gage pressure). These simplifications result in:

$$HA = (P_2/\gamma - P_1/\gamma) + (Z_2 - Z_1) + HL_t$$

or
$$HA = (Z_2 - Z_1) + HL_t$$

and
$$HL_t = HL_p + HL_{fp} + HL_m$$

where Z_2 (elevation of the water discharge) minus Z_1 (elevation of the water surface of the water body containing the pump intake) is the net elevation difference between the effluent and influent of the pressurized flow stream. HA is the total dynamic head (TDH) that must be supplied by a pump for the specified system and given water flow rate.

5.5.6 Friction energy losses

Total energy losses due to flow friction (HL_t) consist of losses for (1) straight sections of pipe, (2) pressurized facility units, with or without internal media, and (3) pipe fittings associated with pipes and pressurized facility units. For calculating head losses in pipes (HL_p), the simpler Hazen-Williams method (Hammer, 1977) is used rather than the more rigorous Darcy-Weisbach method (Mott, 1978). Head losses, and associated pump power requirements, are proportional to water velocity squared, for a given length of pipe of consistent material and inside diameter, and are inversely proportional to the Hazen-Williams coefficient (Table 5.8). This approach is also used for pressurized facility units other than pipes, but water-wall friction in these units is likely negligible compared to that of fittings and internal media. The Hazen-Williams method is:

$$HL_p = 1.279e-7 \{ [Q (1000 \text{ L/m}^3) (\text{day}/1440 \text{ min}) L^{0.54}] / (\pi \text{ HWC ID}^{2.63}) \}^{1.85}$$

Biological fouling of pipes may be considerable, especially in seawater systems, and may significantly increase head losses in pipes. If needed, low or high biofouling conditions can be designated for a facility unit. For low biofouling conditions, friction losses for clean pipe are multiplied by a factor 1.3, and for high biofouling conditions, this factor is 2.0. In practice,

biofouling is controlled by duplicated, independent, pump suction and discharge lines. These lines are alternately cycled to create anoxic conditions to kill fouling organisms in the inactive line.

Minor losses for pipe fittings associated with pipes and pressurized facility units include (1) change in flow direction (e.g., bends, elbows, T's, and Y's), (2) change in cross-sectional flow area (sudden and gradual reducers and expanders), (3) entrance losses (reservoir to pipe) and exit losses (pipe to reservoir), and (4) obstructions (e.g., valves, screens, flow meters, and specialized units such UV water sterilizers). Rigorous modeling of these losses would require specification of all fittings, including internal dimensions and friction coefficients, where losses are proportional to water velocity squared. This level of detail is not supported by AquaFarm, and fitting losses are calculated as a given proportion (HL_{fp} ; value can be specified for each facility unit; default 10%) of the associated pipe/vessel wall friction loss by:

$$HL_f = HL_p HL_{fp} / 100.0$$

For head losses in pressurized facility units containing internal media and accumulated particulate solids (e.g., mechanical filters), head loss values are normally available from the filter manufacturer for clean and maximum solid loading conditions (HL_{ml} and HL_{mc}). These values can be specified in terms of water head (m) or pressure (kPa), where the latter is converted at point of use by the water specific weight (γ). Media is periodically cleaned of solids as a function of the specified solids loading set-point with respect to PS_{max} (%; ≤ 100 ; see Chapter 3). The ratio PS / PS_{max} is equivalent to the fraction of the service cycle completed, and HL_{ml} minus HL_{mc} is equivalent to the allowable increase in pressure loss per service cycle. Head loss of media and accumulated solids is calculated by:

$$HL_m = HL_{mc} + (HL_{ml} - HL_{mc}) PS / PS_{max}$$

5.5.7 Water pumping

The required net positive suction head ($NPSH_R$; m, absolute pressure) for a water pump inlet is a pump specification. In practice, $NPSH_R$ is used as a design and management criterion to limit pump cavitation and pump wear and to maintain the rated pump efficiency (Mott, 1979; Jensen, 1983). The available net positive suction head ($NPSH_A$; m, absolute pressure) at the pump inlet is calculated using the general energy balance model, where point 1 is at the surface of the water body

supplying the pump suction line and point 2 is at the pump inlet. The condition that must be satisfied is $NPSH_A \geq NPSH_R$. $NPSH_A$ is calculated by:

$$NPSH_A = P_s + (Z_2 - Z_1) - HL_p - HL_f - P_w / [\gamma (7.5006 \text{ mm Hg/kPa})]$$

where $P_s = BP / [\gamma (7.5006 \text{ mm Hg/kPa})]$

P_s is at the surface of the pump intake water, normally the local barometric pressure. HL_p and HL_f are the head loss in the suction pipe and fittings, and P_w is calculated at the existing water temperature and salinity. $NPSH_R$ and intake head losses are not considered for submerged pumps.

Pumps may be installed as single units or in parallel arrays of similar or different pumps (see Chapter 3). Centrifugal water pumps are normally used in aquaculture, but the methods used here are not specific to a particular pump type. Pumps may be submerged or out of water, where for the latter the pump suction may be flooded or the pump elevated above its source water. Pump specifications used in AquaFarm are minimum and maximum flow rate (L/min), maximum head (m), $NPSH_r$, and power efficiency (%). Rigorously, pump flow-head curves should be used in conjunction with system flow-head curves to find the operating point of the pump at the intersection of the curves. In addition, pump power efficiency should be calculated as a function of flow rate (Jensen, 1983). However, the simplifications are used that the pump can achieve the existing flowrate and TDH of the system and that power efficiency is a constant value. The rationale for these simplifications is based on the objectives stated earlier, i.e. to generate energy requirements and operation conditions for water pumping that can be used for selecting specific water pumps

Power consumption rate of a water pump (PW; kW) is a function of the water flow rate, total dynamic head (TDH; m), and rated efficiency of the pump (Mott, 1979; Jensen, 1983):

$$PW = [\gamma Q (\text{day}/86400 \text{ s}) TDH] / [(e_p/100.0) (e_m/100.0)]$$

or $PW = [\gamma Q (\text{day}/86400 \text{ s}) TDH] / (e / 100.0)$

5.6 Water budgets

Water is a major resource requirement of all larger aquaculture systems, while its availability and associated costs are highly site specific. Discharge water from aquaculture facilities is also important, mainly with respect to environmental impacts. To support analyses addressing these concerns, water budgets are maintained for individual facility units, and by their combination, total water consumption and discharge rates are maintained for whole facilities. Facility unit water budgets are used (1) to manage influent flow rates, as required to maintain water depths (water makeup) or overflow rates (water exchange), and (2) to quantify water resource requirements. In addition, water transfer rates and volume changes of a facility unit are used in heat and mass transfer calculations.

5.6.1 Water budget model

Facility unit water budgets (water mass balances) include terms for influent and effluent flow rates (Q_i and Q_e), net seepage infiltration and loss (Q_s), precipitation and watershed runoff (Q_p and Q_r), and evaporation (Q_{evp}). Water seepage may be a source of water when local water tables are high relative to pond elevations, but seepage is typically a water loss. Water lost by splashing and leaks is not considered. For flow-through systems, Q_i and Q_e dominate water budgets for both individual facility units and the whole system. For recirculating systems, especially when heated, Q_{evp} may represent a considerable water loss for the whole system, while Q_i and Q_e dominate water budgets for individual facility units. For housed systems, Q_s , Q_p , and Q_r can be ignored, and Q_{evp} is typically reduced considerably unless air humidity is controlled. In contrast, for static water exposed to the environment, Q_i is limited to that required to replace water losses and Q_s , Q_p , Q_r , and/or Q_{evp} can be major water budget terms.

Given the dominance of water advection for flowing water aquaculture systems, water budgets are of limited interest. For static water aquaculture, however, a number of research efforts have developed water budgets for various pond systems and climatic regimes (e.g., Boyd, 1982b; Teichert-Coddington et al., 1988; Green and Boyd, 1995b; Nath, 1996; Nath and Bolte, 1998). Accurate prediction of precipitation, evaporation, and seepage are required to ensure accurate water budgets.

For calculating change in water volume per time (dV/dt ; m^3/day), expression of a generic water budget in terms of a differential equation gives:

$$dV/dt = Q_i - Q_e + Q_p + Q_r - Q_{evp} \pm Q_s$$

The unknown term of this equation depends on the water management strategy used. In general, two conditions exist: (1) for flowing water systems, dV/dt is zero, Q_i is supplied continuously to maintain desired through-flow rates, and Q_e represents the continuous over flow rate of the facility unit, or (2) for static water systems, dV/dt varies, Q_i is supplied periodically to maintain minimum water volumes, and Q_e is normally zero except when precipitation and runoff exceed water losses for a sufficient period. For the first condition, Q_e is calculated given Q_i . For the second condition, dV/dt and Q_i or Q_e are calculated using various arrangements of the water budget equation. When water is to be added because a minimum management depth has been reached, dV/dt is equivalent to the volume at the desired depth minus the volume at the current depth, divided by the period over which water is to be added. In AquaFarm, this period is initially set to the simulation step size and then the calculated Q_i is limited depending on available water supply rates. Based on these two, typical scenarios, typical forms of the water budget equation used for flowing and static water bodies, respectively, are

flowing: $Q_e = Q_i + Q_p + Q_r - Q_{evp} \pm Q_s$

where $dV/dt = 0$, and $Q_e \cong Q_i$ for high exchange rates

static: $Q_i = dV/dt - Q_p - Q_r + Q_{evp} \pm Q_s$

where $Q_e = 0$

5.6.2 Precipitation and evaporation

Precipitation can be approximated using given seasonal mean values or values can be specified in a climate data file. For direct input of precipitation to the water surface, climate values ($Q_{p,mm}$; mm/day) are converted to water budget terms (Q_p ; m^3/day) based on the air-water surface area (SA_{aw} ; m^2). Watershed runoff (Q_r ; m^3/day) is estimated by (U.S. Soil Conservation Service, 1972; Yoo and Boyd, 1994; Nath, 1996):

$$Q_p = Q_{p,mm} SA_{aw} \text{ (m/1000 mm)}$$

$$Q_r = WA \{[(Q_{p,mm} - 0.2 MWR)^2 / (Q_{p,mm} + 0.8 MWR)] / 1000\}$$

where $MWR = 25.4 (1000/CN - 10)$

and MWR = maximum watershed retention (mm/day), CN = curve number (dimensionless), and WA = effective watershed area around a pond (m^2). CN is based on soil type(s), land use, and hydrologic conditions (U.S. Soil Conservation Service, 1972; Yoo and Boyd, 1994). For example, a CN of 85 was used by Nath (1996), corresponding to the hydrologic soil group D and the pasture soil use type. WA values are also highly site specific, and Q_r varies directly with WA .

Calculation of evaporation was described earlier in this chapter under Heat transfer (Q_{evp} ; m^3 /day; $Q_{evp,mm}$; mm/day). Alternatively, values can be specified in the climate data file (empirical pan evaporation rates). Specified water seepage values ($Q_{s,mm}$; mm/day) are converted to water budget terms (Q_s ; m^3 /day) based on the air-water surface area (SA_{aw} ; m^2):

$$Q_s = Q_{s,mm} SA_{aw} \text{ (m/1000 mm)}$$

5.7 Gas transfer

Passive and active mass transfer of gases by diffusion across gas-liquid interfaces is found in all types of aquaculture systems. Gas transfer is often limiting to fish production and is an area of considerable management concern and resource consumption. Gases considered here include dissolved oxygen (O_2 ; DO), nitrogen and argon (N_2+Ar ; DN), carbon dioxide (CO_2 ; DC), ammonia (NH_3), hydrogen sulfide (H_2S), chlorine (Cl_2), and ozone (O_3). Gas diffusion may be passive (natural, open surface) or active (enhanced transfer for gas addition and removal). Primary concerns in aquaculture are (1) the addition of DO (fish metabolic substrate), (2) the removal of DN (supersaturated source waters), DC (fish metabolite), NH_3 (fish metabolite), H_2S (source water contaminant), and Cl_2 (source water contaminant), and (3) addition and removal of O_3 (water disinfection). DO levels are a potential concern in most types of systems, while DC levels are mainly a concern in intensive systems using pure oxygen absorption units. In intensive aquaculture systems, DO saturation levels of $\leq 50\%$ and DC saturation levels of $\geq 2000\%$ are not uncommon.

5.7.1 Gas transfer model

The theoretical basis of gas transfer consists of four steps, consisting of molecular diffusion through the gas and liquid bulk phases and across the gas and liquid films at the gas-liquid interface (Montgomery, 1985; Tchobanoglous and Burton, 1991). For conditions found in aquaculture systems, the bulk phases are assumed to be well mixed and the transfer model reduces to the common two-film model. The thickness of either the gas or liquid boundary layer and the molecular diffusivity of the gas in this layer controls the rate of gas transfer between the bulk phases. For high solubility gases, the gas film transfer represents the rate limiting step, and transfer is increased by stirring of the gas bulk phase and reduction of the gas film thickness. For low solubility gases, diffusion across the liquid film is the rate limiting step, and transfer is increased by stirring of the water bulk phase and reduction of the liquid film thickness. Based on a ranking of Henry's constants (Montgomery, 1985), the ranking of solubilities from highest to lowest is $\text{NH}_3 > \text{CO}_2 > \text{H}_2\text{S} > \text{Cl}_2 > \text{O}_3 > \text{O}_2 > \text{N}_2$. Given that CO_2 diffusion is reported to be liquid film controlled (Stumm and Morgan, 1981), all gases are considered liquid film controlled except NH_3 .

Gas transfer rate (dC/dt ; $\text{g/m}^3\text{-day}$) is proportional to the difference between the existing and equilibrium concentrations of the gas in solution, which expressed as a differential equation is:

$$dm/dt = K_L A (C_s - C)$$

$$dC/dt = K_L (A/V) (C_s - C)$$

$$dC/dt = K_L a (C_s - C)$$

Integration between the limits C_0 and C_t and 0 and t , yields:

$$C_t = C_s - [e^{(-K_L a \cdot t)} (C_s - C_0)]$$

$$K_L a = \ln [(C_s - C_t) / (C_s - C_0)] / t$$

The second equation, derived from the first, is used to determine gas transfer coefficients from empirical, operational data (e.g., aerator tests). Regardless of the additional gas sources and sinks that are usually added to these mass balance equations, modeling applications of diffusive gas transfer require the calculation of values for gas equilibrium concentrations (C_s) and overall mass transfer coefficients ($K_L a$). The latter exercise is a primary objective of this section, along with methods used to model gas transfer and resource requirements of active gas transfer. Method variables are listed in Table 5.9.

Table 5.9. Method variables for gas transfer

Symbol	Definition
A	Gas-liquid interface area of control volume (m^2)
AE	Field corrected aerator efficiency (kg O ₂ /kWhr)
C	Gas concentration (mg/L)
C ₂₀	Air equilibrium DO for test conditions (freshwater, 20 C, 9.08 g/m ³)
CDOD	Change in dissolved oxygen deficit across the aerator (%)
C ₀	Gas concentration at time zero (g/m ³)
C _s	Gas concentration at equilibrium (g/m ³)
C _t	Gas concentration at time t (g/m ³)
D	Water depth (m)
G/L	Gas-liquid, volumetric flow rate ratio (dimensionless)
H	Elevation drop (m)
K _L	Gas diffusion coefficient (m/day)
K _L a	Overall gas transfer coefficient (1/day)
K _{O2-STD}	Standard, passive oxygen transfer coefficient (1/day; 1.0 m water depth, clean water, 20 °C)
M _{air}	Mass air flow rate (kg/hr)
OTE	Field corrected oxygen transfer efficiency (%; used for diffusers)
OTR	Field corrected oxygen transfer rate (kg O ₂ /hr)
POAE	Pure oxygen absorption efficiency (%): 100 x O ₂ transferred / O ₂ used
POTE	Pure oxygen transfer efficiency (kg O ₂ /kWhr): O ₂ transferred / energy used, not including power requirements for O ₂ generation
PW _a	Air power supply rate to aerator (kWhr/day)
PW _t	Total power supply rate to aerator (kWhr/day)
PW _w	Water power supply rate to aerator (kWhr/day)
Q	Water flow rate (m ³ /day)
SAE	Standard aerator efficiency (kg O ₂ /kWhr): mass oxygen transferred per energy consumed by aerator
SOTE	Standard oxygen transfer efficiency (%; used for diffusers)
SOTR	Standard oxygen transfer rate (kg O ₂ /hr)
t	Time (day)
T	Water temperature (C)
T	Water temperature (C)
U	Water velocity (m/s)
V	Facility unit water volume or volume of control volume (m ³)
V _{air}	Volumetric air flow rate (m ³ /hr)
WS	Wind speed (m/s)
α	Gas transfer rate scaling coefficient for waste water (dimensionless)
β	Gas equilibrium concentration scaling coefficient for waste water (dimensionless)
θ	Temperature correction coefficient
ρ _{air}	Mass density of wet air (kg/m ³)
σ	Water specific weight (kn/m ³)

The modeling procedure for gas diffusion is: (1) determine equilibrium concentrations for all participating gases (C_s), (2) determine passive and active gas diffusion coefficients for oxygen (K_{O_2} ; $K_L a$ for O_2 ; 1/day), and (3) determine gas diffusion coefficients for gases other than oxygen by use of gas diffusivity ratios. Over the course of a simulation, at each simulation step, equilibrium concentrations and passive and active transfer coefficients for a given gas (i) and facility unit are calculated. Total transfer coefficients ($K_{i, \text{total}}$) are additive, assuming parallel transfer (Thibodeaux, 1979) of passive ($K_{i, \text{passive}}$) and active ($K_{i, \text{active}}$) diffusion, where $K_{i, \text{total}} = K_{i, \text{passive}} + K_{i, \text{active}}$. The parameters θ , α , and β are applied uniformly to all gases for passive and active aeration and are assigned constant values (explained later).

Gas transfer coefficients and rates are used in gas mass balances and to calculate power, compressed air, and oxygen requirements of gas exchangers. For passive gas transfer, predicted water temperatures, water velocities, and wind speeds are most critical. For active transfer of air and pure-oxygen contact units, method validity is largely dependent on given specifications. Similar to other managed processes, required mass transfer rates are based on specified set points (DO, DN, DC % sat.) and other process control variables (see Chapter 3, Process management). Peak and total mass and energy requirements (power, oxygen, and air flow) are maintained during simulations for use in facility resource budgets and user review.

A variety of conditions may exist regarding equilibrium gas concentrations. If a facility unit is closed with respect to gas transfer (e.g., pressurized filters), then the gas phase (if any) is assumed to be at equilibrium with the liquid phase and gas transfer is not considered. If a facility unit is open to the atmosphere (e.g., ponds), then equilibrium gas concentrations are based on air partial pressures for N_2+Ar , O_2 , and CO_2 (see Chapter 4, Dissolved gases). If a facility unit is closed to the atmosphere and supplied with pumped air (e.g. packed column aerators), then partial pressures in the gas phase may deviate from air values. This normally reduces gas transfer rates, as gases either accumulate or are depleted in the gas phase. However, a simplifying assumption is made that gas partial pressures are equivalent to air values and that given specifications account for this assumption. In all cases, gas phase partial pressures of NH_3 , H_2S , CL_2 , and O_3 are considered to be zero. For pure oxygen contact systems, the gas phase is assumed to be pure O_2 .

5.7.2 Passive gas transfer

Oxygen diffusion coefficients (K_{O_2} ; 1/day) are a function of water depth, water velocity, wind speed, precipitation (not considered here), water temperature, and presence of dissolved and particulate constituents (α ; dimensionless). α is a waste water correction factor, typically applied to active aeration, and has a value of 1.0 for clean water. Reported methods for calculating K_{O_2} are intended for flowing waters (streams) or relatively static waters (lakes). With respect to aquaculture, these application conditions are represented by facility units such as raceways and ponds, respectively. The simplest method is to use a given, standard K_{O_2} ($K_{O_2}\text{-STD}$; e.g. 0.7/day) where:

$$K_{O_2} = K_{O_2\text{-STD}} \theta^{(T-20)} \alpha / D$$

A number of reported methods are available for flowing water (Rathbun, 1977), which mainly differ in their parameters rather than functional form. These methods give a wide range of predicted K_{O_2} values for a particular set of conditions. Using the basic functional form reported in Rathbun (1977) and adding the α term, the method for horizontal flowing water is:

$$K_{O_2} = a U^b D^{-c} \theta^{(T-20)} \alpha$$

where a = scaling coefficient (6.49, 4.20 – 12.29), b = velocity exponent (0.78, 0.5 – 1.0), and c = depth exponent (1.47, 0.85 – 1.85). The values shown for parameters a , b , and c (mean and ranges) are mean values for nine studies reported in Rathbun (1977). Lacking a better alternative, these parameter means are used as default values in AquaFarm. A default value of 1.024 is used for θ , as commonly used for both passive aeration (Rathbun, 1977) and active aeration (Tchobanoglous and Burton, 1991). However, reported values of θ vary from 1.015 to 1.040, apparently due to variable test conditions (Tchobanoglous and Burton, 1991). Using this method, for $T = 20^\circ\text{C}$ and $\alpha = 1.0$, resulting K_{O_2} values are 0.0, 0.18, 1.08, and 6.49 per day, at U values of 0.0, 0.01, 0.1, and 1.0 m/s, respectively.

For passive gas transfer in relatively static waters, Boyd and Teichert-Coddington (1992; BTC method) provide a method developed for fish ponds (1000 m² area), where for wind speeds ≤ 1.0 m/s and 1.0 – 4.5 m/s, respectively:

$$K_{O_2} = 0.008 \theta^{(T-20)} \alpha \text{ 24 hr/day} / D$$

$$K_{O_2} = (0.017 \text{ WS} - 0.014) \theta^{(T-20)} \alpha \text{ 24 hr/day} / D$$

For wind speeds exceeding 4.5 m/s, K_{O_2} is limited to 1.5/day. An alternative method intended for larger water bodies and higher wind speeds is provided by Banks and Herrera (1977; BH method), where for wind speeds of 2 - 20 m/s:

$$K_{O_2} = 1.0e-6 (8.43 WS^{0.5} - 3.67 WS + 0.43 WS^2) \theta^{(T-20)} \alpha (86400 \text{ s/day}) / D$$

The precipitation term available in the BH method is not used, given the poor accuracy of predicting specific precipitation events and a preference for conservative estimates for K_{O_2} . The $\theta^{(T-20)}$ term was added to the BH method and the α term was added to both methods. At 20 °C and $\alpha = 1.0$, the two methods agree at $WS = 2.2$ m/s, where K_{O_2} is 0.56/day. At $WS < 2.2$ m/s, the BH method gives higher values, and at $WS > 2.2$ m/s, the BTC method gives higher values. Both of these methods are available in AquaFarm, but the BTC method is likely best due to its specific development for smaller water bodies such as fish ponds. For large ponds (>10 ha), the BH method may be best. Switching between methods based on their wind speed ranges creates a significant discontinuity in K_{O_2} values and is not used. Overall, the maximum of the calculated values based on water velocity and wind speed is used, and a minimum K_{O_2} of 0.1/day is used in all cases.

5.7.3 Active gas transfer by air-water contactors

Active gas transfer utilizes increased mixing of the liquid bulk phase, reduced liquid film thickness, increased interfacial surface area per unit volume, and/or increased gas phase partial pressures and concentration gradients. Air-water contactors available in AquaFarm include a variety of aerators and gas strippers (Colt and Tchobanoglous, 1979; Boyd and Watten, 1989; Colt and Orwicz, 1991a; Watten, 1994). Active aeration can be performed in any type of facility unit, as a primary or secondary process. Facility units that are not primarily intended for active gas transfer may act as air-water contactors, including water flow over weirs, pipe discharges, airlift pumps, foam fractionators, and trickling biofilters. Aerators meant to add oxygen will remove oxygen when oxygen is super saturated, and aeration efficiencies decrease considerably at $DO > 90\%$. As evident in the equations below, field corrected transfer efficiencies approach zero as DO levels approach 100% saturation. Poor management practices such as these are prevented through the use of appropriate process control variables.

Operational variables for air-water contactors are based on given specifications (SAE, SOTR, SOTE, and CDOD; Tables 5.10 and 5.11). These specifications are available from manufacturers

Table 5.10. Reported standard aerator efficiencies (SAE, kg O₂/kWhr; means and ranges)^a

Aerator Type ^b	SAE (kg O ₂ /kWhr) ^c
Subsurface Aerators	
Air diffuser: fine bubble	1.6 (1.2 – 2.0)
Air diffuser: medium bubble	1.3 (1.0 – 1.6)
Air diffuser: coarse bubble	0.9 (0.6 – 1.2)
Various aquaculture diffusers, depth 1.0 – 1.2 m	< 1.0
Airlift pump	2.0 – 2.1, 1 – 4
Foam fractionators	
Static tube systems (air lift pumps with internal deflection plates or turbine impellers)	2.1 (1.2 – 1.6, 1.8 – 2.4, 2.0 – 3.0)
Gravity Aerators	
Weirs, inclined falls, and vertical arrays of perforated flow obstructions (water head loss)	1.5 (1.2 – 1.8, 0.6 – 2.4)
Cascade weir (45°)	1.5 – 1.8
Corrugated incline plane (20°)	1.0 – 1.9
Horizontal screens	1.2 – 2.6
Lattice aerator	1.8 – 2.6
Packed column aerator, vertical column with media and blown air (water head loss and air pumping)	1.8 (1.2 – 2.4)
Trickling biofilters	1.2 – 2.6
U-tube aerator (water head loss and air pumping)	0.72 – 2.3
U-tube aerator (water head loss, venturi aerator)	2.0 – 3.3
Surface Aerators	
Pipe discharge fittings and nozzles (e.g. jet exhauster with venturi air intake)	1.9 (1.2 – 2.6)
Propeller aspirator pump (uses venturi to aspirate air into water)	1.42 (1.16 – 1.58, 1.7 – 1.9)
Vertical pump (water propelled into air, low velocity)	1.15 (0.61 – 1.58)
Pump sprayer (water propelled into air, high velocity)	1.15 (0.79 – 1.70)
Paddle wheel: all types	1.95 (1.0 – 2.9)
Paddle wheel: Auburn University design	2.25 (2.12 – 2.33)
Paddle wheel: “Taiwanese” style	1.17
Paddle wheel: “Japanese” style	1.03
Water destratifiers	in terms of m ³ /kWhr (see text)

^a Listed values compiled from Colt and Tchobanoglous (1979), Hackney (1981), Boyd and Watten, (1989), Colt and Orwicz (1991a), Loyless and Malone (1998), Auburn University (p.c.)

^b See references for descriptions of aerator types and additional performance data

^c lb/hp-hr = 1.6440 kg/kWhr

Table 5.11. Reported CDOD values for gravity and surface aerators (20 °C) ^a

Aerator Type ^b	CDOD (%)
Gravity Aerators	
Simple weir (30 cm height)	7 - 10
Cascade (25°, 24 cm height)	22 - 26
Cascade (45°, 50 cm height)	36 - 38
Splash board (30 cm height)	23 - 25
Splash board (60 cm height)	36 - 41
Corrugated inclined plane (20°, 30 cm height)	18 - 29
Corrugated inclined plane (20°, 60 cm height)	30 - 50
Lattice aerator (30 cm height)	29 - 37
Lattice aerator (60 cm height)	48 - 61
PCA (30 cm height)	94 - 96
PCA (60 cm height)	96 - 98
Horizontal perforated trays (110 cm height)	95 - 100
Surface Aerators – Pipe Discharge Fittings	
Straight pipe	25
Screen cover	52
Slotted cap	65
Tee aspirator (3.8 cm)	72
Half-open gate valve	76
Ell aspirator (3.8 cm)	83

^a Listed values compiled from Chesness and Stephens (1971), Moore and Boyd (1984), Colt and Orwicz (1991a)

^b See references for descriptions of aerator types and additional performance data

and/or are reported in the literature for standard conditions (initial DO 0.0 mg/L, tap water, $\alpha = 1$, $\beta = 1$, temperature 20 °C, BP 760 mm Hg). Calculation of these functional specifications from more fundamental design variables is complex and not considered in AquaFarm. Rather, Tables 5.10 and 5.11 are available to assist users in specifying air-water contactors during facility construction.

For air-water contact units, standard specifications (SAE, SOTR, and SOTE) are corrected to field conditions by (Colt and Tchobanoglous, 1979, Tchobanoglous and Burton, 1991; Boyd and Watten, 1989; Colt and Orwicz, 1991a; Watten, 1994):

$$AE = SAE (\beta C_s - C) \theta^{T-20} \alpha / C_{20}$$

$$OTR = SOTR (\beta C_s - C) \theta^{T-20} \alpha / C_{20}$$

and $OTE = SOTE (\beta C_s - C) \theta^{T-20} \alpha / C_{20}$

The fundamental relationship inherent in these methods is the ratio equality:

$$\text{standard rate or efficiency} / (C_s - 0.0) = \text{corrected rate or efficiency} / (C_s - C)$$

If water salinity is greater than zero, then both C_s and C_{20} values must be based on that salinity.

Barometric pressure is assumed to approximate 760 mm Hg for the aerator test conditions and the current local value is accounted for in C_{20} and C_s values. Additional, related functions include:

$$AE = \text{OTR (24 hr/day)} / PW_t$$

$$\text{or } PW_t = \text{OTR (24 hr/day)} / AE$$

$$\text{or } \text{OTR} = PW_t AE / (24 \text{ hr/day})$$

$$\text{and } PW_t = PW_w + PW_a$$

$$\text{SOTR} = K_{O_2, 20} C_{20} V \text{ (kg/1000g) (day/24 hr)}$$

$$\text{SOTE} = 100 \text{ (air-to-water oxygen transfer rate / oxygen supply rate in pumped air)}$$

Active aeration can be used at a constant rate, on a demand basis, or continuously. For air-water contactors such as pipe discharge fittings, gravity aerators, and packed column aerators, existing water flow rates are utilized, specified G/L ratios (if used) are automatically maintained, and oxygen transfer rates are not directly controlled. For these aerators, the modeling procedure at each simulation step is: (1) correct SAE to field conditions, (2) determine available PW_t , and (3) determine existing OTR based on the relationship between SAE and PW_t . Alternatively, gravity aerators and pipe discharge fittings may be modeled using CDOD values (described later). The other possible types of air-water contactors can be controlled by their energy input rate. For these aerators, the modeling procedure at each simulation step is: (1) correct SAE to field conditions, (2) determine required OTR based on process control variables (see Chapter 3, Process management), and (3) determine required PW_t based on the relationship between SAE and OTR. For all types of aerators, following step (3), additional tasks are (4) express oxygen transfer rates as equivalent K_{O_2} values and (5) determine diffusion coefficients for other gases using gas diffusivity ratios.

5.7.3.1 α and β coefficients

By the methods here, α and β coefficients are applied uniformly to all passive and active gas transfer calculations, using constant, given values. The α coefficient is the ratio of the oxygen transfer coefficient for water containing dissolved and particulate compounds relative to clean water (K_{O_2} wastewater / K_{O_2} tap water). Impurities in the water, especially surface-active materials such as dissolved organic compounds, tend to decrease gas transfer rates. Typical values of α for municipal waste water are 0.82 and 0.98 for BOD₅ levels of 180 and 3 mg/L, respectively (Tchobanoglous and Burton, 1991). For aquaculture pond water, Shelton and Boyd (1983) reported α values ranging from 0.66 to 1.07, with a mean of 0.94, but could find no relationship between α and water quality variables. As a result, no attempt is made to calculate α , and α values are specified along with other aerator variables (default $\alpha = 0.94$).

The α coefficient can also be used to account for impacts of water salinity. For surface aerators, Boyd and Daniels (1987) showed that OTR values were not significantly affected by salinities up to 40 ppt. However, for diffused aeration, Boyd and Watten (1989) report that OTR values increased to a maximum at 15 ppt and then declined, as salinity was increased from 0 to 40 ppt. This relationship is apparently due to the impact of salinity on surface tension and bubble size, where K_{O_2} is maximized at intermediate bubble sizes (Boyd and Watten, 1989).

The β coefficient is the ratio of C_s of wastewater to C_s of tap water, with a typical range of 0.9–1.0 and design value of 0.95 (Tchobanoglous and Burton, 1991). Given its use as a scalar for C_s , which is a function of salinity, it is used to account for reduced DO equilibrium concentrations for waters with considerable dissolved solids that are not expressed as salinity. For aquaculture pond waters, Shelton and Boyd (1983) reported values ranging from 0.92 to 1.0, with a mean of 0.98, but could find no relationship between β and water quality variables. As a result, no attempt is made to calculate β , and values are specified along with other aerator variables (default value = 0.98). When salinity is > 0.0 ppt, β is set to 1.0, where it is assumed that salinity adequately accounts for total dissolved solids. β is applied to equilibrium DO values for both passive and active aeration. β is not applied to other gases.

5.7.3.2 Subsurface aerators

Air diffusers release air bubbles below the water surface, providing air-water interfacial area (number and size of bubbles) and the air-water contact time (bubble release depth and ascension velocity) for gas transfer (Table 5.10; Colt and Tchobanoglous, 1979, Tchobanoglous and Burton, 1991; Boyd and Watten, 1989). Compared to surface aerators, diffused aeration is likely to be less energy efficient but is often preferred for multiple points of application that can be supplied by a single air pump. Air pressures required to supply diffusers are normally low (e.g. < 2.0 m water), and regenerative, centrifugal air blowers are often used for larger applications (e.g. > 100 L/min air flow rate). A variety of diffusers are commercially available, including air stones, porous tubing, and slit tubing, classified by bubble size (e.g. coarse, medium, and fine) and required air-release pressure. Airlift pumps and foam fractionators also act as air diffusers, for which air is released by a diffuser or sparger at the base of a vertical tube.

Energy components included in reported SAE values for diffusers are often not clearly stated. It is assumed that SAE values include all energy components, including the diffuser air-release pressure, static water head over the diffuser, friction losses in the air supply plumbing, and the efficiency of the air pump. Impacts of diffuser fouling (often significant) can be accounted for in given SAE values. Based on this approach, calculated diffuser AE values represent energy consumption rates of air pumping.

For aquaculture applications of diffused aeration, submergence depths are typically ≤ 2.0 m and OTE values typically range well below 10%. For example, at a depth of 1.5 m, reported OTE values range from 2.0% (diffuser type not given; Mavinic and Bewtra, 1976) to 6.0% (medium pore silica glass diffusers; AES, 1999). Reported OTE values for wastewater treatment applications are typically for water depths of 3 – 8 m and are not directly applicable to aquaculture, e.g., fine bubble (10 - 30+ %), medium bubble (6 – 15%), and coarse bubble (4 – 8%) (e.g. Tchobanoglous and Burton, 1991).

As diffuser depth is increased, AE is reported to remain relatively constant, as increases in gas transfer are offset by increases in applied power (Mavinic and Bewtra, 1976). Thus, in the AE equation, it is assumed that both C_S and C_{20} are based on the application depth. In contrast, OTE increases with diffuser depth, and thus the SOTE test depth is used for the C_{20} value while the application depth is used for the C_S value. The diffuser application depth is assumed to equal the

water depth of the facility unit. If SOTE is available and SAE is not, then power use is based on air flow rate and the adiabatic compression formula.

In addition to energy use, required air flow rates (M_{air} ; m^3/hr) are needed for specifying air pumps, air delivery systems, and required numbers of diffusers (e.g., air stones) or lengths of diffusers (e.g., porous tubing). Airflow rates are calculated by different methods, depending on available specifications. If SOTE is available, then airflow is calculated by:

$$M_{\text{air}} = \text{OTR} / [(0.23 \text{ kg O}_2/\text{kg air}) * \text{OTE} / 100]$$

$$V_{\text{air}} = M_{\text{air}} / \rho_{\text{air}}$$

where air is 23% oxygen on a mass basis and OTR is calculated by simulation. Alternatively, if AE is available and OTE is not, then the adiabatic compression formula is rearranged to calculate M_{air} based on applied energy and V_{air} is then calculated as above. In using the adiabatic compression formula, the outlet pressure is the sum of the diffuser air release pressure (e.g. 0.5 psi), the static water head over the diffuser (e.g. 1.5 psi at 40 in water depth), and friction losses in the air supply plumbing (e.g. 0.5 – 3.0 psi).

5.7.3.3 Gravity Aerators

Gravity aerators include cascades, packed column aerators, and U-tube aerators (Tables 5.10 and 5.11). Cascade and packed column aerators utilize head loss to create water turbulence, splashing, and air entrainment, and media may be used to increase air-water interface area (Boyd and Watten, 1989; Watten, 1994). For packed column and U-tube aerators, air pumping requirements are determined by given G/L ratios and other variables in the adiabatic air compression formula. U-tube aerators utilize a temporary hydrostatic head to increase the concentration gradient of oxygen transfer (Speece, 1969; Speece, 1970). For U-tube aerators, some water head loss is incurred, entrained air is added by pumping or venturis, recommended G/L ratios are ≤ 0.20 to avoid discharge surging, and energy use includes water head losses and air pumping.

Cascade type gravity aerators include weirs, inclined cascades, and vertical arrays of perforated flow obstructions. The water is open to the atmosphere, air pumps are not used, and energy use is limited to water head loss (PW_w). Packed column aerators (PCA) consist of enclosed, vertical, columns with packing media. Columns are supplied with counter-current air flow at given

G/L ratios, usually ≥ 3 (Hackney, 1981; Hackney and Colt, 1982). Energy use includes water head loss (PW_w) and air pumping (PW_a).

All types of gravity aerators typically utilize available water head (e.g., $\leq 1.5\text{m}$) and flow rate at some point in the system. Correspondingly, water flow control to achieve a desired aeration level is not considered, process control is not used, and OTR is a product of AE and PW_t . PW_w is calculated by:

$$PW_w = Q (\text{day}/86400 \text{ s}) H \sigma (24 \text{ hr/day})$$

PW_a is calculated using the adiabatic compression formula, including the air pressure drop across the column, friction losses in the air supply plumbing, and the efficiency of the air pump. Air pressure drops through columns depend on hydraulic loading rates and media size and are typically low (e.g. $0.1 - 0.4 \text{ kPa}$). Thus, air pumping power requirements are generally a minor component (e.g. $\leq 5\%$) of total energy use (Hackney, 1981). SAE values for gravity aerators (Table 5.10) are assumed to include water head loss in the aerator but not energy losses in the water supply. SAE values include the energy consumption of air pumping if pumped air is used.

As an alternative to the SAE approach, a gravity aerator can be specified by a CDOD value (Table 5.11; Boyd and Watten, 1989; Watten, 1994), where DO_0 is the influent DO (time 0) and DO_t is the effluent DO (time t). This method is provided due to the availability of reported CDOD values for gravity and pipe-discharge aerators and the simplification that PW_w does not have to be calculated. CDOD is defined and applied by:

$$CDOD = 100.0 (DO_t - DO_0) / (DO_{sat} - DO_0)$$

$$DO_t = DO_0 + CDOD (DO_{sat} - DO_0) / 100.0$$

$$K_{O_2} = \ln [(DO_{sat} - DO_t) / (DO_{sat} - DO_0)] / t$$

5.7.3.4 Surface aerators

Surface aerators are maintained at the water surface (by floatation or support) and increase air-water surface area by spraying or splashing water into the air. Surface aerators include discharge fittings, propeller aspirators, vertical pumps, pump sprayers, and horizontal paddle wheels (Tables 5.10 and 5.11; Boyd and Watten, 1989). Surface aerators other than discharge fittings are powered

by electrical motors, gasoline or diesel engines, or tractor power takeoffs (PTO). SAE values for these aerators are assumed to represent the power consumption rate of the motor that drives the aerator, as opposed to the brake power applied to the aerator shaft.

Pipe discharge fittings include various terminal devices that utilize water pressure, velocity, and elevation head loss to create a water spray or air entrainment (Boyd and Watten, 1989). The energy consumption of discharge fitting consists of water head loss only. Similar to simple gravity aerators, existing water head is utilized, process control is not used, OTR is a product of AE and P_{tw} , given SAE values should only consider energy losses across the aerator, and CDOD values may be used instead of SAE values.

Surface aerators may be used for water mixing for vertically stratified pond waters. Mixing of a stratified water column can have a significant impact on effective AE values, as oxygen depleted water at the bottom of the water column is exchanged with higher oxygen water at the surface. Capacities for mixing are not necessarily correlated to capacities for aeration, however, and SAE performance tests are not performed in stratified waters. To support the simulation of active destratification, effective water mixing rates ($m^3/kWhr$) may be specified for surface aerators and specifically designed water destratifiers in conjunction with other aerator variables. For example, mixing and rates of 305, 1778, and $3235 m^3/kWhr$, for vertical pumps, propeller aspirators, and paddle wheels, respectively, have been reported (Boyd and Watten, 1989).

Surface aerators typically act as point sources of oxygen. Fish are known to congregate around aerators when DO levels near the aerator exceed the mean DO of the whole pond and mean DO falls below fish tolerance levels. Thus, aeration levels that are not adequate on a whole pond basis may be adequate to maintain fish under practical conditions. However, with respect to modeling and the prediction of aeration requirements, complete horizontal mixing is assumed. Therefore, in order to simulate these conditions, the DO set-point level must be reduced to the adequate whole-pond mean DO. In addition, since fish respond to the mean DO with respect to fish performance modeling, it may also be necessary to reduce the low DO tolerance level for fish. Without these corrections, predicted aeration requirements will likely exceed those used under practical conditions.

5.7.4 Diffusion coefficients for air-water contactors

Active gas transfer of air-water contactors is modeled as a diffusion process across a concentration gradient, as used for passive gas transfer. Combining equations for AE and dC/dt , the oxygen transfer coefficient is calculated by:

$$K_{O_2} = PW_t \text{ SAE } (\beta C_s - C) \theta^{T-20} \alpha (1000 \text{ g/kg}) / [C_{20} (\beta C_s - C) V]$$

or
$$K_{O_2} = PW_t \text{ SAE } \theta^{T-20} \alpha (1000 \text{ g/kg}) / (C_{20} V)$$

As volume (V) is increased, the impact of a given aeration effort on K_{O_2} is decreased. As aeration power use (PW_t) is increased, K_{O_2} is increased.

5.7.5 Diffusivity transformations

Based on calculated K_{O_2} values, diffusion transfer coefficients for other gases (K_i) are calculated from K_{O_2} using a multiplicative factor. This factor can be based on ratios of gas molecule diameters, molecular weights, or diffusivity values, where the latter approach is used here (Thibodeaux, 1979). Since O_2 is a liquid film controlled gas, diffusivity transformations are used for other liquid film controlled gases (i.e., not NH_3). The diffusion transfer coefficient for a gas i (K_i) is calculated using a diffusivity factor for gas i relative to O_2 (DF_i ; Table 5.12):

$$K_i = K_{O_2} DF_i$$

where
$$DF_i = D_i / D_{O_2}$$

5.7.6 Diffusion of gases participating in acid-base equilibria

Gas absorption (transfer from gas to water phase) is increased for gases participating in chemical reactions in the liquid film layer (i.e. CO_2 , NH_3 , H_2S , CL_2 , and O_3) (Montgomery, 1985; Stumm and Morgan, 1981). For the purposes of AquaFarm, the only reactive gas for which absorption is considered is CO_2 , where gas phase partial pressures of the other reactive gases are always zero (if used, O_3 is added directly). A typical example in aquaculture is CO_2 absorption in solar algae ponds. Absorbed CO_2 reacts with H_2O (hydration) and/or OH^- (hydroxylation) and is

Table 5.12. Diffusivity factors for gas i relative to O₂ (DF_i)

Gas i	Thibodeaux (1979) ^a	Colt and Bouck (1984) ^b	Grace and Piedrahita (1994) ^c	AquaFarm ^d
CO ₂	0.98 = 1.77 / 1.80	1.0	DF _i = 1.96 ± 1% / 2.5 ± 20% DF _i = 0.78 (0.65 – 0.99) DF _i value used = 1.0	1.0
N ₂	0.91 = 1.64 / 1.80	0.85	NR	0.85
NH ₃	0.98 = 1.76 / 1.80	NR ^e	NR	not used
Cl ₂	0.68 = 1.22 / 1.80	NR	NR	0.68
H ₂ S	0.78 = 1.41 / 1.80	NR	NR	0.78
O ₃	NR ^e	NR	NR	1.0

^a Calculated DF_i values using diffusivity values (cm²/s x 10e5 at 20 °C) relative to O₂ (1.80)

^b DF_i values used for packed column aerators

^c Diffusivity and DF_i values (1/atm x 10e5) used for packed column aerators

^d Constants used in AquaFarm

^e Not reported

thereby transformed to HCO₃⁻, by ionization of H₂CO₃ or directly. As a result, CO₂ is depleted in the liquid film layer and CO₂ diffusion is enhanced. The magnitude of this chemical enhancement depends on the relative rates of simultaneous diffusion and reaction kinetics. Since the hydration and hydroxylation rate of CO₂ (K_{RCO2}) is relatively slow, enhancement of CO₂ diffusion is relatively low compared to a highly reactive gas such as Cl₂. However, enhancement of CO₂ diffusion may still be considerable. The chemical enhancement factor (CEF; ≥ 1.0; dimensionless) is defined as the actual transfer rate divided by the transfer rate without reaction. Applying CEF and ionization fraction (α₀; 0-1; see Chapter 4), where the unionized gas fraction is the driving force of diffusion, yields:

$$d\text{CO}_2\text{-C}/dt = \text{CEF } K_{\text{CO}_2} [(\alpha_{0s} \text{ DIC}_s) - (\alpha_0 \text{ DIC})]$$

$$d\text{CO}_2\text{-C}/dt = \text{CEF } K_{\text{CO}_2} (\text{CO}_2\text{-C}_s - \text{CO}_2\text{-C})$$

where α_{0s} is at the equilibrium pH, CO₂-C_s is a function of air CO₂, CEF and α₀ are a function of pH, and pH is a function of DIC. Rigorous methods for determination of CEF values are complex,

requiring finite-element division of the liquid film into multiple layers and numerical solution procedures at small time steps (e.g. 0.02 s; Emerson, 1975). This approach is not suitable for purposes here and a method intended for industrial conditions (Danckwerts, 1970) is used:

$$dCO_2-C/dt = K_{CO_2} [CO_2-C_s - (CO_2-C / \cosh (M^{0.5}))] (M^{0.5} / \tanh (M^{0.5}))$$

$$M = D_{CO_2} K_{RCO_2} \theta^{(T-20)} / (K_{CO_2} (V/A) (\text{day}/86400 \text{ s}))^2$$

$$K_{RCO_2} = [0.03/\text{s} + (8500 \text{ L}/(\text{mol s}) [\text{OH}])]$$

where $\cosh x$ (hyperbolic cosine of x) = $[\exp(x) + \exp(-x)] / 2$

and $\tanh x$ (hyperbolic tangent of x) = $[\exp(x) - \exp(-x)] / [\exp(x) + \exp(-x)]$

and D_{CO_2} = molecular diffusivity of CO_2 in water ($1.77 \times 10^{-9} \text{ m}^2/\text{s}$; Table 5.12), K_{RCO_2} = hydration/hydroxylation reaction rate coefficient (1/s), and $[\text{OH}]$ is expressed as mol/L. K_{RCO_2} is calculated by a method given in Grace and Piedrahita (1994), which yields values comparable to reported values (e.g., 0.025 – 0.04/s at 25 C; Stumm and Morgan, 1981). In the development and testing of this method, it was found that a simplification of the Danckwerts equation, as used by Montgomery (1985), provided essentially equivalent results for absorption and allowed the Danckwerts equation to be uniformly applied to both CO_2 absorption and desorption:

$$dCO_2-C/dt = K_{CO_2} (CO_2-C_s - CO_2-C) [M^{0.5} / \tanh (M^{0.5})]$$

$$CEF = [M^{0.5} / \tanh (M^{0.5})]$$

For example, at a pH of 8.5, CEF values are 4.4, 1.9, and 1.2 at K_{CO_2} values of 0.2, 0.5, and 1.0/day, respectively, showing that CEF is maximized when diffusion rates are low. As a function of pH, CEF is decreased at lower pH levels and increased at higher pH levels. Emerson (1975) calculated very high CEF values (up to 21) for a particular lake, but these values are apparently specific to the extreme study conditions (low alkalinity, pH 10, and relatively stagnant liquid film at $600 \pm 400 \text{ um}$). In agreement, application of the Danckwerts method to the conditions of Emerson (1975), using a K_{CO_2} of 0.165/day, gives an equivalent CEF of 21. As K_{CO_2} declines relative to K_{RCO_2} , CEF for CO_2 increases, but overall transfer decreases (Emerson, 1975). The upper limit to CEF is the value corresponding to that where the CO_2 concentration gradient is represented as total carbonates.

For desorption (from water to gas phase) of reactive gases, chemical enhancement to diffusive transfer occurs due to the generation of the gas in the liquid layer, again depending on the relative rates of simultaneous diffusion and reaction kinetics. CEF values for H_2S , Cl_2 , and O_3 are based on given, constant values (default value 1.0, no effect). CO_2 desorption is modeled by more rigorous methods (below). CO_2 levels in intensive aquaculture systems may exceed equilibrium levels by 20 fold or more. For active degassing of CO_2 , high G/L ratios (e.g. ≥ 3.0) are required to carry off the transferred CO_2 in the gas phase and maintain adequate desorption rates (Grace and Piedrahita, 1994). Paddle wheel and packed column aerators (with blown air) are most likely to provide required G/L ratios, and other types of gas exchangers do not generally represent effective CO_2 management tools (Grace and Piedrahita, 1994). However, CO_2 transfer rates of devices other than packed column aerators are not well documented in the literature.

As with CO_2 absorption, fully rigorous methods for CO_2 desorption require finite-element division of the reactor (e.g., PCA) into multiple layers and numerical solution procedures at small time-steps (e.g., Grace and Piedrahita, 1994). The simplified approach of the Danckwerts method is used here. K_{RCO_2} is the CO_2 dehydration and dehydroxylation reaction rate coefficient (e.g., 10 – 20/s at 25 °C; Stumm and Morgan, 1981). These reactions are relatively fast compared to hydration and hydroxylation and result in correspondingly higher CEF values. A function for calculating K_{RCO_2} has not yet been developed for purposes here, and a constant K_{RCO_2} value of 15/s (20 °C) with respect to pH is used. For example, application of this method gives CEF values declining from 70.4 to 1.6, as K_{CO_2} values are increased from 0.2 to 10.0. This behavior was shown by Grace and Piedrahita (1994) for packed column aerators, where CEF values close to 1.0 were found for these high-rate gas exchangers. As with absorption, it is assumed that the upper limit to CEF is the value corresponding to that where CO_2 is represented as DIC.

5.7.7 Ammonia desorption

Ammonia desorption is a gas film controlled process and operates according to different conditions than liquid film controlled gases. Due to the high solubility of ammonia, high G/L ratios are required for significant ammonia desorption to occur. Supporting this argument, Ver and Chiu (1988) reported that use of paddlewheel aerators significantly impacted DO and DC dynamics in

fish ponds but ammonia dynamics were unchanged. For flow through aquaculture systems, ammonia desorption is generally considered insignificant (e.g., Burrows and Combs, 1968). However, there is a lack of rigorous studies regarding ammonia desorption in aquaculture systems, and ammonia desorption is highly dependent on pH, wind speed, and G/L ratios.

NH₃ diffusion is estimated independently of other gases, where K_{NH_3} (1/day) is estimated by the method of Folkman and Wachs (1972):

$$d\text{TAN}/dt = K_{\text{NH}_3} [(\alpha_{1s} \text{TAN}_s) - (\alpha_1 \text{TAN})]$$

$$d\text{TAN}/dt = K_{\text{NH}_3} (\text{NH}_3\text{-N}_s - \text{NH}_3\text{-N})$$

$$d\text{TAN}/dt = -K_{\text{NH}_3} \text{NH}_3\text{-N}$$

$$\text{where } K_{\text{NH}_3} = 0.14 \{1.0 + [0.41 \text{ WS (km/1000 m) (3600 s/hr)}]\} (24 \text{ hr/day}) \theta^{(T-20)} \\ / (D \text{ 100 cm/m})$$

The equilibrium (saturation) ammonia concentration ($\text{NH}_3\text{-N}_s$) is zero and α_1 is a function of pH. For example, at $\text{WS} = 3.0 \text{ m/s}$, $T = 20^\circ\text{C}$, and $D = 1.0 \text{ m}$, the calculated K_{NH_3} is 0.18/day. This formulation shows why reported ammonia desorption rates for aquaculture system are low, given typically low values for TAN ($\leq 2.0 \text{ mg TAN/L}$), α_1 (≤ 0.2), and K_{NH_3} ($\leq 0.2/\text{day}$). Impacts of active aeration on K_{NH_3} are ignored, due to insufficient support in the literature. Depending on the type of aeration method, the resulting under estimation of ammonia desorption may be insignificant or provide a small safety factor for predicted ammonia concentrations.

5.7.8 Active gas transfer – pure oxygen contact systems

Pure oxygen contact systems (oxygenators) include a variety of mechanical devices, variably employing pressurized contact systems, multiple stage transfer, and off-gas recycling (Colt and Watten, 1988; Watten et al., 1991; Watten, 1994). Oxygen may be supplied from high pressure cylinders, liquid oxygen tanks, or generated on site. For purposes here, oxygenators are modeled as a zero-order, chemical addition process, rather than as a gas diffusion process. Given specifications include pure oxygen absorption efficiency (POAE; %) and pure oxygen transfer efficiency (POTE; $\text{kg O}_2/\text{kWhr}$) (Table 5.13). POAE and POTE values are used as specified, rather than as standard values corrected to field conditions. Any significant impact of influent DN levels on POAE and POTE values must be included in the given values. Removal (stripping) rates of nitrogen (e.g., 10 –

50%) and carbon dioxide (e.g., 1 – 10%) are additional oxygenator specifications. In practice, these stripping rates depend on G/L ratios, off-gas recycling, and other design variables. For water pumps used with high-pressure contactors, pump energy consumption must be included in the POTE value.

Table 5.13. Reported pure-oxygen absorption efficiencies (POAE, %), pure-oxygen transfer efficiencies (POTE, kg O₂/kWhr), and potential DN stripping capabilities for pure oxygen systems (Watten, 1994)

System	POAE (%)	POTE (kg O ₂ /kWhr)	Potential DN stripping capacity
U-tube	30 – 50	1.0 – 1.5	fair
U-tube with off-gas recycling	60 – 90	2.0 – 3.0	poor
Down flow bubble contactor	80 – 90	3.9	fair
Packed column	40 – 80	0.5 – 2.0	good
Pressurized packed column	95 – 100	1.0	poor
Spray tower	40 – 55	0.5 – 1.0	good
Multi-stage low head oxygenation	30 – 95	2.0 – 5.5	fair
Side stream injection	15 – 70	< 0.5	poor
Enclosed surface agitation	30 – 70	0.3 – 1.0	fair

5.8 Sedimentation, filtration, and fractionation of particulate solids

Particulate solids considered in AquaFarm include (1) suspended (non-settleable) inorganic solids (clay turbidity) and (2) settleable inorganic and organic solids from added compounds, fish feeds, fish fecal material, and dead phytoplankton (see Chapter 2, Facility unit state variables). Processes that may be used to remove particulate solids include sedimentation, mechanical filtration, and fractionation. Particulate solids in aquaculture systems range from $\leq 10 \mu\text{m}$ to $\geq 1000 \mu\text{m}$ in size, and alternative solid removal processes are characterized by particle size ranges for which they are best suited. Listed in order of the capacity to remove solids, from larger to smaller particle sizes ($> 100 \mu\text{m}$ to $< 30 \mu\text{m}$), solid removal techniques typically employed in aquaculture include: coarse screens, sedimentation, tube/plate sedimentation, microscreens, granular media, porous media, and foam fractionators (Chen et al., 1994). The solid removal methods described below are used to calculate terms used in solid mass balance equations and to quantify the accumulation of filtered and settled solids and production of solid wastes.

5.8.1 Solid sedimentation

Settleable, particulate solids, typically $> 100\mu\text{m}$ in size (Chen et al., 1994), are removed from the water column and accumulate on benthic surfaces due to gravity sedimentation. Solid sedimentation may be intended and therefore enhanced by design (e.g., sedimentation basins for solids removal) or unwanted and therefore minimized by design (e.g., self-cleaning fish rearing units). While relatively simple in design and operation, two main disadvantages of sedimentation for intended solids removal are low hydraulic loading rates and low removal efficiencies of smaller particles ($\leq 100\mu\text{m}$). In aquaculture systems, sedimentation is mainly used to treat facility effluents, when prolonged water retention times are acceptable.

If flow baffles or dual-drain effluent configurations are used for continuous, hydraulic removal of settled solids (Timmons et al., 1998), then settled solids are routed to the designated effluent port and do not accumulate on benthic surfaces. Otherwise, accumulated settled solids are removed by periodic events, as specified by the maximum allowed solids accumulation and other management variables (see Chapter 3, Process management). When media is present in the water column, solid sedimentation is enhanced by interception and diffusion (Chen et al., 1994). This may be intended (e.g., parallel tube/plate clarifiers,) or undesired (e.g., biological filters). This enhancement to sedimentation is accounted for by given solid filtration efficiencies.

Rigorous quantification of solids sedimentation, whether intended or not, requires consideration of (1) distributions of particle sizes, particle densities, and settling velocities, (2) particle interaction (e.g., flocculation), (3) water velocity profiles within a facility unit, (4) particle retention time, and (5) particle re-suspension by scouring and fish activity (James, 1984b; Tchobanoglous and Schroeder, 1985; Chen et al., 1994). A rigorous, mechanistic modeling approach to solid sedimentation is further complicated by variable particle characteristics, which are impacted by system hydraulics and shear forces. In addition, detailed specifications are required for facility unit hydraulics, which typically cannot be represented by ideal flow patterns.

A simplified approach to solids sedimentation is used here, where solid removal rate by sedimentation (dC/dt ; $\text{g/m}^3\text{-day}$) is:

$$dC/dt = C (\text{fraction removed}) (\text{exchange rate, } 1/\text{day})$$

$$dC/dt = C (\text{MSV} / \text{HLR}) (Q / V)$$

$$dC/dt = C (\text{MSV} / D)$$

where C = solid concentration (g/m^3 , dry weight), MSV = particle mean settling velocity (m/day), D = water depth (m), HLR = hydraulic loading rate ($\text{m}^3/\text{m}^2\text{-day}$), Q = water flow rate (m^3/day), and V = water volume (m^3). This derivation represents solid sedimentation in terms of first-order, exponential decay kinetics, a simplification that has been used by others (e.g., Fritz et al., 1979; Fritz, 1985; James, 1984; Piedrahita, 1989). The sedimentation term represents one term in the differential equation for C , with additional sources and sinks added as needed. If the water body is stratified, then solids settle from the top layer to the bottom layer and from the bottom layer to the bottom surface of the facility unit. Any upward vertical mixing of solids is considered by the use of reduced settling velocities.

A weighted-mean particle settling velocity is calculated according to the contributing solid sources. Two major pools of solids are considered, consisting of (1) solids originating from dead phytoplankton and (2) all other sources (fish fecal material, fertilizers, and inert solids). Settling velocities for solids of phytoplankton origin are about an order of magnitude smaller than solids of fish origin due to their smaller size and density. Typical particle settling velocities and default velocities used in AquaFarm are given in Table 5.14. These settling velocities are applied to all of the settleable, particulate solids present in the water column, and thus settling velocities at the lower end of reported ranges are used.

Two cases are used with respect to mean particle settling velocities: (1) facility units specifically designed and intended for solids sedimentation and (2) all other facility units. The latter case is used to account for reduced solid sedimentation rates in facility units stocked with fish, using aeration, exposed to wind, and other impacts on internal water velocities or perturbation of the benthic zone. For example, for static, earthen fish ponds stocked with carp or tilapia, Avnimelech et al. (1999) reported that sediment resuspension accounted for 60-90% of the total solids settling flux (e.g., $1000 \text{ g}/\text{m}^2/\text{day}$). In this study, sediment resuspension was due to fish foraging behavior, rather than wind induced water currents, and increased with mean fish weight and biomass density. In the approach used here, the resuspension of sediments is considered by use of reduced particle settling velocities. For example, for sediment resuspension amounts ranging from 50 to 90% of the total solids settling flux, settling velocities are reduced by factors ranging from 0.5 to 0.1. For sediment resuspension due to advective water currents, settling velocities are set to zero if the water velocity exceeds the given settled-solid scouring velocity (cm/s). Reported scouring velocities for settled solids of fish origin range widely, from 2 to 40 cm/s (Chen et al., 1994). The default value used here is 25 cm/s .

Table 5.14. Reported settling rates (1/day) and velocities (m/day) for particulate solids

Reported values
Solids of fish origin in basins designed for sedimentation: 20 to 120 m/day for 65 to 90% of the total particulate solids present (Chesness et al., 1975; Chen et al., 1994)
Solids of bacteria and phytoplankton origin in wastewater stabilization ponds: 0.05/day (first-order constant; Fritz et al., 1979; Fritz, 1985)
Solids of detrital origin in natural water bodies: 0.2 m/day (Chen and Orlob, 1975)
Solids of phytoplankton origin in natural water bodies: 0.05 - 0.2 m/day (Chen and Orlob, 1975)
Default settling velocities used in AquaFarm
Fish origin, intended settling: 50 m/day
Fish origin, unintended settling: 5 m/day
Phytoplankton origin, intended settling: 1 m/day
Phytoplankton origin, unintended settling: 0.2 - 0.3 m/day

5.8.2 Solid filtration and fractionation

For intensive applications such as the treatment of recirculated water, mechanical filtration and fractionation techniques are typically used for solids removal. Common mechanical filters include microscreen filters (typically self cleaning and gravity flow), granular media filters (pressurized sand and bead filters), and porous media filters (pressurized diatomaceous earth and cartridge filters). Fractionation techniques for particulate solids include foam fractionation and centrifugal particle separation (hydroclones or swirl separators).

These solid removal processes are mechanistically complex and dependent on a host of design variables (Tchobanoglous and Schroeder, 1985; Chen et al., 1994; Timmons, 1994). For the purposes here, mechanical filtration and fractionation rates of particulate solids are based on given solid removal efficiencies (percent removal per water pass through filter). Solid filtration efficiencies are also assigned to facility units that are not primarily intended as solid filters (e.g., chemical and biological filters) and to account for particle interception and diffusion (e.g., parallel tube or plate clarifiers). These solid removal efficiencies are available in the literature (e.g., Chen et al., 1994) and from filter manufacturers.

Accumulated solids are periodically removed from filters according to specified holding capacities and other management variables. The impact of accumulated solids on water head losses through filters is considered. Airflow rate requirements of foam fractionators are based on specified gas-liquid flow rate ratios (G/L). Energy requirements of air pumping are calculated using the adiabatic air compression formula, including the required air-release pressure and static water head,

friction losses in the air supply plumbing, and the efficiency of the air pump and motor (similar to airlift pumps). Facility units up and down stream of foam fractionators and centrifugal separators are normally non-pressurized.

5.9 Chemical filtration and reactions rates

Chemical filtration is occasionally used in aquaculture systems to remove selected compounds by adsorption. Two chemical filtration processes considered by AquaFarm are (1) removal of ammonium (NH_4^+) by ion-exchange using clinoptilolite (zeolite) and (2) removal of chlorine by granular activated carbon (GAC) (Liao and Lin, 1981; Tchobanoglous and Schroeder, 1985). Filtration rates are based on given compound removal efficiencies (% per pass). Filter media is periodically regenerated according to the compound holding capacity of the media (90% of maximum used) and accumulation of particulate solids. Removal of ammonium by clinoptilolite is less efficient in seawater systems due to the presence of competing sodium ions (Na^+). Some hydrogen, calcium, and magnesium ions are also removed by clinoptilolite but impacts on pH and hardness are considered negligible. For both types of chemical filtration, either particulate solid levels must be low or pre-filtration of solids is required to prevent clogging of media. Compound filtration rates are used in mass balances and to quantify the accumulation of filtered compounds and media regeneration requirements. Calculations include:

$$\text{TCC} = \text{SCC} \text{ BD } V_m$$

and
$$\text{TC}_t = \text{TC}_0 + \text{FR } V \text{ (kg/1000 g) } t$$

where
$$\text{FR} = C \text{ (RE/100) } Q / V$$

where TCC = compound capacity of a given volume of media (kg), SCC = specific compound capacity per unit media (kg compound / kg media), BD = bulk density of media (kg media/m^3), V_m = volume of media (m^3), FR = filtration rate ($\text{g cmpd/ m}^3\text{-day}$), C = influent compound concentration (g/m^3), RE = removal efficiency (%/pass), Q = influent water flow rate (m^3/day), V = water volume (m^3), and TC_0 and TC_t are the quantities of compound held in the media (kg) at the beginning and end of a simulation time-step of length t (days).

Most chemical transformations in facility units are biologically mediated and are described in other chapters. In addition, user defined treatment chemicals (e.g., chlorine and ozone) may undergo

first-order decay at specified rates (%/day). Chemical equilibria reactions that may occur in facility units are described in Chapter 4. Acid-base reactions are considered instantaneous, except in regards to carbon dioxide transfer. Rates of calcium carbonate dissolution and precipitation are related to water quality in complex ways (Stumm and Morgan, 1981). In the approach used here, these rates are based on (1) calculated, total amounts that will dissolve or precipitate if the solution goes to equilibrium ($\text{g CaCO}_3/\text{L}$) and (2) a specified rate of dissolution and precipitation (%/day; e.g., 5%/day) relative to calculated, total amounts. If calcium carbonate is added for alkalinity or pH adjustment, then the required amount is assumed to dissolve instantaneously at its given purity and solubility levels. Water sources and facility units may have infinite calcium carbonate phases (i.e. calcium carbonate soil).

5.10 Compound addition

A variety of compounds can be added to static or flowing water for water conditioning and treatment. Compounds considered include (1) inorganic and organic fertilizers, (2) pH and alkalinity adjustment compounds, and (3) pure oxygen, sea salt, and various user-defined fish/egg treatment, water conditioning, and water disinfection compounds. Compound addition rates are based on given set-point concentrations and other process control variables (see Chapter 3, Process management). Compounds may be in gas, liquid, or solid forms and compound (1) purity (%) or molarity (mol/L) and (2) solubility (%; solids only) are specified. Compound addition rates are used in their respective mass balances and to calculate required compound quantities for resource budgets.

Fertilizers can include mixed inorganic and/or organic compounds and their addition can be based on DIC, DIN, or DIP set points. Fertilizer composition is user specified, as percent dry weights of various compounds, including inorganic urea nitrogen (urea-N), inorganic ammonia nitrogen ($\text{NH}_4\text{-N}$), inorganic nitrate nitrogen ($\text{NO}_3\text{-N}$), inorganic phosphorous ($\text{PO}_4\text{-P}$), and organic solids (dry weight), the latter with specified nitrogen and phosphorous contents. Given percent dry weights are summed ($\leq 100\%$) and any remaining material is considered to be inert. For inorganic fertilizers, active, soluble ingredients are assumed to become fully available when the fertilizer is applied. For organic fertilizers, O_2 is consumed and N, P, and CO_2 are released, as the fertilizer degrades over time. The organic carbon content of added particulate solids (dry weight; e.g., animal manures) is assumed equal to that of phytoplankton.

pH and alkalinity adjustment compounds include carbon dioxide, nitric, sulfuric, and phosphoric acid, sodium hydroxide, sodium bicarbonate and carbonate, agricultural limestone, and hydrated and burnt lime (see Chapter 4). Water disinfection compounds include chlorination-dechlorination (e.g., 2.0 mg Cl_2/L and dechlorination by 7.4 mg sodium thiosulfate per mg Cl_2), ozone (e.g., added to achieve 0.5 mg/L), ultra violet light (e.g., applied at $0.75 \text{ W/m}^3\text{-day}$), or any user defined compound. User defined compounds can be assigned first-order decay coefficients but are otherwise considered to be non-reactive and non-volatile.

6. Methods of Aquatic Biology

Methods of aquatic biology used in AquaFarm concern processes of pond soils, various types of bacteria, and unicellular algae (phytoplankton). Mass transfer rates of these processes are applied to the mass balance differential equations used to model facility units. The methods described below are based in the aquaculture literature, and method derivations and additional developments are included. Overall, an integrated analytical framework is constructed for the application of aquatic biology to the simulation of aquaculture systems.

6.1 Environmental scalars

The temperature dependence of biological rate constants, as well as physical (e.g. gas diffusion) and chemical (e.g. acid-base equilibria) processes, can be expressed by the Van't Hoff-Arrhenius Rate Law (Tchobanoglous and Schroeder, 1987):

$$K_T = A e^{[-E/(R T_K)]}$$

where K_T = rate constant (1/day) at temperature T_K (°K), A = coefficient (1/day), E = activation energy (J/mol), and R = universal gas constant (8.314 J/mol-K). For practical use, this relationship is expressed in terms of application and standard temperatures (T_1 and T_2 ; °C):

$$K_{T1} = K_{T2} e^{[E/(R T_1 T_2)(T_1 - T_2)]}$$

where K_{T1} is at the application temperature T_1 , and K_{T2} is at the standard temperature T_2 . If it is assumed that the term $[E/(R T_1 T_2)]$ is constant over the temperature range of interest (e.g., 0-40 °C), and T_2 is set to 20 °C, then the relationship typically used in environmental engineering can be derived (e.g., Chen and Orlob, 1975; Tchobanoglous and Schroeder, 1987; Tchobanoglous and Burton, 1991):

$$K_T = K_{T20} \theta^{(T - 20)}$$

where K_T is at the application temperature (T ; °C), K_{T20} is at the standard temperature (20 °C), and θ is the temperature correction coefficient.

In the application of this simplified relationship to bacterial processes, it was found that the response of bacteria over the temperature range 0 - 40 °C was not adequately represented. Use of a single θ value over this range gave rates that were too high at low temperatures and too low at high temperatures. Thus, different values for θ are used based on whether the application temperature is above or below 20 °C (Figures 6.1 and 6.2). In addition, the simplified Van't Hoff-Arrhenius method does not give a decline in rate constants at excessively high temperatures. Justification for this simplification depends on the type of biological process. Given that maximum optimum temperatures for heterotrophic and nitrifying bacteria are reported to be 35 - 40 °C (Tchobanoglous and Burton, 1991; Hagopian and Riley, 1998), this simplification is warranted for bacteria. In contrast, the literature suggests that phytoplankton performance at higher temperatures (e.g. > 35 °C) is decreased (Svirezhev et al., 1984).

To support low-high temperature scaling, biological responses to other environmental conditions (e.g., salinity and pH), and environmental scaling to fish performance (Chapter 7), linear, exponential, and polynomial functions are available (Table 6.1; Figure 6.3). These functions (scalars) provide concave-down profiles, with intermediate regions where biological rates are maximized. Paired, discontinuous functions are often required to adequately express biological response over full ranges of driving variables. The width of the intermediate optimal zone represents the adaptive capacity of an organism to the variable. In general, 1) linear scalars are often adequate, especially when criteria values are approximate, 2) exponential scalars may be preferred when criteria values are better known, and 3) polynomial are used when it is not required to capture full ascending and descending legs (ranges $C_{\min} - C_{\max 0}$ and $C_{\min 0} - C_{\max}$) and a single, continuous function is desired to facilitate the generation of scalar parameters by regression.

Table 6.1. Typical functional forms used to calculate environmental scalars as a function of given water quality criteria and variable values.

Parameters and variables		Definition
C_{mint}		Minimum tolerance criterion
C_{mino}		Minimum optimum criterion
C_{maxo}		Maximum optimum criterion
C_{maxt}		Maximum tolerance criterion
V		Water quality variable (same units as associated criteria)
S		Individual scalar value (0 – 1)
CS		Combined scalar value (0 – 1) = minimum of individual scalars and/or products of interactive scalars

Scalar	Condition	Function
All	$V \leq C_{\text{mint}}$ or $V \geq C_{\text{maxt}}$	$S = 0$
Linear	$C_{\text{mint}} < V < C_{\text{mino}}$	$S = (V - C_{\text{mint}}) / (C_{\text{mino}} - C_{\text{mint}})$
	$C_{\text{mino}} \leq V \leq C_{\text{maxo}}$	$S = 1.0$
	$C_{\text{maxo}} < V < C_{\text{maxt}}$	$S = (C_{\text{maxt}} - V) / (C_{\text{maxt}} - C_{\text{maxo}})$
Exponential ¹	$C_{\text{mint}} < V < C_{\text{mino}}$	$S = \exp\{-k_1 [(C_{\text{mino}} - V) / (C_{\text{mino}} - C_{\text{mint}})]^{k_2}\}$
	$C_{\text{mino}} \leq V \leq C_{\text{maxo}}$	$S = 1.0$
	$C_{\text{maxo}} < V < C_{\text{maxt}}$	$S = \exp\{-k_1 [(V - C_{\text{maxo}}) / (C_{\text{maxt}} - C_{\text{maxo}})]^{k_2}\}$
Polynomial (second order and higher)	$C_{\text{mint}} < V \leq C_{\text{maxo}}$	$S = a + b V + c V^2$
	$C_{\text{mino}} \leq V < C_{\text{maxt}}$	$S = d + e V + f V^2$

¹ Adapted from Svirezhev et al. (1984), where $k_1 = 4.6$ and $k_2 = 4$ were reported for phytoplankton response to temperature and the intermediate region where $S = 1.0$ was added here. Due to the latter development, k_2 values of about 2.5 to 3 appear to provide better results (2.8 was used for examples of this method presented here and in Chapter 7).

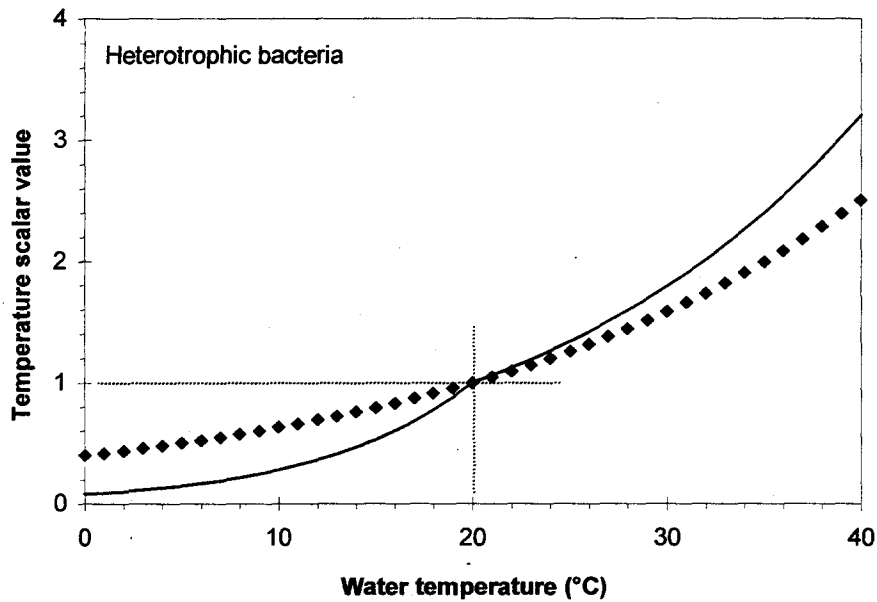


Figure 6.1. Response of heterotrophic bacteria to water temperature (simplified Van't Hoff-Arrhenius method), using one value for θ (points) and two values for θ above and below 20 °C (line) (θ values from Table 6.3)

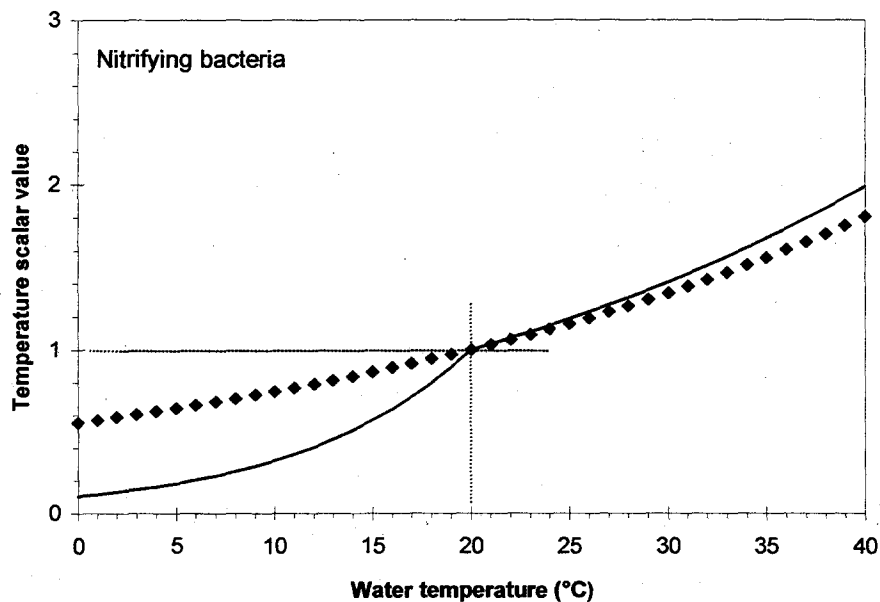


Figure 6.2. Response of nitrifying bacteria to water temperature (simplified Van't Hoff-Arrhenius method), using one value for θ (points) and two values for θ above and below 20 °C (line) (θ values from Table 6.4)

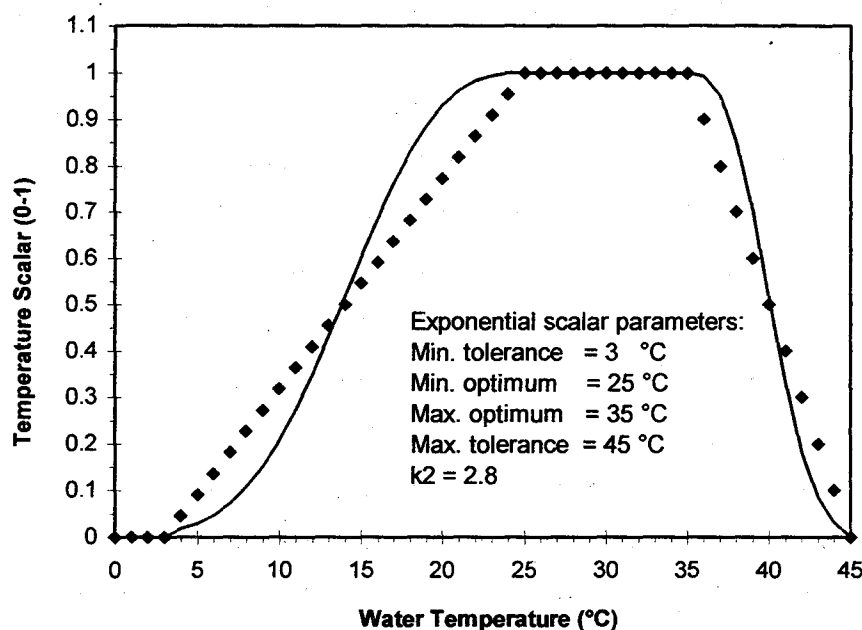


Figure 6.3. Response of phytoplankton to water temperature, using the given scalar parameters and linear (points) and exponential (line) scalar functions

6.2 Soil processes

Processes of water-body soils and sediments (settled solids) include (1) particle advection, diffusion, and resuspension, (2) compound adsorption and desorption, and dissolution and precipitation, and (3) bacterial and other biological processes (Colman and Jacobson, 1991). Soil and sediment processes are complicated by the simultaneous presence of aerobic surface layers and anoxic subsurface layers, where these two conditions favor different processes. Soil and sediment processes can show significant impact on water column concentrations of organic matter, alkalinity, DO, DIN, and DIP (Boyd, 1990; Schroeder et al., 1991).

In the modeling approach used here, soil processes can be used in place of or in addition to bacterial degradation of organic sediments (described below). If the latter alternative is used, soil processes may be essentially limited to alkalinity and DIP uptake. For all methods, soil-water and sediment-water compound flux rates are included in compound mass balances. Compound transfer due to water seepage is considered separately from soil and sediment processes.

Soil processes are mechanistically complex and depend on physical and chemical soil properties (Boyd, 1990). Soil properties are both site specific (e.g., texture and bulk density, pH, mineral content, and cation exchange capacity) and management specific (e.g., history of pond use, organic and phosphorous loading, and lime application) (Boyd, 1982; Boyd, 1990; Boyd and Bowman, 1997). A simplified, empirically based approach to soil processes is used here. Daily mean compound uptake (%/day) and release ($\text{g/m}^2\text{-day}$) rates of the soil layer of a given facility unit (e.g., pond) are interpolated from given annual regimes of monthly mean values. Compounds considered include O_2 , CO_2 , alkalinity, NH_4 , NO_3 , and HPO_4 . Typically, the uptake of oxygen, alkalinity, and DIP and the release of DIN are most important. Compound flux rates are based on reported values, which have been measured by whole pond respiration budgets, in-vitro incubation of removed cores, and in-situ respirometry (Table 6.2). Reported rates show seasonality and vary from site to site. Reported rates typically combine soil and sediment rates to single values, and therefore reported rates require adjustment if soil processes and sediment degradation are used together in a simulation.

Table 6.2. Soil process rates for soil-lined water bodies (reported mean values and ranges)

Compound	Flux Rate	Reference
DO consumption, shrimp ponds	$4.4 \text{ g O}_2/\text{m}^2\text{-day}$	Steeby, 1998
DO consumption, commercial catfish ponds	$5.7 \text{ g O}_2/\text{m}^2\text{-day}$	Steeby, 1998
	$2.6 - 6.7 \text{ g O}_2/\text{m}^2\text{-day}$	Berthelson et al., 1996
DO, intensive ponds	$0.1\text{-}1.3 \text{ g O}_2/\text{m}^2\text{-day}$	Epes, 1989
DO consumption, typical range	$0.5 - 5.0 \text{ g O}_2/\text{m}^2\text{-day}$	Schroeder, 1975; Boyd, C. E., 1982a; Boyd, 1990; Berthelson, 1993
DO consumption, extreme range	$<0.5 \text{ to } >20.0 \text{ g O}_2/\text{m}^2\text{-day}$	Boyd, 1990
DIC production, tilapia ponds	$0.5 \text{ g C}/\text{m}^2\text{-day}$	Boyd and Bowman, 1997
DIC production, typical range	$0.17 - 1.7 \text{ g C}/\text{m}^2\text{-day}$	Based on typical range for DO and $3.0 \text{ g O}_2/\text{g C}$
Alkalinity consumption, in terms of lime requirement to achieve water alkalinity levels $\geq 20 \text{ mg CaCO}_3/\text{L}$	$500 - 5000 \text{ kg CaCO}_3/\text{ha}$	Boyd, 1990
DIN (primarily TAN) production	$11 - 15 \text{ mg N}/\text{m}^2\text{-day}$	Szabo and Olah, 1998
DIP (ortho-phosphate) production	$0.004 - 0.105 \text{ mg P}/\text{m}^2\text{-day}$	Szabo and Olah, 1998
DIP(ortho-phosphate) consumption, when soil not saturated with phosphorous	10%/day removal rate	Boyd and Musig, 1981

6.3 Bacterial processes

Bacterial processes are typically major processes in all types of aquaculture systems. Bacterial processes can occur in the water column, in settled solids, and on water-containment and filter-media surfaces. Bacterial processes considered here include oxidation of organic solids by heterotrophic bacteria (HB), nitrification (oxidation) of ammonia and nitrite by nitrifying bacteria (NB), and denitrification of nitrate by denitrifying bacteria (DB). Nitrogen fixing blue-green algae (Cyanobacteria) are considered under phytoplankton processes. Hydrolysis of urea to ammonia and carbon dioxide by bacterial action is ignored ($\text{CO}(\text{NH}_2)_2 + \text{H}_2\text{O} \rightarrow 2 \text{NH}_3 + \text{CO}_2$). Urea is assumed to spontaneously degrade to carbon dioxide and ammonia when added to water (e.g., fish excretion and addition of urea as fertilizer).

In solar algae ponds, HB oxidize dead phytoplankton and solids associated with fish production. Since the oxygen demand of dead phytoplankton is equivalent to the oxygen produced by these phytoplankton, HB processes in ponds can be on the same order of magnitude as phytoplankton processes. In addition, while relatively less important, NB and DB processes normally represent significant components of pond nitrogen budgets. Bacterial processes in pond sediments occur in conjunction with any designated soil processes. Bacteria and detritus (bacterial-detrital aggregate; BDA) in pond systems can be an important food resource for detritivores such as tilapia. In intensive aquaculture systems, the HB mediated oxidation of organic solids produced by added feeds and fish wastes consumes about 1.0 g O₂/g dw solids and produces CO₂ and TAN, all of which are deleterious to fish production. Ammonia nitrification by specifically designed biofilters is the primary ammonia removal method used in intensive aquaculture.

For all HB, NB, and DB processes, bacterial process rates are used in mass balances for DO, DIC, DIN, DIP, alkalinity, and particulate and settled solids. Substrate consumption rates are a function of kinetic parameters, substrate concentrations, and additional environmental variables (e.g., temperature and pH). The substrates used for a given bacterial process consist of the terminal electron donor and acceptor, and multiple-substrate saturation kinetics are used in the models developed below. Saturation kinetics may also be referred to as (1) Michaelis-Menten kinetics, when based on volumetric mass transfer rates ($R = R_{\max} [S / (K_S + S)]$) or (2) Monod kinetics, when based on bacterial growth rates ($\mu = \mu_{\max} [S / (K_S + S)]$). Consumption and excretion rates of secondary substrates are based on the stoichiometry of bacterial metabolism.

6.4 Heterotrophic bacteria

Heterotrophic (carbonaceous) bacteria (HB) oxidize organic particulate solids in the water column (PS; g dry weight solids/m³) and particulate settled solids on benthic surfaces (PSS; g dry weight solids /m²). HB can also oxidize dissolved organic compounds, but these compounds are ignored here. PS can originate from a variety of sources, such as influent water, waste feed, fish feces, dead phytoplankton, and added fertilizers. PSS accumulate due to the settling of PS (see Chapter 5, Solid sedimentation). In relatively clean water systems such as salmon hatcheries, PS levels are typically < 5-10 mg/L. In eutrophic pond systems, PS levels above 50 mg/L are not uncommon (in addition to phytoplankton). PSS values are highly specific to the type of aquaculture system and facility units within these systems. In general, PSS levels can range from negligible to 1.0 kg/m², and much higher levels can exist in specialized facility units such as waste sludge collection basins.

6.4.1 Suspended heterotrophic bacteria

For wastewater treatment in activated sludge reactors and stabilization ponds (e.g., Fritz et al., 1979; James, 1984; Fritz, 1985; Tchobanoglous and Burton, 1991), explicit accounting of both organic substrate (PS) and bacterial (HB) concentrations is typically used. Typical mass balances used in wastewater treatment for HB and PS are:

$$dHB/dt = \mu_{HBmax} HB [PS / (K_{PS-HB} + PS)] - K_{DHB} HB$$

$$dPS/dt = (\mu_{HBmax} HB / Y_{HB}) [PS / (K_{PS-HB} + PS)]$$

where dHB/dt = HB growth rate (g HB/m³/day) and dPS/dt = PS oxidation rate (g PS/m³/day). These differential equations may also include scalar terms for temperature and DO and other sources and sinks of HB and PS. Method variables for HB processes are listed in Table 6.3. For both natural system and aquaculture models, while the presence of bacteria is implicit in the consideration of HB processes, explicit accounting of bacterial populations is not commonly used (Chen and Orlob, 1975; Meyer and Brune, 1982; Svirezhev et al., 1984; Piedrahita, 1989). In general, the rationales and derivations for the simplified methods that are used in these published models are lacking. For intensive aquaculture systems, HB processes are often ignored except for facility units where solids are concentrated for removal.

Table 6.3. Parameters and variables for processes of heterotrophic bacteria ^a

Symbol	Value ^b	Definition, units, and reported values (mean and/or range)
BDA	C	Combined HB and detritus, bacterial-detrital aggregate (g BDA/m ³)
F _{HB}	C	HB concentration expressed as a fraction of PS (g HB/g PS; 0-1)
HB	C	Heterotrophic bacteria concentration (g dw cells/m ³)
K _{DHB}	0.06	Endogenous decay coefficient of HB (1/day): 0.06, 0.025 – 0.075 (20 °C; Tchobanoglous and Burton, 1991); 0.07 (Fritz et al., 1979; Fritz, 1985)
K _{DO-HB}	2.0	Half-saturation constant of DO for PS (g O ₂ /m ³): 1.0 (Fritz et al., 1979)
K _{DO-SHB}	5 – 10	Half-saturation constant of DO for PSS (g O ₂ /m ³): estimated
K _{PS}	0.1 - 0.2	First-order solids decay constant of PS for unlimiting conditions (1/day): 0.28 – 0.71 (Malone et al., 1993); 0.23, 0.05-0.3 (20 °C; Tchobanoglous and Burton, 1991); 0.1 – 0.3 (Fritz et al., 1979); 0.2 (Chen and Orlob, 1975); 0.12 (used without consideration of saturation kinetics; Piedrahita, 1989)
K _{PSS}	0.02 - 0.1	First-order solids decay constant of PSS (1/day): estimated
K _{PS-HB}	50	Half-saturation constant for PS (g PS/m ³): 50 (Fritz et al., 1979; Fritz, 1985); 60 (James, 1984); 60, 25-100 (20 °C; Tchobanoglous and Burton, 1991)
K _{PSS-SHB}	50	Half-saturation constant for PSS (g PSS/m ²): estimated
PS	C	Organic particulate solids in the water column (PS; g dry weight solids/m ³)
PSS	C	Organic, settled particulate solids on benthic surfaces (PSS; g dry weight solids/m ²): value based on bottom surface area (regardless of presence of media)
PSS _D	C	Depth (wet) of settled solids (mm)
SCL _S	C	Substrate scalar (0-1; dimensionless)
Y _{HB}	0.6	HB cell mass formed per mass of substrate consumed (g HB/g PS): 0.6, 0.4-0.8 (20 °C; Tchobanoglous and Burton, 1991); 0.5 (20 °C; Fritz et al., 1979; Fritz, 1985)
μ _{HBmax}	4	Maximum specific growth rate of HB (1/day): 3, 1.2-6 (20 °C; Tchobanoglous and Burton, 1991); 5 (Fritz et al., 1979; Fritz, 1985); 0.2 (for PSS; Svirezhev et al., 1984)
θ _{HB}	1.135 @ ≤ 20 °C, 1.056 @ > 20 °C	Temperature correction coefficient (dimensionless): 1.047, 1.04 – 1.08 (Tchobanoglous and Burton, 1991); 1.135 (4-20 °C; Tchobanoglous and Burton, 1991); 1.056 (20-30 °C; Tchobanoglous and Burton, 1991)
ρ _{PSS}	300	Bulk density of PSS (kg dry weight/ m ³ wet volume): 300 (equivalent to 0.3 g/cm ³ cited in Avnimelech et al., 1999); 1300 for kg wet weight/ m ³ wet volume (Piedrahita, 1990)

^a Cited values are mainly based on municipal waste; reporting temperature shown when available^b Numerical values are default values used in AquaFarm and “C” denotes a calculated variable

In the approach used here, HB biomass levels (bacterial populations) are not explicitly accounted, HB biomass (dry weight) is included with PS, and net HB production is a source of BDA. In the derivation below, combined HB-PS is temporarily termed bacterial-detrital aggregate (BDA), and then PS is redefined as BDA. A second simplifying assumption used here is that a substantial (equilibrium) HB biomass is always present, as a constant proportion of BDA, including new solids entering the system. The derivation of a mass balance for BDA begins with the fundamental process equations given earlier, for which scalar terms for environmental conditions and substrate levels are combined to a single scalar term (SCL):

$$dHB/dt = \mu_{HBmax} HB SCL_S - K_{DHB} HB$$

$$dPS/dt = -(\mu_{HBmax} HB / Y_{HB}) SCL_S$$

Equations for HB and PS are combined to yield:

$$dBDA/dt = \mu_{HBmax} HB SCL_S - K_{DHB} HB - (\mu_{HBmax} HB / Y_{HB}) SCL_S$$

$$\text{or } dBDA/dt = \mu_{HBmax} HB (1 - 1/Y_{HB}) SCL_S - K_{DHB} HB$$

If HB is represented as the product of BDA and F_{HB} , then:

$$dBDA/dt = \mu_{HBmax} BDA F_{HB} (1 - 1/Y_{HB}) SCL_S - K_{DHB} BDA F_{HB}$$

$$\text{or } dBDA/dt = BDA [\mu_{HBmax} F_{HB} (1 - 1/Y_{HB}) SCL_S - K_{DHB} F_{HB}]$$

Finally, redefining PS as BDA and adding the temperature scalar gives:

$$dPS/dt = PS \theta_{HB}^{(T-20)} [\mu_{HBmax} F_{HB} (1 - 1/Y_{HB}) SCL_S - K_{DHB} F_{HB}]$$

$$\text{or } dPS/dt = PS \theta_{HB}^{(T-20)} [K_1 SCL_S - K_2]$$

$$\text{where } K_1 = \mu_{HBmax} F_{HB} (1 - 1/Y_{HB})$$

$$K_2 = K_{DHB} F_{HB}$$

$$SCL_S = \text{minimum} \{ [PS / (K_{PS-HB} + PS)], [DO / (K_{DO-HB} + DO)] \}$$

K_1 and K_2 are combined constants used in simulations. The derived function for dPS/dt represents a combination of first-order and saturation kinetics. As expected, if Y_{HB} is equal to 1.0, then the decline in PS over time is limited to bacterial endogenous decay (K_{DHB}). It is emphasized that while F_{HB} and Y_{HB} have the same units (g HB/g PS), they represent a concentration fraction and a

yield ratio, respectively. It is assumed that HB rates are independent of pH values for the pH range of aquaculture systems (5 – 10), and a scalar term for pH is not used for HB processes.

Given values for K_{PS} , μ_{HBmax} , Y_{HB} , and K_{DHB} are used to calculate F_{HB} , K_1 , and K_2 . To accomplish these calculations, saturated conditions are used ($SCL_S \cong 1.0$), where PS kinetics approximate first-order carbonaceous (CBOD) decay. K_{PS} represents a combination of constants and is itself constant, and F_{HB} can be estimated from the other parameters:

$$dPS/dt = PS \theta_{R,HB}^{(T-20)} K_{PS}$$

where $K_{PS} = \mu_{HBmax} F_{HB} (1 - 1/Y_{HB}) - K_{DHB} F_{HB}$

rearrange $F_{HB} = K_{PS} / [\mu_{HBmax} (1 - 1/Y_{HB}) - K_{DHB}]$

Using parameter values in Table 6.3, F_{HB} , K_1 , and K_2 are calculated:

$$F_{HB} = -0.3 / [4 (1 - 1/0.6) - 0.06] = 0.1100$$

$$K_1 = \mu_{HBmax} F_{HB} (1 - 1/Y_{HB}) = 4 \times 0.11 (1 - 1/0.6) = -0.2933$$

$$K_2 = K_{DHB} F_{HB} = 0.06 \times 0.11 = 0.0066$$

and thus $dPS/dt = PS \theta_{HB}^{(T-20)} [-0.2933 SCL_S - 0.0066]$

Examination of this derived function shows that (1) the decay term (K_2 ; e.g., 0.0066) is small relative to the growth term ($K_1 SCL_S$; e.g., 0.2933×0.7) and (2) as SCL_S approaches one, K_1 approaches K_{PS} . As shown in the application of this equation to appreciable PS concentrations (e.g., ≥ 10 mg/L), PS oxidation rates are relatively insensitive to μ_{HBmax} , Y_{HB} , and K_{DHB} values and are mainly dependent on K_{PS} .

6.4.2 Settled heterotrophic bacteria

The approach used for settled solids is identical to that used for suspended solids, including given values for K_{PSS} , μ_{HBmax} , Y_{HB} , and K_{DHB} and calculated values for F_{HB} , K_1 , and K_2 :

$$dPSS/dt = PSS \theta_{HB}^{(T-20)} [\mu_{HBmax} F_{HB} (1 - 1/Y_{HB}) SCL_S - K_{DHB} F_{HB}]$$

$$dPSS/dt = PSS \theta_{HB}^{(T-20)} [K_1 SCL_S - K_2]$$

where $SCL_S = \text{minimum} \{ [PSS / (K_{PSS-SHB} + PSS)], [DO / (K_{DO-SHB} + DO)] \}$

The aquaculture literature regarding empirical observations of PSS oxidation rates is mainly limited to oxygen consumption rates of combined soil and sediment processes, and reported K_{PSS} and half-saturation constants are not available. $K_{PSS-SHB}$ is based on an areal concentration (g PSS/m^2), as opposed to the volumetric basis of K_{PS-HB} (g PS/m^3), and thus $K_{PSS-SHB}$ may be lower in value than K_{PS-HB} . For dissolved oxygen, higher values are assumed for K_{DO-SHB} relative to K_{DO-HB} , given the constraint imposed by oxygen transfer from the water column to the sediment layer. K_{PSS} can be set independently of K_{PS} , supporting additional rate control.

As described in Chapter 5 (Solids sedimentation), sediment resuspension due to fish activity and water currents is considered by the use of reduced solid settling velocities. Consideration of resuspension by use of reduced settling rates emulates the turnover of the surface sediment layer. For tilapia and carp ponds, a conservative estimate of 3.0 mm/day of surface sediment resuspension and resettling due to fish feeding activity has been reported (Avnimelech et al., 1999). For the sediment layer that does accumulate, it is assumed that only a given surface depth of the sediment remains aerobic and is subject to oxidation. For this purpose, PSS mass (kg dw/m^2) and depth (PSS_D ; mm) of wet solids (mm) are related by: $PSS_D = (1000 \text{ mm/m}) PSS / \rho_{PSS}$

For example, at a ρ_{PSS} of 300 kg/m^3 , a PSS of 1.0 kg/m^2 is equivalent to a sediment layer depth of 3.3 mm. In terms of oxygen consumption, if this 1.0 kg/m^2 of PSS is oxidized at a relatively low rate (e.g., $K_{PSS} = 0.05/\text{day}$) and consumes $1.105 \text{ g O}_2/\text{g dw solids}$, then the initial oxygen demand is $55 \text{ g O}_2/\text{m}^2\text{-day}$. This value greatly exceeds even the highest reported pond sediment respiration rates (e.g., $6.7 \text{ g O}_2/\text{m}^2\text{-day}$; see Soil processes), indicating that the depth of the aerobic surface layer is much less than 3.3 mm and or K_{PSS} is well below $0.05/\text{day}$. Observed surface depths of aerobic sediments were not found in the literature. In method testing performed here, depths of about 1.0 mm were found to provide good results. In practice, significant accumulation of sediments is mainly limited to pond-based systems and the water treatment systems of intensive systems. In ponds, however, carp and tilapia are known to resuspend accumulated sediments, and ponds may be periodically drained and PSS either removed or allowed to oxidize in the open air.

6.5 Nitrifying bacteria

Nitrification is a two-step process (Wheaton et al., 1994a). In the first step, ammonia is oxidized to nitrite by *Nitrosomonas* and related genera. In the second step, nitrite is oxidized to nitrate by *Nitrobacter* and related genera. In aquaculture systems, ammonia can originate from influent water, biological production, soil processes, and fertilizer addition. Nitrite originates primarily from incomplete nitrification. Transient nitrite spikes are known to occur during biofilter conditioning (Westerman et al., 1993) and seasonally in solar algae ponds (Boyd, 1990), due to imbalances in bacterial populations. Nitrifying bacteria (NB) are highly sensitive to changes in environmental conditions (e.g. temperature and pH), and their slow growth causes slow adaptation rates to new environmental conditions (Hagopian and Riley, 1998). Reported DO levels required to support nitrification are $\geq 1 - 2$ mg O₂/L (Wheaton et al., 1994). Reported pH levels required to support high nitrification rates are 7.2 - 9.0, with an optimum at 7.8 (Tchobanoglous and Burton, 1991; Wheaton et al., 1994a; Hagopian and Riley, 1998). When organic substrates are available, relatively fast growing HB typically out-compete NB for habitat and reduce NB process rates.

Due to the slow growth of NB bacteria, it is likely that significant levels of suspended NB in aquaculture systems occur only in eutrophic, static or recirculated, waters where substrate levels and cell retention times support significant cell populations. Attached (fixed film) NB on water-containment surfaces, for example pipe and tank walls and pond benthic surfaces, are likely to represent the most significant NB biomass in most water bodies. Ammonia biofilters rely totally on attached NB. Fixed-film nitrification rates may be primarily controlled by diffusion rates of ammonia into the bacterial film (Lu and Piedrahita, 1993), which in turn are dependent on a host of design and management variables. Variables impacting biofilter nitrification rates include ammonia levels, hydraulic and TAN loading, non-ideal flow distribution, and NB film thickness and fouling. In turn, NB film thickness and fouling are a function of hydraulic loading, particulate solid levels in the influent water, media characteristics, media cleaning cycles, and degree of media scrubbing per cleaning event. Nitrification rates can be reduced considerably by poor filter design and excessive filter cleaning (Malone et al., 1993).

In sum, the sensitivity of NB to environmental conditions and the ammonia diffusion rates of fixed-film nitrification are mechanistically complex and difficult to quantify. In response, reported methods for suspended and fixed-film nitrification in aquaculture systems are highly simplified. For suspended NB in pond systems, the literature shows that either nitrification is ignored (e.g., Chen

and Orlob, 1975; Meyer and Brune, 1982; Svirezhev et al., 1984), or first-order decay of ammonia is assumed while ignoring NB populations. For example, Piedrahita (1989) used a constant, specific TAN oxidation rate of 0.024/day and made no distinction between suspended and attached NB. Other than ammonia biofilters, no studies were found in the aquaculture literature concerning nitrification rates of attached NB on water-containment surfaces. However, such open surfaces are likely to provide good conditions for attached NB, given their exposure to water flow and lack of accumulated solids. The significance of attached NB on water-containment surfaces depends on the combined wall-surface to volume ratio of the system. Ammonia nitrification in biofilters of aquaculture systems has been well studied, but design procedures and models developed from this work generally consist of simplified, empirically based, formulations (e.g., Malone et al., 1993; Wheaton et al., 1994b).

In the modeling approach used here, similar to HB processes, NB are not explicitly modeled as a bacterial population, and it is assumed that suspended NB concentrations are proportional to ammonia concentrations as defined by F_{NB} . Method variables for NB processes are listed in Table 6.4. The relative proportions of TAN and NO_2 nitrifying bacteria are assumed to be at steady state conditions and nitrification is modeled as a combined process, for which TAN is oxidized directly to NO_3 . This simplification is commonly used in aquaculture and waste treatment modeling (e.g., Fritz et al., 1979; Fritz, 1985; Piedrahita, 1989; James, 1984), where it has been shown that rates of nitrite oxidation exceed those of ammonia and therefore ammonia oxidation represents the limiting kinetics (James, 1984).

6.5.1 Suspended nitrifying bacteria

Derivation of the method used for suspended NB begins with the fundamental process equation (Tchobanoglous and Burton, 1991):

$$dTAN/dt = -\theta_{NB}^{(T-20)} (\mu_{mNB} NB / Y_{NB}) SCL$$

where $SCL = SCL_S SCL_{pH}$

$$SCL_S = \text{minimum} \{ [TAN / (K_{TAN-NB} + TAN)], [DO / (K_{DO-NB} + DO)] \}$$

Table 6.4. Parameters and variables for processes of nitrifying bacteria ^a

Symbol	Value ^b	Definition, units, and reported values (mean and/or range)
FLT _{CC}	10	Biofilter conditioning time from cleaning (days)
FLT _{CD}	0.67	Biofilter rate decrease factor for filter cleaning (0-1; dimensionless)
FLT _{MI}	10	Maximum limit to rate of increase in nitrification rates (%/day)
FLT _{SM}	C	Biofilter maximum solids holding capacity (kg, dry weight; based on filter water volume)
FLT _{SO}	30	Biofilter solids capacity at which nitrification is reduced to zero (% of FLT _{SM})
F _{NB}	C	Suspended NB concentration expressed as a fraction of TAN (g NB/ g TAN; 0-1; dimensionless)
K _{DNB}	0.05	Endogenous decay coefficient of NB (1/day): 0.05 (cited by Zhu and Chen, 1999)
K _{DO-ANB}	3.0	Attached NB half-saturation constant for oxygen (g O ₂ /m ³): estimated
K _{DO-NB}	1.0	Suspended NB half-saturation constant for oxygen (g O ₂ /m ³): 0.20 (NTS, minimum value; Hagopian and Riley, 1998); 0.25 (NTB, minimum value; Hagopian and Riley, 1998); 1.3 (NTS; Fritz et al., 1979)
K _{NO2-NTB}	5.0	Suspended NTB half-saturation constant for nitrite (g NO ₂ -N/m ³): 5.0 (25 °C; Wheaton et al., 1994); 2.8 (minimum value; Hagopian and Riley, 1998); 1.4, 0.2 – 5.0 (20 °C; Tchobanoglous and Burton, 1991)
K _{TAN}	0.05	Suspended NB first-order TAN decay constant for unlimiting conditions (1/day): 0.03 (NTB; Chen and Orlob, 1975); 0.09 (NTS; Chen and Orlob, 1975); 0.05, 0.03 – 0.06 (20 °C; Tchobanoglous and Burton, 1991)
K _{TAN-ANB}	C	Attached NB half-saturation constant for TAN (g TAN/m ³): 2.0 (27 °C; value used by Zhu and Chen, 1999); 1.3, 3.5 (25 °C; values cited by Zhu and Chen, 1999)
K _{TAN-NB}	1.4	Suspended NB half-saturation constant for TAN (g TAN/m ³): 1.4, 0.2 – 5.0 (20 °C; Tchobanoglous and Burton, 1991)
K _{TAN-NTS}	1.0	Suspended NTS half-saturation constant for TAN (g TAN/m ³): 0.73 – 1.0 (20 °C; Wheaton et al., 1994); 0.275 (20 °C, Fritz p. 198); 0.6 (minimum value; Hagopian and Riley, 1998); 0.6, 0.2 – 2.0 (20 °C; Tchobanoglous and Burton, 1991); 1.0 (James, 1984)
R _{TAN-max}	S	Attached NB maximum TAN nitrification rate (g N/m ² -day): 4 (Brune and Gunther, 1981); 1.9 (27 °C; Zhu and Chen, 1999)
R _{TAN-std}	S	Attached NB standard nitrification rate (g N/ m ² -day): at 20 °C, non-limiting operating conditions, and corresponding to TAN _{std}

Table 6.4. Continued

Symbol	Value	Definition, units, and reported values (mean and/or range)
SA_M	C	Attached NB media surface area (m^2)
SCL_F	C	Biofilter fouling scalar (0-1; dimensionless)
SCL_L	C	Biofilter loading scalar (0-1; dimensionless)
SCL_{pH}	C	Nitrification pH scalar (0-1; dimensionless)
SCL_R	C	Biofilter regeneration scalar (0-1; dimensionless)
SCL_S	C	Nitrification substrate scalar (0-1; dimensionless)
SVR	S	Attached NB - media surface area to bulk volume ratio (m^2/m^3)
TAN_{min}	0.07	Attached NB - Minimum TAN level for nitrification ($g\ TAN/m^3$): 0.07 (27 °C; Zhu and Chen, 1999)
TAN_{std}	S	Attached NB - standard TAN level where $R_{TAN-std}$ is achieved ($g\ TAN/m^3$)
t_R	C	Biofilter - elapsed time since filter regeneration (day)
t_S	C	Biofilter - elapsed time since filter started (day)
V	C	Attached NB - water volume (m^3)
V_M	S	Biofilter - bulk volume media (m^3): specified as percent of available water volume filled with media
Y_{NB}	0.157	Cell yield coefficient ($g\ cell/g\ TAN$): value used is based on given stoichiometry ($cell = PS$); 0.05 (Tchobanoglous and Schroeder, 1987); 0.2, 0.1 – 0.3 (20 °C, suspended growth; Tchobanoglous and Burton, 1991); 0.17 (Wheaton et al., 1994); 0.15 (NTS; Fritz et al., 1979; Fritz, 1985); 0.17 – 0.21 (values cited by Zhu and Chen, 1999)
μ_{NBmax}	0.7	Suspended NB - maximum growth rate for (1/day): 0.7, 0.3 – 2.0 (NTS, 20 °C; Tchobanoglous and Burton, 1991); 1.0, 0.4 – 3.0 (NTB, 20 °C; Tchobanoglous and Burton, 1991); 1.0, 0.3 – 3.0 (overall, 20 °C; Tchobanoglous and Burton, 1991)
μ_{ANBmax}	1.5	Attached NB - maximum growth rate (1/day): 0.77 – 2.0 (NTS, 20 °C; Wheaton et al., 1994); 1.48 (27 °C; value used by Zhu and Chen, 1999); 1.25-1.5 (25 °C; values cited by Zhu and Chen, 1999)
θ_{NB}	1.12 @ $\leq 20\ ^\circ C$, 1.035 @ $> 20\ ^\circ C$	Temperature correction coefficient (dimensionless): 1.03 (derived from data cited in Wheaton et al., 1994); 1.035 (trickling filters; Tchobanoglous and Burton, 1991); 1.12 (derived from data cited in Wheaton et al., 1994); 1.02 (Chen and Orlob, 1975)

^a *Nitrosomonas* is abbreviated as NTS and *Nitrobacter* is abbreviated as NTB; reporting temperature shown when available

^b Numerical values are default values used in AquaFarm, C denotes a calculated variable, and S denotes a biofilter specification

Using the simplification that $F_{NB} = NB / TAN$, substitution yields:

$$dTAN/dt = -TAN \theta_{NB}^{(T-20)} (\mu_{mNB} F_{NB} / Y_{NB}) SCL$$

$$dTAN/dt = -TAN \theta_{NB}^{(T-20)} K_{TAN} SCL$$

where $K_{TAN} = \mu_{mNB} F_{NB} / Y_{NB}$

The derived function for $dTAN/dt$ represents a combination of first-order decay and saturation kinetics. K_{TAN} is a product of constants and is therefore a constant. K_{TAN} is assigned a value directly, and thus μ_{mNB} , F_{NB} , and Y_{NB} are not needed to calculate K_{TAN} . F_{NB} can be estimated from parameter values in Table 6.4:

$$F_{NB} = K_{TAN} Y_{NB} / \mu_{mNB} = 0.05 \times 0.157 / 0.7 = 0.0112$$

As expected, F_{NB} is much smaller than F_{HB} (e.g., 0.1100). The dynamics of NB cell biomass is ignored, except that cell yield per substrate oxidized, Y_{NB} (g NB/g TAN), is considered as a source for PS, where the contributed PS is equivalent to the product of Y_{NB} and $dTAN/dt$. Outside of the optimal pH range of 7.2 – 9.0, the pH scalar term (SCL_{pH}) is assumed to decline linearly from 1.0 to 0.0, as pH declines to 6.0 or increases to 10.0.

6.5.2 Attached nitrifying bacteria

For attached (fixed film) NB on water containment surfaces and biofilter media, an empirically based modeling approach is taken here which utilizes variables typically reported for biofilters (Table 6.5). In addition, scalar terms are added for various operational variables impacting nitrification rates. The normalized nitrification rate (R_{NRM} ; g N/m²-day per g N/m³) is a useful, overall performance parameter, where $R_{NRM} = R_{TAN-std} / TAN_{std}$. Malone et al. (1993) report that R_{NRM} values of 0.50 are appropriate for moderate to lightly loaded bead filters, but that this value should be reduced to 0.25 for heavily loaded filters subject to backwashing frequencies of 2 to 4 times per day.

Biofilters contain media and may be flooded or trickling. In fluidized-bed biofilters, the packing medium is expanded by the upward movement of water through the bed, and the level of bed expansion and porosity depends on the water flow rate. However, expansion and porosity of

Table 6.5. Reported performance variables for ammonia biofilters *

Filter type	Mean pH	SVR (m ² /m ³)	TAN _{std} Mean effluent TAN (g N/m ³)	R _{TAN-std} Nitrification rate (g N/m ² -day)	R _{NRM} Normalized nitrification rate (g N/m ² -day per g N/m ³)
Upflow sand filter	7.15	2350	0.31	0.064	0.21
Hydraulic washed bead filter	7.54	1230	0.62	0.231	0.37
Mechanical washed bead filter	7.38	1050	1.10	0.291	0.26
Rotating biological contactor	7.51	150	0.53	0.280	0.53
	NA	223	0.2–2.0	0.020–0.2	0.1
Fluidized bed filter	7.47	2350	0.30	0.284	0.95
Mean	—	—	0.66	0.21	0.40

* Reported in Malone et al. (1993) and Wheaton et al. (1994)

fluidized-bed filters are not explicitly considered here, and these filters are specified similar to fixed media filters. NB attached to biofilter media are essentially no different than NB attached to water-containment surfaces, except that the latter are assumed to always be fully conditioned.

Nitrification rates for attached NB are limited by a maximum absolute rate ($R_{TAN-max}$; Brune and Gunther, 1981; Zhu and Chen, 1999), based on constraints to water-film ammonia diffusion and limits to the maximum, active film thickness (James, 1984; Lu and Piedrahita, 1993). Related to the diffusion constraint, ammonia half-saturation coefficients for fixed-film bacteria are reported to be about 2 to 3 times higher than those used for suspended bacteria (James, 1984, p 201). The modeling method for attached (fixed film) NB is:

$$dTAN/dt = -R_{TAN-max} (S_{AM} / V) \theta_{NB}^{(T-20)} SCL$$

where $S_{AM} = SVR V_M$

$$SCL = SCL_S SCL_{pH} SCL_{DO} SCL_L SCL_R SCL_F$$

$$SCL_S = \text{minimum} \left\{ \frac{[TAN - TAN_{min}]}{[K_{TAN,ANB} + TAN - TAN_{min}]}, \right. \\ \left. [DO / (K_{DO,ANB} + DO)] \right\}$$

$K_{TAN,ANB}$ is based on the four filter specifications: $R_{TAN-max}$, $R_{TAN-std}$, TAN_{std} , and TAN_{min} (Tables 6.4 and 6.5). It is assumed that these specifications apply to a temperature of 20 °C and non-limiting operating conditions, with respect to DO, pH, filter conditioning, and filter fouling. $K_{TAN,ANB}$ is calculated by:

$$dTAN/dt = R_{TAN-max} [(TAN - TAN_{min}) / (K_{TAN-ANB} + TAN - TAN_{min})]$$

$$R_{TAN-std} = R_{TAN-max} [(TAN_{std} - TAN_{min}) / (K_{TAN-ANB} + TAN_{std} - TAN_{min})]$$

and therefore

$$K_{TAN-ANB} = (TAN_{std} - TAN_{min}) (R_{TAN-max} / R_{TAN-std} - 1)$$

For example, using typical biofilter specifications, calculated values of $K_{TAN,ANB}$ range from about 2.0 to 5.3. A $K_{TAN-ANB}$ value of 3.9 is about 2.8 times K_{TAN-NB} (1.4), which is within the expected range for this factor (2 - 3).

$$K_{TAN-ANB} = (0.50 - 0.07) (4.0 / 0.30 - 1) = 5.3 \quad (R_{NRM} = 0.60; \text{various sources})$$

$$K_{TAN-ANB} = (2.25 - 0.07) (1.87 / 1.00 - 1) = 1.9 \quad (R_{NRM} = 0.44; \text{Zhu and Chen, 1999})$$

$$K_{TAN-ANB} = (1.00 - 0.07) (3.0 / 0.5 - 1) = 3.9 \quad (R_{NRM} = 0.50; \text{active nitrification})$$

$$K_{TAN-ANB} = (2.00 - 0.07) (0.5 / 0.1 - 1) = 7.7 \quad (R_{NRM} = 0.05; \text{passive nitrification})$$

The last two sets of parameters are used as AquaFarm default values. For passive, fixed-film nitrification on water containment surfaces, values shown are intended for soil-lined ponds. For intensive systems, higher nitrification rates are likely to exist and may approach active nitrification rates.

Scalar terms in addition to SCL_S are given a value of 1.0, unless calculated according to the conditions described below. The pH scalar term is calculated as described for suspended NB. For DO, in addition to consideration of saturation kinetics, the DO scalar term (SCL_{DO}) declines from 1.0 to 0.0 as DO declines from 2.0 to 0.5 (using a linear scalar). The filter loading scalar (SCL_L) accounts for the required response time of a biofilter to increases in ammonia loading. For example, sudden increases in ammonia loading occur at filter start-up and when fish lots are added to a system. In this case, some finite amount of time is required for an increase in bacterial biomass in response to the additional substrate. SCL_L is calculated such that the nitrification rate of a filter (g

$\text{N/m}^2\text{-day}$) cannot increase faster than a given limit (FLT_{MI} ; %/day). The filter regeneration scalar (SCL_{R}) accounts for the negative impact of media cleaning on NB biomass. If $t_{\text{R}} < \text{FLT}_{\text{CC}}$, then:

$$\text{SCL}_{\text{R}} = 1.0 + [\text{FLT}_{\text{CD}} (t_{\text{R}} / \text{FLT}_{\text{CC}} - 1.0)]$$

The filter fouling scalar (SCL_{F}) accounts for solids accumulation in the filter (PSS ; kg dw) relative to a given maximum operational capacity (PSS_{max} ; kg dw):

$$\text{PSS}_{\text{max}} = \text{FLT}_{\text{SM}} \text{FLT}_{\text{SO}} / 100$$

If $\text{PSS} > \text{PSS}_{\text{max}}$, then $\text{SCL}_{\text{F}} = 0$. Otherwise:

$$\text{SCL}_{\text{F}} = (\text{PSS}_{\text{max}} - \text{PSS}) / \text{PSS}_{\text{max}}$$

6.6 Denitrifying bacteria

Denitrifying bacteria (DB) convert nitrate (NO_3) to nitrogen gas (N_2) under anaerobic conditions (Tchobanoglous and Burton, 1991). Organic solids are used as a source of carbon and hydrogen ions are consumed (alkalinity produced). The importance of DB processes in aquaculture systems includes (1) impacts on alkalinity and pH and (2) nitrogen losses due to NO_3 conversion to N_2 and N_2 diffusion out of the system. Denitrification rates in soil lined, solar algae ponds can apparently represent a major component of the nitrogen budget (e.g., Boyd, 1985). These rates have been estimated from other nitrogen budget terms, and direct measurements are not available. Denitrification has been offered as a likely mechanism for unexplained nitrogen losses in intensive systems (Tom Losordo, North Carolina State University), where aerobic conditions exist throughout the system but anaerobic microcosms can apparently develop in relatively small volumes of accumulated settled solids. Denitrification biofilters show some use in facility effluent treatment systems (e.g., Solar Aqua Farms, CA) and recirculation treatment systems (Kaiser and Schmitz, 1988), to reduce nitrate levels and to provide a process to offset the acidification of nitrification.

In AquaFarm, consideration of denitrification is optional, like all bacterial processes, and can occur when settled organic solids exist and nitrate is available. Method variables are listed in Table 6.6. Highly simplified methods are used. Cell production and organic carbon consumption are ignored. With respect to required anaerobic conditions (Tchobanoglous and Burton, 1991), DO levels within the sediment layer are not modeled and are not applied to denitrification rates.

Table 6.6. Parameters and variables for processes of denitrifying bacteria^{1,2}

Symbol	Value ³	Definition, units, and reported values (mean and/or range)
F _{DB}	0.1	DB concentration expressed as a fraction of NO ₃ (g DB/g NO ₃ ; 0-1; dimensionless): calculated
K _{DB}	0.05	First-order NO ₃ decay constant for unlimiting conditions (1/day): estimated
K _{NO3-DB}	1.0	Half-saturation constant for nitrate (g NO ₃ -N / m ³): 0.1, 0.06 – 0.20 (20 °C; Tchobanoglous and Burton, 1991)
K _{PSS-DB}	30	Half-saturation for PSS (g PS/m ³ and g PSS/m ²): estimated
SCL _S	C	Denitrification substrate scalar (0-1; dimensionless)
Y _{DB}	0.6	Cell yield coefficient (g PS/g NO ₃ -N): 0.8, 0.4 – 0.9 (20 °C; Tchobanoglous and Burton, 1991)
μ _{max}	0.3	Maximum DB growth rate (1/day): 0.3, 0.3 – 0.9 (20 °C; Tchobanoglous and Burton, 1991)
θ	1.12 @ ≤ 20 °C, 1.03 @ > 20 °C	Temperature correction coefficient (dimensionless): 1.09: (Tchobanoglous and Burton, 1991)

¹ Cited values are mainly based on municipal waste

² Reporting temperature shown when available

³ Numerical values are default values used in AquaFarm and C denotes a calculated variable

While consideration of an anoxic-aerobic partition was found to be necessary for modeling the oxidation of settled solids (described earlier), its use here did not result in sufficient denitrification rates. Apparently, denitrification in soil-lined ponds is occurring in sub-benthic, mixed sediment and soil layers or in sediment microcosms. Since water column NO₃ levels are used, the value used for K_{NO3,DB} must account for water-solid NO₃ transfer. Denitrification rates are estimated by:

$$d\text{NO}_3\text{-N}/dt = -\theta_{DB}^{(T-20)} (\mu_{DB\max} \text{DB} / Y_{DB}) \text{SCL}_S$$

where $\text{SCL}_S = \text{minimum}\{[\text{NO}_3\text{-N} / (\text{K}_{\text{NO3-DB}} + \text{NO}_3\text{-N})], [\text{PSS} / (\text{K}_{\text{PSS-DB}} + \text{PSS})]\}$

Using the simplification that $F_{DB} = \text{DB} / \text{NO}_3\text{-N}$, substitution yields:

$$d\text{NO}_3\text{-N}/dt = -\text{NO}_3\text{-N} \theta_{DB}^{(T-20)} (\mu_{DB\max} F_{DB} / Y_{DB}) \text{SCL}_S$$

$$d\text{NO}_3\text{-N}/dt = -\text{NO}_3\text{-N} \theta_{DB}^{(T-20)} K_{DB} \text{SCL}_S$$

where $K_{DB} = \mu_{DB\max} F_{DB} / Y_{DB} = 0.05$ (assigned value)

and $F_{DB} = K_{DB} Y_{DB} / \mu_{DB\max} = 0.05 \times 0.6 / 0.3 = 0.1000$

6.7 Phytoplankton

The importance of phytoplankton processes in aquaculture varies with system type and management intensity. In fertilized, solar-algae ponds with no added feed, primary production is the primary basis of the food chain (Coleman and Edwards, 1987; Schroeder et al., 1990). The positive relationship between primary and fish productivity has been demonstrated by empirical studies (e.g., Oglesby, 1977; McConnell et al., 1977; Almazan and Boyd, 1978b; McNabb et al., 1990; Knud-Hansen et al., 1990). Phytoplankton processes in solar-algae ponds typically dominate water quality dynamics, including diurnal and seasonal regimes of dissolved oxygen (Piedrahita, 1990; Piedrahita and Giovannini, 1991), the major nutrients of photosynthesis (DIC, DIN, DIP) (Boyd, 1979; King and Garling, 1983), and pH and alkalinity. For solar-algae ponds receiving prepared fish feeds, the role of phytoplankton as a food resource diminishes accordingly, but the major impact of phytoplankton on water quality remains (Boyd, 1990). Eutrophic ponds are characterized by large diurnal changes in primary productivity rates and in the resulting oxygen, carbon dioxide, pH, and unionized-ammonia levels, all of which impact fish performance. In fed ponds at night, the combined oxygen demand of phytoplankton, bacteria, and fish require increasing levels of nightly aeration as feeding rates increase above 50 kg/ha-day. For static ponds, a net benefit is not achieved from phytoplankton processes, as the oxygen produced by phytoplankton is re-consumed when the phytoplankton die and are oxidized by heterotrophic bacteria. For a relatively new class of aquaculture systems, termed "green water recirculation systems" or "partitioned aquaculture systems", algal cell retention times are controlled by continuous algal cropping and removal from the system. A net benefit from phytoplankton processes is therefore achieved, yielding a net addition of oxygen and net removal of fish metabolites. In contrast, flow-through aquaculture systems and housed recirculation systems are typically devoid of any phytoplankton processes, due to inadequate cell retention times and/or solar radiation levels.

Given this background, prediction of primary productivity and related processes is clearly an important task in aquaculture modeling. Primary productivity is mechanistically complex and influenced by a number of factors, including solar radiation, water turbidity, temperature, and nutrient availability. These factors can vary temporally and spatially, over diurnal and seasonal periods, and over the depth of the water column. Furthermore, these factors can vary stochastically (Straskraba, 1980), depending on the degree of environmental control that is applied to the system. It is well known in aquaculture research and production that identically managed solar-algae ponds can show significantly different behavior for no apparent reason. Nevertheless, a large amount of

phytoplankton modeling work applicable to the purposes here has been accomplished (e.g., Steele, 1962; Bannister, 1974; James, 1984; Straskraba and Gnauck, 1985; Piedrahita and Giovannini, 1991; Piedrahita et al., 1993; Giovannini and Piedrahita, 1994). This work shows that a sufficiently rigorous, deterministic modeling approach to phytoplankton processes can approximate primary productivity rates to a degree of accuracy such that the predicted rates are useful to facility design and management.

In the modeling procedure described below, phytoplankton is modeled as a single functional group of combined species (e.g. diatoms, green algae, and blue-green algae). Gross primary productivity (GPP; $\text{g C/m}^3\text{-day}$) is a function of (1) phytoplankton density, (2) maximum potential growth rate, (3) light intensity penetrating the water surface and column, (4) water temperature, and (5) concentrations of DIC (CO_2), DIN (NH_4^+ , NO_3^- , and N_2), and DIP (HPO_4^{2-}). Potassium, calcium, magnesium, and other minor nutrients are assumed non-limiting. Net primary productivity (NPP; $\text{g C/m}^3\text{-day}$) is a function of GPP, minus losses due to phytoplankton respiration. Rates of compound consumption and excretion by phytoplankton are based on metabolic stoichiometry. The presence of zooplankton is not considered, and the loss of phytoplankton due to zooplankton grazing is considered indirectly through the phytoplankton death rate. The loss of phytoplankton due to fish grazing is considered explicitly. Predicted phytoplankton process rates are used in mass balances for phytoplankton, particulate solids, and the metabolic compounds listed above. Dead phytoplankton contribute directly to particulate organic solids. Method variables for phytoplankton processes are listed in Table 6.7.

6.7.1 Gross and net primary productivity

Based on the sources and sinks of phytoplankton considered, the following differential equation is used to express the change in phytoplankton over time (dP/dt ; $\text{g C/m}^3\text{-day}$):

$$dP/dt = Q_i P_i - Q_e P_e + \text{GPP} - \text{PR} - \text{PD} - \text{FC}$$

where $\text{NPP} = \text{GPP} - \text{PR}$

Gross primary productivity (GPP) is calculated as a function of temperature, light, and the most limiting nutrient (e.g., Steele, 1962; Straskraba and Gnauck, 1985), assuming that these three scalars are multiplicative (Svirezhev et al., 1984):

$$\text{GPP} = \mu_{\max} \text{PC SCL}_T \text{ SCL}_L \min\{\text{SCL}_{\text{DIC}}, \text{SCL}_{\text{DIN}}, \text{SCL}_{\text{DIP}}\}$$

Table 6.7. Parameters and variables for phytoplankton processes

Symbol	Value ¹	Definition, units, and reported values (mean and/or range)
AOR _L	C	Adjustment for relative change in length of light travel due to refraction (dimensionless)
CCR	30	Carbon to chlorophyll-a ratio (g C/g chl a): 12.5 – 50 (Reynolds, 1984); 30 (Nath, 1996); 24 (Piedrahita, 1990)
chl a	C	Chlorophyll-a concentration (mg chl-a/m ³)
D	C	Pond depth (m)
FC	C	Consumption rate of phytoplankton by fish (gC/m ³ -day)
GPP	C	Gross primary productivity (gC/m ³ -day)
I ₀	C	PAR incident on the water surface (Einst/m ² -day)
I _{0D}	C	PAR at a given depth in the water column (Einst/m ² -day)
I _{0DM}	C	Mean PAR over a given depth of the water column (Einst/m ² -day)
I _S	50	Saturation PAR for phytoplankton (Einst/m ² -day): PAR intensity where maximum GPP occurs; 20.7 (Fritz et al., 1979); 23.7 – 142.4 (Piedrahita et al., 1993); 86, 60 – 173 (Giovannini and Piedrahita, 1994)
K _{DIC}	1.0	Half-saturation constant for carbon dioxide (g CO ₂ -C/ m ³): 1.0 (Fritz et al., 1979; Fritz, 1985); 6.0 (Nath, 1996); 0.5-0.6 (Chen and Orlob, 1975)
K _{DIP}	0.02	Half-saturation constant for ortho-phosphate (g HPO ₄ -P/ m ³): 0.02 (Fritz et al., 1979; Fritz, 1985); 0.035 (Nath, 1996); 0.03-0.05 (Chen and Orlob, 1975)
K _{N2}	20	Half-saturation constant for nitrogen gas (g N ₂ /m ³): estimated
K _{NO3}	0.3	Half-saturation constant for nitrate (g NO ₃ -N/m ³): 0.3-0.4 (Chen and Orlob, 1975); 0.3 (for DIN; Nath, 1996)
K _{TAN}	0.1	Half-saturation constant for TAN (g TAN/m ³): 0.1 (Fritz et al., 1979; Fritz, 1985)
K _{O2}	1.0	Half-saturation constant for oxygen for phytoplankton respiration (g O ₂ /m ³): estimated
LEC	C	Light extinction coefficient (1/m)
NPP	C	Net primary productivity (NPP; g C/m ³ -day)
PC	C	Phytoplankton concentration in terms of carbon (g C/m ³)
PD	C	Phytoplankton death rate (g C/m ³ -day)
PD _K	0.1	Phytoplankton specific death rate (1/day; included settling): 0.1 - 0.2 (based on typical cell age of 5-10 days); 0.05 (Nath, 1996; mortality only); 0.05 (used as a settling rate: Fritz et al., 1979; Fritz, 1985); 0.09 (Svirezhev et al., 1984)
P _e	C	Effluent phytoplankton concentration (g C/m ³)
P _i	C	Influent phytoplankton concentration (g C/m ³)
PR	C	Phytoplankton respiration rate (g C/m ³ -day)
PR _B	0.05	Phytoplankton base respiration rate (1/day): 0.08 (Fritz et al., 1979; Fritz, 1985); 0.1 (Nath, 1996); 0.05 (Chen and Orlob, 1975)

Table 6.7. Continued

Symbol	Value ¹	Definition, units, and reported values (mean and/or range)
PR _D	C	Daytime phytoplankton respiration rate (g C/m ³ -day)
PR _{GPP}	10	Phytoplankton respiration rate as a proportion of GPP (%): 10.0 (Culberson and Piedrahita, 1993)
PR _N	C	Nighttime phytoplankton respiration rate (g C/m ³ -day)
PS	C	Particulate solid concentration (g dw/m ³)
PS _C	C	Equivalent phytoplankton concentration of particulate solids (g C/m ³)
PS _{TS}	0.5	Particulate solids turbidity scalar (0-1; dimensionless)
Q _e	C	Effluent water flow rate (m ³ /day)
Q _I	C	Influent water flow rate (m ³ /day)
SC	2.0	Secchi constant (dimensionless): 1.7 (Giovannini and Piedrahita, 1994); 2.0 (Nath, 1996); range 1.2 – 2.7 (Straskraba and Gnauck, 1985)
SCL _{DIC}	C	GPP DIC scalar (0-1; dimensionless)
SCL _{DIN}	C	GPP DIN scalar (0-1; dimensionless)
SCL _{DIP}	C	GPP DIP scalar (0-1; dimensionless)
SCL _L	C	GPP light scalar (0-1; dimensionless)
SCL _{L-bot}	C	GPP light scalar, bottom layer water column (0-1; dimensionless)
SCL _{L-top}	C	GPP light scalar, top layer water column (0-1; dimensionless)
SCL _{NO3}	C	GPP NO3 scalar (0-1; dimensionless)
SCL _T	C	GPP temperature scalar (0-1; dimensionless)
SCL _{TAN}	C	GPP TAN scalar (0-1; dimensionless)
SDV	C	Secchi disk visibility (cm; range 1 - 1000)
T _{maxt}	45	Maximum temperature tolerance range (°C): 34 (Svirezhev et al., 1984); 35 (Nath, 1996)
T _{maxo}	35	Maximum temperature optimum range (°C): 24 (Svirezhev et al., 1984) 30 (Nath, 1996)
T _{mint}	3	Minimum temperature tolerance range (°C): 9 (Svirezhev et al., 1984) 20 (Nath, 1996)
T _{mino}	25-30	Minimum temperature optimum range (°C): 24 (Svirezhev et al., 1984) 30 (Nath, 1996)
α	1150	SDV-chlorophyll coefficient: 80 - 120 (Nath, 1996); 445 (Almazan and Boyd, 1978a)
β	0.67	SDV-chlorophyll exponent: 0.33 (Nath, 1996); 0.51 (Almazan and Boyd, 1978a)
φ _s	C	Incident short-wave solar radiation on a horizontal surface on earth (kJ/m ² -day): corrected for use of solar blocking/shading
μ _{max}	3.0	Phytoplankton maximum specific growth rate (g C/g C-day or 1/day): 3.0 (Svirezhev et al., 1984); 2.0 (Fritz et al., 1979; Fritz, 1985); 2.0 (Chen and Orlob, 1975); 2.25 (Nath, 1996)

¹ Numerical values are default values used in AquaFarm and C denotes a calculated variable

Some debate exists regarding the appropriate method for combining nutrient, light, and temperature limitation terms (Nath, 1996). Alternative forms of the GPP equation include placement of SCL_T and SCL_L within the minimum brackets (e.g. Chen and Orlob, 1975; Nath, 1996) and other formulations. For purposes here, it is assumed that (1) Liebig's limiting factor theory is appropriate for DIC, DIN, and DIP (Boyd, 1979), as based on a "building block" view of cell synthesis, and (2) that temperature and light are best represented as multiplicative scalars, since they represent available energy. Methods used for light and nutrient scalars are described below.

The photosynthesis temperature scalar (SCL_T) is calculated using the exponential scalar function described earlier (Svirezhev et al., 1984; see Figure 6.3). Tolerance and optimum temperature criteria were newly estimated for AquaFarm (Table 6.7; T_{\min} , $T_{\min o}$, $T_{\max o}$, and $T_{\max t}$), for which previously reported values (Svirezhev et al., 1984; Nath, 1996) were found to be excessively restrictive for a generally applicable phytoplankton model.

6.7.2 Respiration and death

Phytoplankton respiration rate (PR; $g\ C/m^3$ -day) is calculated during daytime as a proportion of GPP and during nighttime from a baseline respiration rate (Thomann et al., 1975; Culbertson and Piedrahita, 1993). The respiration temperature scalar (SCL_{TR}) is calculated by a different method than the photosynthesis temperature scalar, where the respiration rate continues to increase as temperatures become excessively high (similar to bacteria). Respiration is calculated by:

$$PR_D = GPP\ PR_{GPP} / 100.0$$

$$PR_N = [O_2 / (K_{O_2} + O_2)]\ SCL_{TR}\ PR_B\ PC$$

$$PR = \text{maximum} \{ PR_D, PR_N \}$$

$$\text{where if } T_{\min o} \leq T \leq T_{\max o} \quad \text{then } SCL_{TR} = 1.0$$

$$\text{or if } T < T_{\min o} \quad \text{then } SCL_{TR} = \theta_P (T - T_{\min o})$$

$$\text{or } (T > T_{\max o}) \quad \text{then } SCL_{TR} = \theta_P (T - T_{\max o})$$

The phytoplankton death rate (PD; $g\ C/m^3$ -day) as used here includes death, sedimentation, and grazing by zooplankton. Many species of algae have the ability to control their buoyancy, but some have a tendency to sink (e.g., diatoms; James, 1984). For purposes here, all live algae is considered to be buoyant, no settling occurs until death, the death rate is used to account for

permanent settling (no re-suspension) of live phytoplankton, and phytoplankton are assumed to be vertically mixed. In addition, the death rate is used to account for losses due to grazing by zooplankton. In this simplified form, phytoplankton death rate is calculated by (first-order decay):

$$PD = PD_K PC$$

6.7.3 Light scalar

The light scalar (SCL_L) is determined using a series of calculations that consider the availability of light in the water column and the response to this light by phytoplankton. When solar radiation is zero (night), SCL_L is zero, GPP is zero, and NPP is less than zero. Light scalar calculations are performed for each daylight hour from sunrise to sunset, even when the simulation time step is greater than one hour. The SCL_L for the actual time step (e.g., 1.0 day) is calculated as the mean of the hourly values. This internal, numerical integration procedure was found necessary to achieve consistency between daily and diurnal simulations.

Water turbidity represents the basis of the light scalar term and is expressed as Secchi disk visibility (SDV; cm). SDV is calculated from combined (1) phytoplankton concentration (PC) and chlorophyll-a content and (2) particulate solid concentration expressed as an equivalent phytoplankton concentration. Values used for the carbon to chlorophyll-a ratio (CCR) are reported to range from 12.5 to 50 and vary with phytoplankton condition and available light (Reynolds, 1984). A constant, intermediate CCR value is used here (default value 30). The decline in SDV with increasing PC can be represented as exponential decay (Almazan and Boyd, 1978a; Boyd, 1979; Nath, 1996):

$$PSC = PS \ P_{TS} \ (g \ C / g \ PS)$$

$$chla = (1000 \text{ mg/g}) (PC + PSC) / CCR$$

$$SDV = \alpha \ chla^{-\beta}$$

Reported values for parameters α and β show considerable variability, likely due to subjective errors in SDV measurements, analytical errors in the measurement of chlorophyll-a concentrations, and the presence of particulate solids in addition to phytoplankton. New α and β values were derived here, based on typical solar-algae ponds reported in the literature and when suspended solids consist only of live and dead phytoplankton. This derivation was based on two data points:

(1) PC = 7 g C/m³, chl-a = 233 mg/m³, and SDV = 29.8 cm and (2) PC = 20 g C/m³, chl-a = 667 mg/m³, and SDV = 14.7 cm. Impacts of alternative values for α and β are analyzed further in Chapter 8.

The light extinction coefficient (LEC; 1/m) is based on SDV (Giovannini and Piedrahita, 1994), including a correction term for light refraction (AOR_L; Piedrahita, 1990; see Chapter 5, Facility climate). Reported values for the Secchi constant (SC) range from 1.2 – 2.7 (Straskraba and Gnauck, 1985). LEC is calculated by:

$$\text{LEC} = \text{SC AOR}_L / [\text{SDV (m/100 cm)}]$$

Photosynthetically active radiation (PAR; I_O; Einstein/m²/d; 1.0 Einstein = 1.0 mol of PAR) is calculated as a proportion of incident solar radiation (ϕ_s ; kJ/m²-day; see Chapter 5, Facility climate). The ratio of PAR to solar radiation varies among plant species and ranges from 0.38 – 0.62 (Monteith, 1973). For phytoplankton, a ratio of 0.4 – 0.5 is typically used (Straskraba, 1980; Bernard, 1983). The conversion factor used here (505.67 kJ/Einst) is based on the assumption that 1.0 Einstein equals 217.44 kJ and 43% of overall radiation is photosynthetically active (Bannister, 1974). I_O is calculated by: $I_O = \phi_s / (505.67 \text{ kJ / Einstein})$

For use of the light scalar equation, it is necessary to calculate the ratio between the available PAR intensity (I_O) and the saturation PAR intensity (I_S) for phytoplankton. Smith (1980) assumed that I_S was equal to 30% of the daily mean PAR, while Nath (1996) used 50% of the daily mean PAR. Culbertson and Piedrahita (1993) assumed that I_S was equal to the maximum PAR intensity at a particular site on a given day, which removed consideration of photo-inhibition of phytoplankton by excessive light levels. Using these simplified approaches, the diurnal ratio of I_O/I_S is variable but the daily mean ratio for I_O/I_S is constant. Thus, these methods effectively remove annual variations in PAR from consideration. In the development of methods for purposes here, it was found that these simplified approaches were too simplistic for a generally applicable phytoplankton model and the ratio I_O/I_S is always calculated.

Piedrahita et al. (1993) observed a pronounced diurnal variation in I_S, where I_S increased from dawn to noon and decreased from noon to dusk. These results suggested a short-term (minutes) adaptive response of phytoplankton to light that is distinct from the more generally reported shade

and light adaptation occurring over periods of several hours to several days. However, a suitable method for estimating variable I_S values for diurnal and annual periods was not found in the literature or developed here, and a constant value is used for I_S (e.g., 50 Einstein/m²/d).

Light intensity incident on a water surface (I_0) is attenuated exponentially as it penetrates the water column (I_{OD}), according to Beer's Law (Giovannini and Piedrahita, 1994; Piedrahita et al., 1993). This function can be integrated over a given depth to determine the mean light level over the given depth (I_{ODM}). Assuming that phytoplankton and particulate solids are vertically mixed, I_{OD} and I_{ODM} are calculated by:

$$I_{OD} = I_0 e^{(-LEC * D)}$$

$$I_{ODM} = (I_0 - I_{OD}) / [\ln(I_0 / I_{OD})]$$

The light scalar (SCL_L) is calculated by combining equations for light availability and phytoplankton response to light level, and then integrating the derived function over water depth (Steele, 1962; Piedrahita et al., 1993; Giovannini and Piedrahita, 1994; Field and Effler, 1982):

$$SCL_L = [e^{1.0 / (LEC D)}] [e^{[(-I_0 / I_S) \exp(-LEC D)]} - e^{(-I_0 / I_S)}]$$

This equation was verified to be correct by comparing results to numerical integration procedures. For cases where vertical stratification of the water column is considered, phytoplankton productivity rates in the two horizontal water layers are separately accounted. However, phytoplankton populations are also vertically mixed at each simulation step, as required for the correct use of these light scalar equations. The mean of the top and bottom layer light scalars equals the overall column scalar. Stratified light scalar terms are calculated by:

$$SCL_{L-top} = [e^{1.0 / (LEC D / 2.0)}] [e^{[(-I_0 / I_S) \exp(-LEC D / 2.0)]} - e^{(-I_0 / I_S)}]$$

$$SCL_{L-bot} = (2.0 SCL_L) - SCL_{L-top}$$

For typical values of light extinction and depth in solar-algae aquaculture ponds (high turbidity), the SCL_L equation can be simplified to (Culberson and Piedrahita, 1993):

$$SCL_L = [e^{1.0 / (LEC D)}] [1.0 - e^{(-I_0 / I_S)}]$$

6.7.4 Nutrient scalars

Individual nutrient scalars are calculated by saturation kinetics. TAN, NO₃, and/or N₂ may be used for the DIN requirement (Eppley et al., 1969; Toetz et al., 1973). The half-saturation constant used for TAN (0.1) is lower than that for NO₃ (0.3), corresponding to the preference for TAN (i.e. reduced nitrogen) by phytoplankton. The preference for a substrate is proportional to the reciprocal of its half-saturation constant. The half-saturation constant for N₂ (20.0) is assumed to be relatively large, so that the uptake of fixed nitrogen is dominant, but the aquaculture literature was weak in this area. As expected, ratios between K_{DIC}, K_{DIN}, and K_{DIP} are roughly comparable to the mass uptake ratios of these compounds (see Process stoichiometry). Nutrient scalars are calculated by:

$$SCL_{DIC} = DIC / (K_{DIC} + DIC)$$

$$SCL_{DIN} = SCL_{TAN} + SCL_{NO3} + SCL_{N2}$$

and $SCL_{DIP} = DIP / (K_{DIP} + DIP)$

where $SCL_{TAN} = (TAN / K_{TAN}) / d$

$$SCL_{NO3} = (NO_3 / K_{NO3}) / d$$

$$SCL_{N2} = (N_2 / K_{N2}) / d$$

where $d = 1.0 + (TAN / K_{TAN}) + (NO_3 / K_{NO3}) + (N_2 / K_{N2})$

6.8 Process stoichiometry

The biological processes described in this chapter can be represented as balanced chemical equations, which are used to determine stoichiometric ratios between compounds and the primary substrate (Table 6.8). Stoichiometric ratios are combined with the mass flux rate of the primary substrate (calculated earlier) to determine compound consumption and excretion rates for use in differential equations. In the integrated approach used here, the combined stoichiometries of photosynthetic, heterotrophic, and nitrification processes are considered to be a balanced system (Figure 6.4). This is a critical requirement for realistic modeling, especially for long-term simulations of solar-algae ponds. In particular, when fish and denitrification process are not present and alkalinity is not added or removed from the system, imbalances in photosynthetic, heterotrophic, and nitrification processes cause pH to decrease or increase to unrealistic levels.

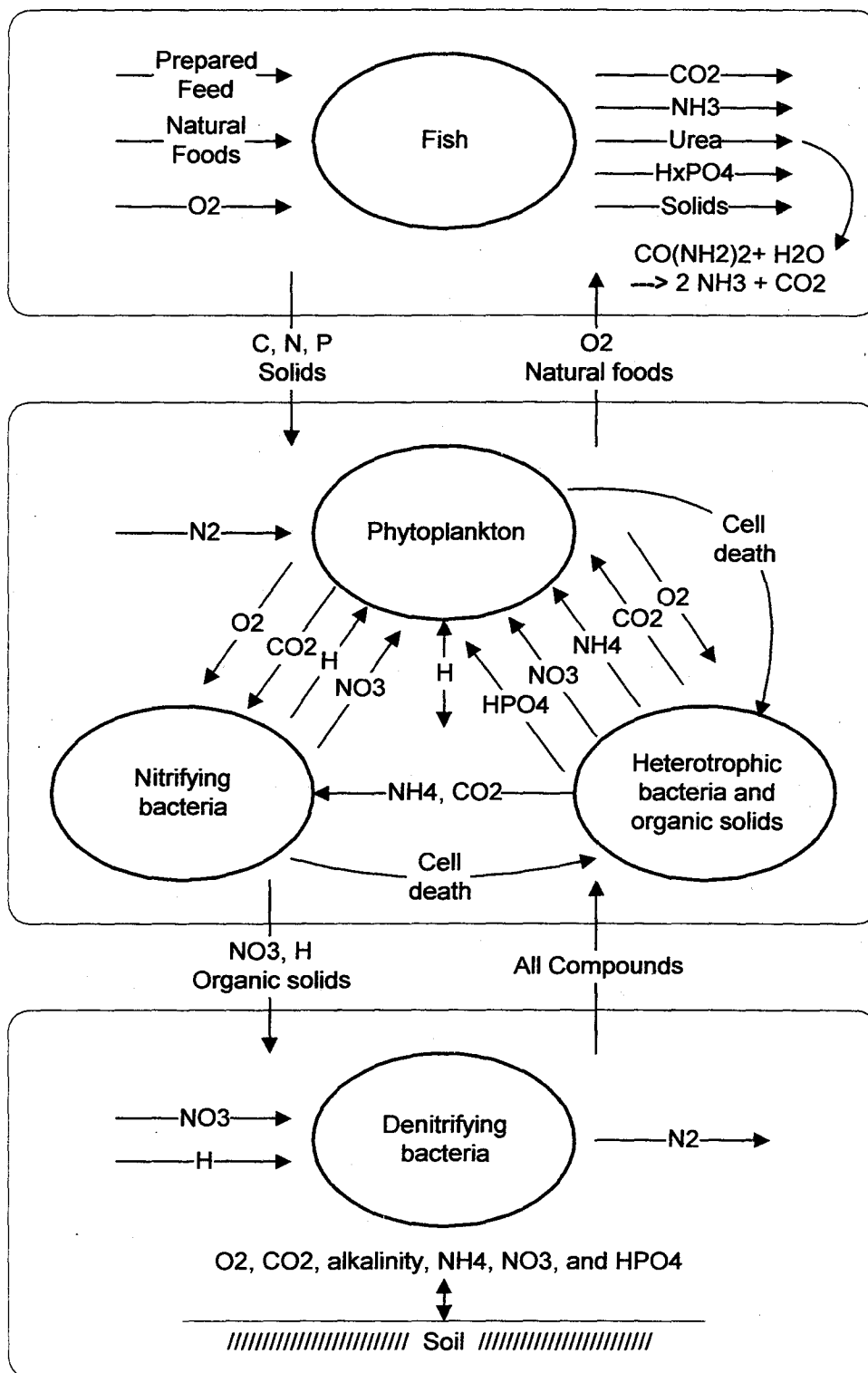
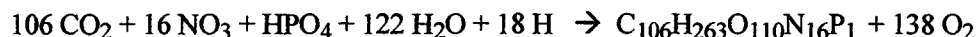
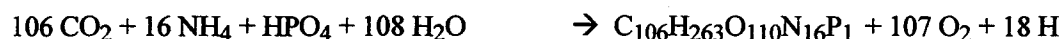


Figure 6.4. Interrelated stoichiometries of fish, photosynthetic, heterotrophic, nitrification, denitrification, and soil processes in a solar-algae pond

6.8.1 Phytoplankton

For phytoplankton, uptake ratios of DIC, DIN, and DIP (CNP ratio) are defined by the molar ratios of these compounds in phytoplankton cells ($C_{106}H_{263}O_{110}N_{16}P_1$; MW 3550 g/mol; Stumm and Morgan, 1981). The molar composition of phytoplankton varies somewhat with species (Fritz, 1985), and the formula used is assumed to represent an average composition. The required CNP ratio on a molar basis is therefore 106 – 16 – 1, which by conversion can be shown to be comparable to the mass CNP ratio of 40 – 7 – 1 (Redfield ratio; Redfield et al., 1963). The photosynthetic stoichiometry of phytoplankton can be represented by three equations, which differ by nitrogen source (NH_4 , NO_3 , and N_2):

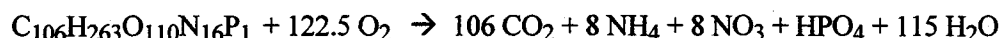


As evident in these equations, the impact of phytoplankton processes on alkalinity (and pH) depends on the nitrogen source. Phytoplankton use of bicarbonate (HCO_3) is not considered in these equations, for which the differential uptake of bicarbonate (HCO_3) versus CO_2 would also impact alkalinity. Phytoplankton are known to use HCO_3 when CO_2 levels are very low, but the related impact on the alkalinity stoichiometry of phytoplankton is not well understood (Goldman et al., 1981). By the approach used here, photosynthetic rates respond to DIC but phytoplankton consume CO_2 . The ability of algae to take up and store nutrients when nutrient levels are high (luxury consumption) and to utilize these nutrients when nutrient levels fall (e.g., James, 1984) is not considered.

The third of the stoichiometric equations listed above represents atmospheric nitrogen (N_2) fixation by blue-green algae (Cyanobacteria; El Samra and Olah, 1979; Lin et al., 1989; Hariyadi et al., 1994). Blue-green algae are known to reach high concentrations in nutrient enriched, solar-algae fish ponds. The relative abundance and dynamics of blue-green algae in aquaculture systems is related to various environmental conditions in complex ways and has not been studied to a degree that supports development of quantitative models. In the approach used here, phytoplankton is modeled as a single functional group of combined species which includes blue-green algae, N_2 can

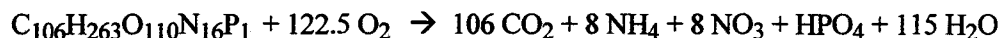
be used as a nitrogen source, and the impact of N_2 fixation on phytoplankton stoichiometry is considered. As the half-saturation constant for N_2 is decreased, the corresponding role of N_2 as a nitrogen source and the implicit, relative abundance of blue-green algae are increased.

If phytoplankton are in a net respiration mode ($NPP < 0$), then the first two of the photosynthetic stoichiometry equations are used together, equal output of NH_4 and NO_3 is assumed, H terms cancel, the impact of HPO_4 on alkalinity is ignored, and respiration has no net impact on alkalinity:

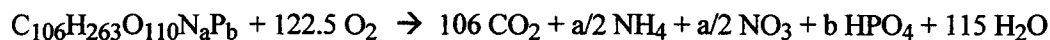


6.8.2 Heterotrophic bacteria

Oxidation of organic particulate solids (PS and PSS) by heterotrophic bacteria is equivalent to phytoplankton respiration, where equal output of NH_4 and NO_3 is assumed and there is no net impact on alkalinity. Oxygen consumption (carbonaceous biochemical oxygen demand) and carbon dioxide production per dry weight solids consumed are equivalent to the associated mass ratios of photosynthesis. However, the DIN and DIP content and associated stoichiometric ratios of PS and PSS are variable and are dependent on the contributing solid sources. Thus, the stoichiometry represented by $C_{106}H_{263}O_{110}N_{16}P_1$:

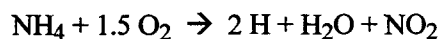


is adjusted to reflect the variable composition of $C_{106}H_{263}O_{110}N_aP_b$:



6.8.3 Nitrifying bacteria

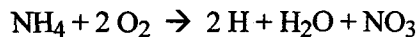
The stoichiometry of nitrification is a combination of two process steps (Wheaton et al., 1994a), where the first step is mediated by *Nitrosomonas* and related genera:



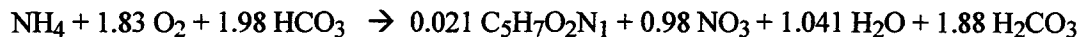
and the second step is mediated by *Nitrobacter* and related genera:



and the combined process is:



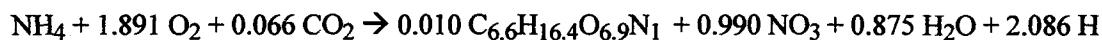
Adding cell production gives:



which can be rearranged in terms of H to give:



In the integrated approach used here, however, the stoichiometry of photosynthetic, heterotrophic, and nitrification processes is considered a balanced system (Figure 6.4). Thus, the stoichiometry of nitrification used here is slightly different from that cited above and uses a bacterial cell composition of $\text{C}_{6.6}\text{H}_{16.4}\text{O}_{6.9}\text{N}_1$ (mw = 220.2; equivalent to $\text{C}_{106}\text{H}_{263}\text{O}_{110}\text{N}_{16}\text{P}_1$ on a per N basis):



6.8.4 Denitrifying bacteria

The stoichiometry of denitrification is given by (Tchobanoglous and Burton, 1991):



The consumption of organic compounds and production of bacterial cells and carbon dioxide are ignored, and the stoichiometry used is therefore: $\text{NO}_3 + \text{H} \rightarrow 0.5 \text{N}_2$

Table 6.8. Stoichiometric ratios (SR) for compound uptake (-) and production (+) by phytoplankton and bacteria

Phytoplankton (net photosynthesis)	SR relative to DIC uptake
g O ₂ / g C (for NH ₄ uptake)	SR _{O2-NH4} = - 2.692
g O ₂ / g C (for NO ₃ uptake)	SR _{O2-NO3} = - 3.472
g O ₂ / g C (for even NO ₃ & NH ₄ uptake)	SR _{O2} = - 3.082
g O ₂ / g C (for N ₂ uptake)	SR _{O2-N2} = - 2.865
g O ₂ / g C (for NH ₄ , NO ₃ , & N ₂ uptake)	SR _{O2} = (SR _{O2-NH4} SR _{NH4} + SR _{O2-NO3} SR _{NO3} + SR _{O2-N2} SR _{N2}) / (SR _{NH4} + SR _{NO3} + SR _{N2})
g N/ g C	SR _N = 0.1759
g NH ₄ -N/ g C	SR _{NH4} = SR _N SCL _{NH4} / SCL _N
g NO ₃ -N/ g C	SR _{NO3} = SR _N SCL _{NO3} / SCL _N
g N ₂ / g C	SR _{N2} = SR _N SCL _{N2} / SCL _N
g HPO ₄ -P/ g C	SR _P = 0.0244
g H/g C (for NH ₄ uptake)	SR _{H-NH4} = 0.014251
g H/g C (for NO ₃ uptake)	SR _{H-NO3} = - 0.014251
g H/g C (for N ₂ uptake)	SR _{H-N2} = - 0.014251
g H/g C (for even NO ₃ & NH ₄ uptake)	SR _H = 0
g H/g C (for NH ₄ , NO ₃ , & N ₂ uptake)	SR _H = (SR _{H-NH4} SR _{NH4} + SR _{H-NO3} SR _{NO3} + SR _{H-N2} SR _{N2}) / (SR _{NH4} + SR _{NO3} + SR _{N2})
Phytoplankton (net respiration)	SR relative to DIC production
g NH ₄ -N/ g C	SR _{NH4} = 0.1759 / 2.0
g NO ₃ -N/ g C	SR _{NO3} = 0.1759 / 2.0
g N ₂ -N/ g C	SR _{N2} = 0
g HPO ₄ -P/ g C	SR _P = 0.0244
g H/ g C (for even NO ₃ & NH ₄ excretion)	SR _H = 0
g O ₂ / g C (for even NO ₃ & NH ₄ excretion)	SR _{O2} = - 3.082

Table 6.8. Continued

Organic solid oxidation	SR relative to solids consumption (dw)
g O ₂ / g dw solids (ultimate CBOD)	SR _{O₂} = 1.105
g CO ₂ -C/ g dw solids	SR _{CO₂-C} = 0.359
g NH ₄ -N and NO ₃ -N/ g dw solids	Balanced; depends on N content of solids
g HPO ₄ -P/ g dw solids	Depends on P content of solids
Nitrification	SR relative to TAN consumption
g O ₂ / g N (nitrogenous biochemical oxygen demand, NBOD)	SR _{O₂} = 4.320; compare 4.18 g O ₂ / g NH ₄ -N (Wheaton et al., 1994a)
g H/ g N	SR _H = 0.150; compare 7.14 g CaCO ₃ /g NH ₄ -N (Wheaton et al., 1994a)
g cell/ g N (based on 0.17, but mol cell in balanced equation rounded from 0.011 to 0.01)	SR _{cell} = 0.157; compare 0.17 g cells/ g NH ₄ -N (Wheaton et al., 1994a)
Denitrification	SR relative to NO₃ consumption
g H/ g NO ₃ -N	SR _H = 0.072
g N ₂ / g NO ₃ -N	SR _{N₂} = -1

7. Methods of Fish Biology

Methods of fish biology used in AquaFarm consist of the application of environmental physiology and bioenergetics to fish performance in aquaculture systems. Areas of interest include fish response to environmental variables and quantitative aspects of fish metabolism, feeding, growth, and survival. Fish performance engineering (Ernst, 2000) is a fundamental component of aquacultural engineering, given that fish growth and biomass support represent the primary processes for which fish culture systems are designed and managed. The methods presented here are applicable to facility design and production management for both finfish and crustaceans (together referred to hereafter as “fish”) in all types of aquaculture systems.

7.1 Fish performance engineering

The fundamental principles of fish performance engineering are based upon physiological energetics (Brett and Groves, 1979; Hepher, 1988; Jobling, 1994). Physiological energetics, commonly referred to as bioenergetics, concerns the rates of energy losses and gains and the efficiencies of energy transformation for a whole organism or group of organisms, as distinguished from cellular energetics (Lehninger, 1965) and ecological energetics (Odum, 1971). In this respect, fish and fish foods can be expressed in terms of their material composition or the energy equivalent of these materials. Fish gain energy through food ingestion (I), store energy as growth (G), lose energy through excretion (E), and expend energy through metabolism (M). To apply physiological energetics to fish performance engineering, these energy sources and sinks are combined into a bioenergetic budget: $I = G + E + M$. In response to analytical objectives, this budget can be rearranged to calculate energetic capacities (or scopes) for fish activity (Fry, 1947; Fry, 1971), growth (Paloheimo and Dickie, 1966; Warren and Davis, 1967; Warren, 1971), or feeding (Cuenco et al., 1985a,b,c). For an average carnivorous fish, Brett and Groves (1978) provide relative proportions of the bioenergetic budget terms per 100 calories of ration ingested (expressed as 95 % confidence intervals). This budget shows that a third or less of ingested energy is channeled to growth:

$$(29 \pm 6) G = 100 I - (27 \pm 3) E - (44 \pm 7) M$$

A flow chart of the sources, sinks, and pathways of fish bioenergetics is presented in Figure 7.1. For an individual fish, energy input begins with ingested energy and food conversion efficiency is the proportion of ingested energy incorporated as growth. In the application of bioenergetics to

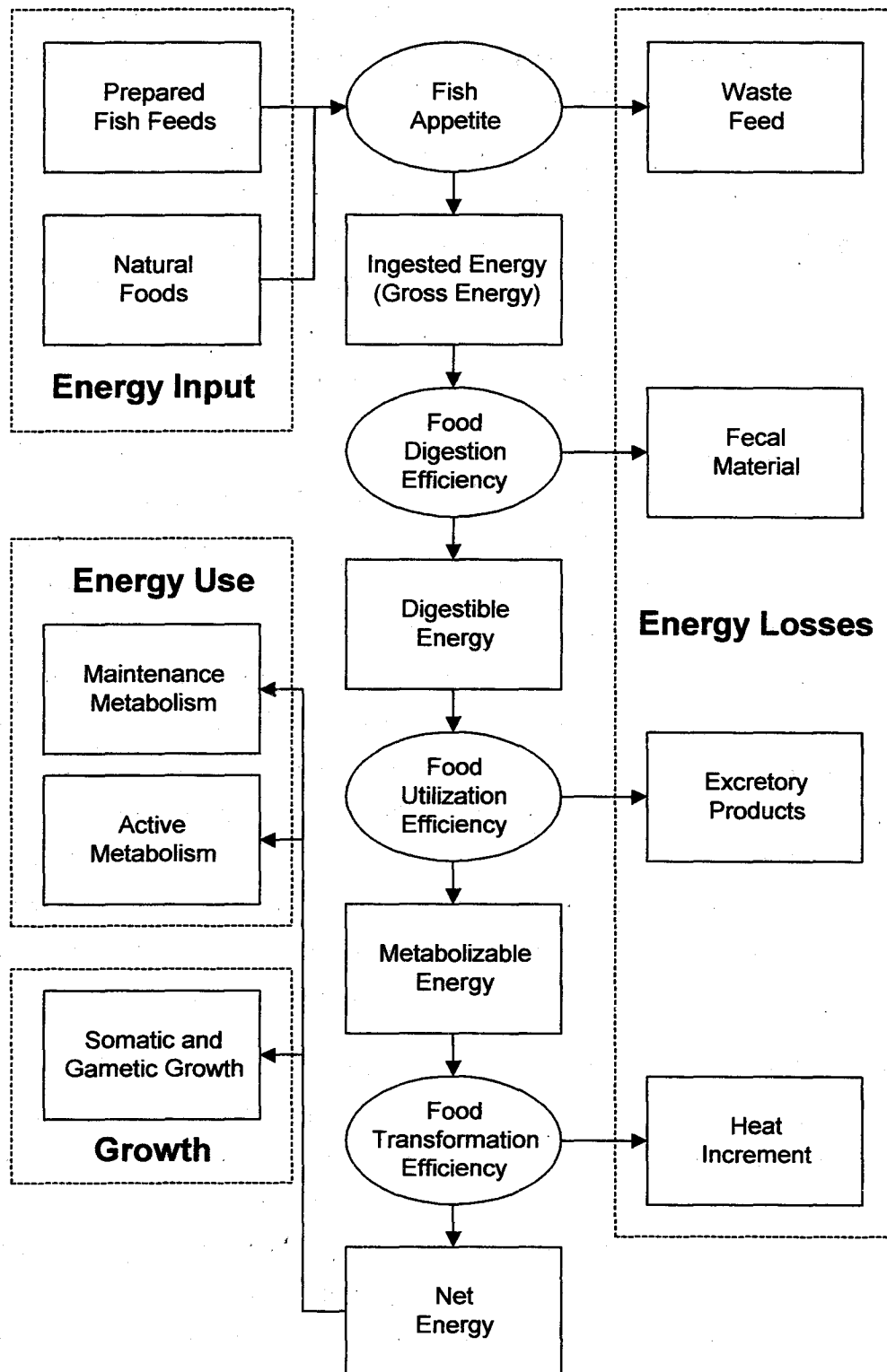


Figure 7.1. Flow diagram of fish bioenergetics showing energy sources, sinks, controlling processes, and distribution paths

aquaculture, however, fish are managed and analyzed as populations (fish production lots), and quantities of feed applied, feed wasted, and fish mortality are also included in food conversion efficiency values. Metabolic energy demands are supported through the catabolism of food substrates, in which oxygen is consumed and metabolites (or catabolites) are produced. Metabolic energy demands are comprised of three major components: (1) Maintenance metabolism includes standard metabolism, defined as the rate of energy use by a fasting fish at rest, and additional demands such as those due to responses to environmental stress. (2) Active metabolism consists of the energy demands of swimming, aggression, and feeding (locomotion). (3) Heat increment (or specific dynamic action) represents the energetic costs of processing and assimilating food.

Rates of fish metabolism, feeding, and growth vary diurnally, seasonally, and over the life of a fish in response to changes in fish and environmental factors (Brett, 1979). Fish performance is a graded response to temporally and spatially graded environmental conditions, and the effect of environmental variables on fish activity, appetite, and growth is mediated through metabolism. The variables driving fish performance include (1) fish rearing-unit shape and dimensions, hydraulic characteristics, and water velocity, (2) water quality, (3) day length and fish exposure to direct light, (4) disturbances from human activity and fish handling practices (e.g. fish grading), (5) fish density as it affects fish behavior and access to food resources, (6) fish development state and size, (7) the availability and quality of natural food, and (8) the application and quality of prepared feeds. The response variables of fish performance include (1) disease resistance, stress accumulation and compensation, and survival, (2) swimming capacity, behavioral aggression, and competition for limited food resources, (3) appetite levels, food ingestion rates, and food assimilation efficiencies, (4) sexual maturation and reproduction (gametic growth), and (5) somatic growth.

In the development of AquaFarm, fish performance methods and models were both collected from the literature and newly developed, as required to construct an integrated, analytical framework for fish performance engineering. Alternative methods are provided in order to support various analysis resolution levels (see Chapter 2) and approaches to fish performance modeling. As in the supporting literature, simplifying assumptions and aggregated processes are utilized regarding the variables and functions used to represent bioenergetic processes. Driving variables are limited to fish size, water quality and photoperiod, and food quantity and quality variables. Response variables are limited to survival, somatic growth, feeding, and total metabolism. In contrast to actual cause and effect relationships, environmental impacts on growth and feeding are calculated directly and metabolic rates are calculated as a function of feeding rates. Feeding and growth rates are related by food conversion efficiencies. Metabolic rates of concern are limited to oxygen consumption and

metabolite excretion, and components of metabolism are combined and expressed as total oxygen consumption and metabolite excretion rates (g compound/kg fish/day or mg compound/kg fish/hr).

7.2 Fish environmental criteria and response

Environmental criteria of fish include water quality and related fish biomass and feed loading variables. Species-specific criteria collected from a wide review of the aquaculture literature (Table 7.1) are provided as default, user accessible values according to the fish species in use. These criteria are mainly intended for application to growth and feeding rates, and specific criteria values should be used as approximate guidelines. Criteria values are dependent on fish nutrition status, stress level, life stage, body size, and environmental acclimation. In addition, criteria for one variable may depend on levels of other variables. For example, minimum criteria for dissolved oxygen increase as carbon dioxide levels increase. Fish biomass and feed loading variables can be used as indicators of water quality, but only when relationships between these loading levels and associated dissolved oxygen and metabolite levels have been determined. Relationships between loading and water quality variables are highly dependent on the specific aquaculture system, but are provided to simplify the simulation of fish biomass support when loading criteria are known.

Up to four criteria are used for each environmental variable, consisting of minimum and maximum values for tolerance and optimum ranges (Fry, 1947; Fry, 1971; Warren and Davis, 1967; Warren, 1971; Brett, 1979; Brett and Groves, 1979; Svirezhev, 1984; Cuenco et al., 1985b). From low to high, these criteria are identified as C_{\min} , $C_{\min o}$, $C_{\max o}$, and C_{\max} . In the optimum range ($C_{\min o}$ to $C_{\max o}$), maximum growth rates are supported with respect to the given variable. The width of the optimum range is related to the capacity for environmental acclimation by the fish. The tolerance range (C_{\min} to C_{\max}) spans beyond the optimum range and conditions here cause a reduction in growth rates, depending on the degree of deviation from optimum limits. The lethal range exists outside of the tolerance range. Conditions here do not support fish growth and, when sustained, result in mortality. For simulation applications, if any variable diverges to the lethal range, the corresponding fish lot is assumed to immediately suffer total mortality. Only lower or upper criteria may be sufficient for some variables, e.g., water temperatures and dissolved oxygen levels often vary below maximum optimum levels. Only maximum criteria need to be considered for fish metabolites.

Table 7.1. Fish environmental criteria, as defined by low and high values for tolerance (C_{mint} and C_{maxt}) and optimum (C_{mino} and C_{maxo}) ranges, with respect to fish growth and feeding *

Physical variables		Criteria			
Temperature	Fish species	C_{mint}	C_{mino}	C_{maxo}	C_{maxt}
(C)	Brook trout	3	8	13	19
	Pacific salmon	3	9	14	22
	Rainbow trout	3	11	17	23
	Atlantic salmon	3	12	18	22
	Yellow perch	8	18	22	27
	White sturgeon	6	19	22	26
	Striped bass	7	20	25	31
	Marine shrimp	10	20	30	36
	Centrarchids	12	20	28	33
	Freshwater prawns	10	22	28	33
	Hybrid striped bass	10	23	28	33
	Common carp	5	24	30	35
	Channel catfish	12	25	30	34
	Tilapia	15	28	33	37
Salinity (ppt)	<i>Basis:</i> primary physiological criterion and highly dependent on fish species and life stage				
	<i>Values:</i> narrow ranges for stenohaline species, wider ranges for euryhaline species, and criteria range from near zero to > 35.0				
pH	<i>Basis:</i> primary controlling factor of fish performance; exerts major impact on other water quality variables (e.g. unionized ammonia of total ammonia) and other facility processes (e.g. biofilter nitrifying bacteria).				
	<i>Values:</i> approximate $C_{\text{mint}} - C_{\text{maxt}}$ range is 6.5 - 8.0 for trout and 6.0 - 9.5 for catfish and tilapia				
Alkalinity (mg CaCO_3/L)	<i>Basis:</i> closely related to pH and water hardness criteria and mainly used as a measure of water buffering capacity for decreases in pH				
	<i>Values:</i> approximate ranges are ≥ 20 for flow through systems, ≥ 50 for phytoplankton systems, ≥ 100 for recirculation systems, and ≤ 500 mg/L for all systems				
Hardness (mg CaCO_3/L)	<i>Basis:</i> calcium and magnesium are required nutrients for body composition and osmoregulation				
	<i>Values:</i> approximate $C_{\text{mint}} - C_{\text{maxt}}$ range is 50 - 350				

* Values represent an approximate consensus of reported values in the aquaculture literature. Use of terms "controlling factor" and "limiting factor" is according to their standard use in bioenergetics (Brett and Groves, 1979).

Table 7.1. Continued

Fish biomass loading variables	Criteria
Biomass density (kg/m ³)	<ul style="list-style-type: none"> • <i>Basis</i>: biomass support and fish behavior; values range widely and depend on fish species, feeding rate, and type of culture system; used for systems with known biomass capacities • <i>Values</i>: expressed as biomass density index (kg/ m³/ cm-length); approximate C_{maxt} are 0.05 for extensive production, 1.5 – 3.0 for salmon hatcheries, and 3.0 – 20.0 for intensive production
Biomass loading (kg/m ³ -d)	<ul style="list-style-type: none"> • <i>Basis</i>: biomass support; values range widely and depend on fish species, influent water quality, and production intensity; used for systems with known biomass loading capacities • <i>Values</i>: expressed as biomass loading index (kg/ m³/ d/ cm-length); approximate C_{maxt} are for 0.1 for intensive trout production and 0.3 for intensive tilapia production
Feed loading (kg feed/m ³ -d)	<ul style="list-style-type: none"> • <i>Basis</i>: system capacity to digest feed and related oxygen demand and metabolite production; highly dependent on fish species and culture system; used for systems with known feed loading capacities • <i>Values</i>: approximate C_{maxt} are for 0.1 for intensive trout production and 0.3 for intensive tilapia production, where these example values are equivalent to biomass loading criteria for a 33-cm fish fed 3.0 % bw/ day
Water exchange rate (no./day)	<ul style="list-style-type: none"> • <i>Basis</i>: biomass support and water velocity, and other considerations similar to biomass loading; used for systems with known water exchange rate requirements. • <i>Values</i>: values range from zero for water-loss makeup only to three exchanges per hour for intensive, flowing water culture (72/day)
Cumulative oxygen consumption (COC, mg O ₂ /L)	<ul style="list-style-type: none"> • <i>Basis</i>: metabolite stoichiometry and criteria in relation to oxygen consumption; used for systems with known relationships between COC values, pH values, and metabolite concentrations. • <i>Values</i>: for a pH range 6.0 - 9.0, approximate C_{maxt} values range 14 – 25 for carbon dioxide constraints and 0.5 - 100 for unionized ammonia constraints

Table 7.1. Continued

Dissolved gases		Criteria			
Dissolved oxygen (DO; mg O ₂ /L)	Fish Species	C _{mint}	C _{mino}	C _{maxo}	C _{maxt}
<i>Basis</i> : primary limiting factor of fish performance	Salmonids	5	7	Use	Use
	Striped/hybrid bass	4	6	percent	percent
	Catfish	3	6	saturation	saturation
	Carp	2	6		
	Tilapia	2	5		
DO (% saturation)	All species	30	50 - 70	200	300
Dissolved carbon dioxide (mg CO ₂ /L)	<ul style="list-style-type: none"> • <i>Basis</i>: primary limiting factor of fish performance, minimum criteria are zero in value, maximum criteria decrease as dissolved oxygen levels decrease below lower optimum levels • <i>Values</i>: approximate C_{maxt} range is 20.0 - 50.0, where values ≥ 100.0 are reported to be tolerated for some species 				
Total gas pressure (TGP; % saturation, or mm-Hg pressure difference between TGP and local barometric pressure)	<ul style="list-style-type: none"> • <i>Basis</i>: gas super saturation can cause gas bubble formation in fish blood and tissues (gas bubble disease) • <i>Values</i>: approximate C_{maxt} range is 105 - 110 % sat. or 38 - 76 mm Hg; approximate C_{maxt} is 102 - 103 % sat. for sensitive species and life stages (e.g. eggs). 				
Metabolites		Criteria			
Unionized ammonia (mg NH ₃ -N/L)	Fish Species	C _{mint}	C _{mino}	C _{maxo}	C _{maxt}
<i>Basis</i> : primary limiting factor of fish performance	Salmonids	0.0	0.0	0.01	0.2
	Striped/hybrid bass	0.0	0.0	0.02	0.3
	Carp	0.0	0.0	0.02	0.5
	Crustaceans	0.0	0.0	0.05	0.7
	Catfish	0.0	0.0	0.05	0.9
	Tilapia	0.0	0.0	0.10	1.0
Nitrite (mg NO ₂ -N/L)	<ul style="list-style-type: none"> • <i>Basis</i>: primary limiting factor of fish performance, minimum criteria are zero, and criteria are highly dependent on fish species and life stage and water salinity, hardness, and dissolved oxygen • <i>Values</i>: approximate C_{maxt} is 0.1 for trout, 2.0 for catfish, and 4.0 for tilapia; C_{maxt} may range from 10 - 20 for tolerant species when sufficient chloride is present as natural or added salts 				
Nitrate (mg NO ₃ -N/L)	<ul style="list-style-type: none"> • <i>Basis</i>: effect on fish is likely limited to impaired osmotic regulation at very high concentrations, which may occur in recirculating fish culture systems with low system exchange rates and no denitrification • <i>Values</i>: approximate C_{maxt} range is ≤ 50 - 300 for all species 				
Particulate solids (mg dry wt./L)	<ul style="list-style-type: none"> • <i>Basis</i>: impaired fish ventilation and gill abrasion and tolerance to solids is highly dependent on fish species. Includes inorganic, organic, and phytoplankton particulate solids. • <i>Values</i>: approximate C_{maxt} is 10 - 80 for solids of feed and fecal origin, e.g. C_{maxo} and C_{maxt} are about 10 and 25 for salmonids, a species with low tolerance to particulate solids 				

7.2.1 Fish response to environmental variables

The criteria values listed in Table 7.1 are used in conjunction with one of the scalar functions (see Chapter 6, Environmental scalars) to calculate a scalar value (range 0 – 1) for each environmental variable that falls outside of its optimum range (Figure 7.2). Individual scalars are combined based on their product (interactive variables; e.g., oxygen and carbon dioxide) and/or minimum (non-interactive variables). This combined scalar is referred to as the water quality scalar (SCL_{WQ}) and may be optionally applied to broodfish maturation rates, egg development rates, and fish growth and feeding rates. Water temperature is typically accounted for explicitly in fish performance models, rather than being included in SCL_{WQ}. Normally, depth-averaged water quality is used. If the cultured organism is a bottom dweller (e.g., shrimp) and water quality is vertically stratified, then benthic water quality is used.

7.2.2 Fish swimming speed

Rearing-unit water velocity (U; cm/s) and fish swimming speed (FSS; body lengths/ s) are important variables regarding fish metabolic rate, exercise, vigor, and meat quality. These variables are related by (Brett 1964):

$$\begin{aligned} \text{FSS} &= U / L \\ M_A &= M_S 10^{(b \text{ FSS})} \end{aligned}$$

where L = fish length (cm), M_A = active (swimming) metabolic rate (mg O₂/kg fish/hr), M_S = standard metabolic rate (mg O₂/kg fish/hr), and b = coefficient (temperature dependant). As FSS increases above 1.0 BL/s, metabolic demands of swimming increasingly dominate bioenergetic budgets. This approach can be misleading, however, as cultured fish swim both slower and faster than the mean water velocity, in the course of diurnal activity levels and due to the existence of velocity gradients and eddies in rearing units that are utilized by resting fish. This is especially true at FSS less than 0.5 to 1.0 BL/s, where spontaneous swimming predominates over swimming required to maintain position (Brett and Glass 1973). For example, in a 30-m long raceway with a complete water exchange every 20 minutes, a relatively high velocity culture environment, U is 2.5 cm/s and FSS is only 0.5 BL/s for a 5.0-cm fish. For purposes here, FSS is not explicitly considered in bioenergetic budgets or used as an environmental criterion. Water velocity is more likely to be managed with respect to the transport of settleable solids than for fish swimming speed.

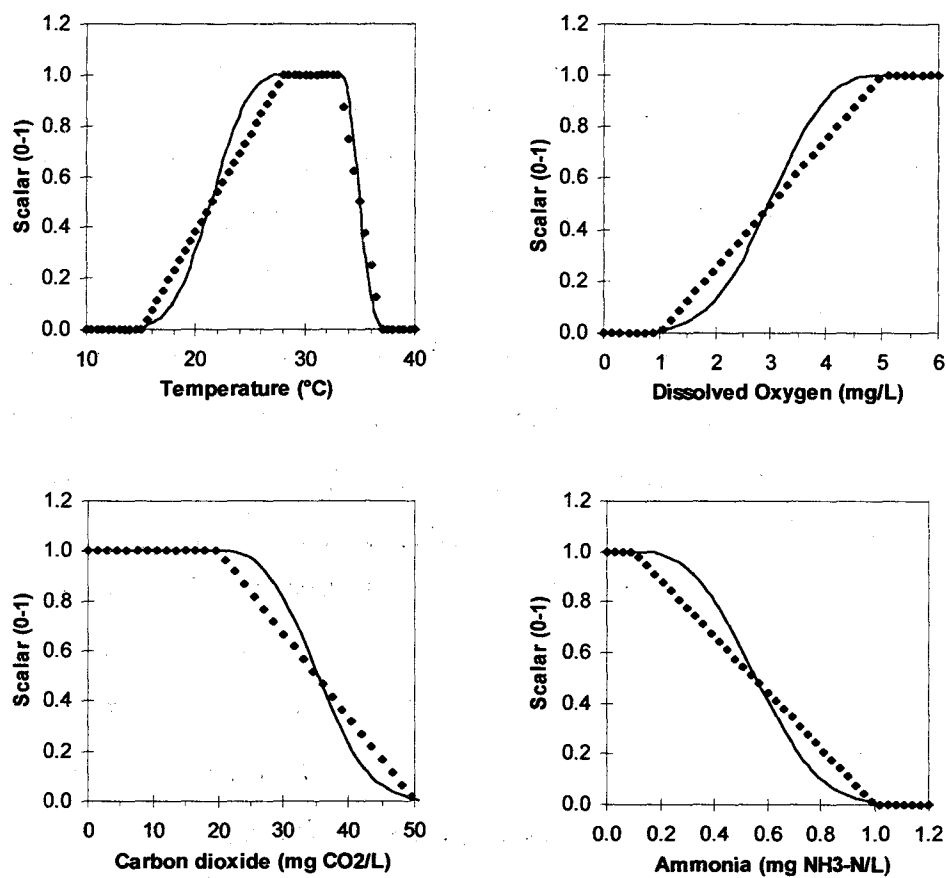


Figure 7.2. Linear (points) and exponential (lines) scalar functions used for modeling fish response to environmental conditions, applied to the response of tilapia to water temperature, dissolved oxygen, dissolved carbon dioxide, and unionized ammonia

7.3 Expressions for fish size, growth, and feeding

The following expressions for fish size, growth rate, and feeding rate are used in fish growth and feeding models. All fish and feed weights are expressed here in terms of wet weight (moisture content included) unless use of dry weights is noted. Specific rates and index values can be expressed as factors (e.g. 0.1) or percents (e.g. 10%), and factors are often used to simplify equations. Variables are defined in Table 7.2

Fish total length (L ; cm) and body weight (W ; g) are related by a length exponent (L_e ; range 2.5 - 3.5, typical value 3.0) and a fish condition factor (FCF ; g/cm^3 ; Table 7.3). FCF varies with fish species, size, nutritional state, and water content (Ricker, 1979; Piper et al., 1986). Parameters L_e and FCF are established by linear regression, utilizing log transformation (base-10 by convention) of geometric mean values (Ricker, 1979). W , L , and FCF are related by:

$$\begin{aligned} W &= FCF (L^{L_e}) \\ \text{or} \quad L &= (W / FCF)^{(1.0 / L_e)} \\ \text{or} \quad FCF &= W / (L^{L_e}) \\ \text{where} \quad \log_{10}(W) &= \log_{10}(FCF) + [L_e \log_{10}(L)] \end{aligned}$$

Length growth rate (LGR ; mm/day) is based on the change in fish length (L_0 to L_t ; cm) over a given time interval (t ; days):

$$LGR = (10 \text{ mm/cm}) (L_t - L_0) / t$$

Absolute fish growth rate (GR ; g fish/day) and specific growth rate (SGR ; g fish/g fish/day; or 1/day or % body weight/ day) are based on the change in fish weight (W_0 to W_t ; g) over a given time interval (t ; days):

$$\begin{aligned} GR &= (W_t - W_0) / t \\ SGR &= [(\ln(W_t) - \ln(W_0)) / t] \end{aligned}$$

Fish growth index (FGI ; range 0 - 1, or 0 - 100%) is based on the target or actual GR relative to the maximum growth rate obtained under satiation feeding (GR_{\max}) for a given growth interval:

$$FGI = GR / GR_{\max} = SGR / SGR_{\max}$$

Table 7.2. Method variables used for fish biology

Symbol	Definition
AC	BIOE method: anabolism coefficient
AE	BIOE method: anabolism exponent (0 - 1)
ANB	BIOE method: anabolism (g ww fish/fish/d)
CAT	BIOE method: catabolism (g ww fish/fish/d)
CC	BIOE method: catabolism coefficient
CE	BIOE method: catabolism exponent (0 - 1)
$C_{\max o}$	Environmental criterion for a given variable: maximum optimum
$C_{\max t}$	Environmental criterion for a given variable: maximum tolerance
$C_{\min o}$	Environmental criterion for a given variable: minimum optimum
$C_{\min t}$	Environmental criterion for a given variable: minimum tolerance
CT	BIOE method: catabolism temperature factor (C)
CV	Coefficient of variation = 100 standard deviation / mean
DE_{\max}	Maximum digestion efficiency occurring at maintenance feeding rate (0-1; e.g. 0.9)
DE_{\min}	Minimum digestion efficiency occurring at maximum feeding rate (0-1; e.g. 0.6)
dw	Dry weight
FB	Fish biomass (kg); subscript "o" and "t" refer to initial and ending times
FBD	Fish biomass density (kg fish/ha)
FBD_{cc}	Carrying capacity FBD (kg fish/ha)
FBD_{csc}	Critical standing crop FBD (kg fish/ha)
FC	BIOE method: feeding catabolism (0 - 1; dimensionless)
FCE	Food conversion efficiency (%; g fish/g feed)
FCE_c	FCE function coefficient
FCE_e	FCE function exponent
FCF	Fish condition factor (g/cm^3)
FCI	Feed competition index (range 1 - 2; e.g., 1.3)
FCR	Food conversion ratio (g feed /g fish)
FD	Quantity of feed fed over a given time interval (kg)
FD_{DIG}	Digested food fraction (0-1)
FD_{GRO}	Growth (stored) food fraction (0-1)
FD_{MET}	Digested, metabolized, and excreted food fraction (0-1)
FD_{mst}	Food moisture content for combined natural and prepared food (range >0 - 1)
FD_{PF-mst}	Food moisture content for prepared feed (range >0 - 1)
FD_{UND}	Undigested food fraction (0-1)
FFI	Fish feeding index (range 0 - 1, or 0 - 100%) = $FFI_{NF} + FFI_{PF}$
FFI_{\max}	FFI at the maximum feeding rate (1.0 or 100%)
FFI_{mnt}	FFI at the maintenance feeding rate (e.g., 0.1 or 10%)
FFI_{NF}	Endogenous (natural food) FFI
FFI_{opt}	FFI at the optimum feeding rate (e.g., 0.6 or 60%)
FFI_{PF}	Exogenous (prepared feed) FFI
FGI	Fish growth index (range 0 - 1, or 0 - 100%) = $FGI_{NF} + FGI_{PF}$
FGI'	Diurnal FGI; corrected for photoperiod and feed application timing (0-1)

Table 7.2. Continued

Symbol	Definition
FGI_B	Individual-bin FGI
FGI_{BL}	FGI_B of the largest fish
FGI_{BS}	FGI_B of the smallest fish
FGI_M	Mean fish lot FGI
FGI_{new}	FGI to be used in an iterative simulation (0-1)
FGI_{NF}	Endogenous (natural food) FGI (0-1)
FGI_{PF}	Exogenous (prepared feed) FGI (0-1)
FGI_{prior}	FGI used in the prior simulation (0-1)
FPI	Fish performance index (range 1 – 2; e.g., 1.1)
FPI_B	Fish performance index of given bin
FPI_{BL}	FPI_B of the largest fish
FPI_{BS}	FPI_B of the smallest fish
FR	Fish feeding rate, wet weight feed (g ww feed/fish/day)
FR_{dw}	Fish feeding rate, dry weight feed (g dw feed/fish/day)
FR_{dw-max}	Maximum FR_{dw} (g dw feed/fish/day)
FR_{max}	Maximum FR (g ww feed/fish/day)
FR_{NF-dw}	Fish feeding rate, dry weight natural foods (g dw natural food/fish/day)
FR_{PF-ww}	Fish feeding rate, wet weight prepared feed (g ww prepared feed/fish/day)
FS_{mst}	Fish moisture content (range >0 - 1)
FSS	Fish swimming speed (fish body lengths/ s)
GR	Absolute fish growth rate (g ww fish/fish/day)
GR_{max}	Maximum GR achieved under satiation feeding (g ww fish/fish/day)
GR_{NF}	GR due to natural food consumption (g ww fish/fish/day)
L	Fish total length (cm); subscript “o” and “t” refer to initial and ending times
L_a	LNGR method: y-intercept (mm/day)
L_b	LNGR method: slope (mm/day/C)
L_e	Length exponent (range 2.5 - 3.5, typical value 3.0)
L_f	Temperature growth factor (%/ °C): decline in LGR from LGR_{maxo} per unit temperature deviation beyond the optimum temperature range
LGR	Length growth rate (mm/day)
LGR_{max}	Maximum LGR (mm/day; used in the LNGR and VBGF methods)
L_{inf}	Inflection fish length with respect to LGR (cm)
L_{max}	Maximum (asymptotic) fish length with respect to LGR (cm)
N_B	Number of fish in the bin defined by W_B
NFP	Natural (endogenous) fish productivity (kg fish/ha/day)
NFP_{max}	Maximum potential NFP (kg fish/ha/day)
N_T	Total number of fish in fish lot
PMR_{FP}	Peak-mean ratio of fish metabolic rate over a 24-hr period based on timing of food processing (range 1.0 – 1.5; use 1.0 to ignore)

Table 7.2. Continued

Symbol	Definition
PMR _{PP}	Peak-mean ratio of fish metabolic rate over a 24-hr period based on photoperiod (range 1.0 – 1.5; use 1.0 to ignore)
POP	Fish number; subscript “o” refers to initial time, subscript “t” refers to ending time
POP _{tp}	Expected fish number after total period tp (days)
SCL _{FP}	Food processing (metabolic) scalar (0-1)
SCL _{FQ}	Feed quality scalar (range 0-1)
SCL _{FS}	Fish size scalar (range 0-1)
SCL _{FBD}	Fish biomass density scalar (range 0-1)
SCL _{PP}	Photoperiod scalar (0-1)
SCL _{WQ}	Water quality scalar (0-1)
SCL _{WT}	Water temperature scalar (0-1)
SD	Standard deviation
SFR	Specific feeding rate (g feed/g fish/day; or 1/day or % body weight/ day)
SFR _c	SFR coefficient (1/day; constant or function)
SFR _e	SFR exponent
SFR _{max}	Maximum (appetite satiation) SFR for a given growth interval (1/day)
SGR	Specific growth rate (g fish/g fish/day; or 1/day or % body weight/ day)
SGR _c	SGR coefficient (1/day; constant or function)
SGR _e	SGR exponent
SGR _{max}	Maximum SGR (1/day)
SMR	Specific mortality rate (1/day)
t	Time interval (days)
T	Water temperature (C)
t _h	Time of day (hr; 0-24)
t _{hmax}	Time of diurnal maximum value (hr)
t _{hmid}	Mid point time between times of diurnal minimum and maximum values (hr)
t _{hmin}	Time of diurnal minimum value (hr)
tp	Target period (days)
U	Rearing-unit water velocity (cm/s)
VB _k	VBGF method: coefficient (1/day)
VB _{to}	VBGF method: theoretical time when length or weight is zero (days, usually < 0)
W	Fish body weight (ww; g/fish); subscript “o” refers to initial time, subscript “t” refers to ending time
W _B	Mean fish weight of given bin (g)
W _{gm}	Geometric-mean W (g) for a given fish growth interval
W _{inf}	Inflection fish weight with respect to GR (g)
W _M	Mean fish weight of the fish lot (g)
W _{max}	Maximum fish weight with respect to GR (g)
W _{tp}	Target fish weight (g) to be achieved at target period tp
ww	Wet weight

Table 7.3. Sampling of reported values for fish condition factor, where $L_e = 3.0$ (Haskell 1959; Piper et al., 1986; Soderberg, 1990)

Fish species	Fish condition factor (g/cm^3)
Northern pike	0.005013
Channel catfish	0.007964
Chinook salmon	0.008191
Steelhead	0.009425
Coho salmon	0.01034
Rainbow, brook, and brown trout	0.01122
Largemouth bass	0.01275
Blue tilapia	0.0233

For the simulation of fish growth over extended periods, it is often desired to achieve a specified date and weight target (by control of feeding rates), but varying temperatures and other environmental conditions make it difficult to predetermine the FGI to be used. Thus, required FGI values are converged upon by the use of iterative simulations, where:

$$\text{FGI}_{\text{new}} = \text{FGI}_{\text{prior}} [(W_{\text{tp}} - W_0) / \text{tp}] / [(W_t - W_0) / t]$$

and FGI_{new} = FGI to be used in an iterative simulation, $\text{FGI}_{\text{prior}}$ = FGI used in the prior simulation, W_{tp} = target fish weight (g) to be achieved at target period tp (days), W_t = fish weight achieved in prior simulation (g) at time t (days), and W_0 = initial fish weight (g).

Specific feeding rate (SFR; g feed/g fish/day; or 1/day or % body weight/ day) is based on the quantity of feed fed (FD; kg) over a given time interval (t , days) relative to total fish biomass (FB; kg) at the beginning or mid-point of the time interval:

$$\text{SFR} = \text{FD} / (\text{FB } t)$$

Fish feeding index (FFI; range 0 - 1, or 0 - 100%) is based on the target or actual fish feeding rate (SFR) relative to the maximum (appetite satiation) feeding rate (SFR_{max}) for a given growth interval:

$$\text{FFI} = \text{SFR} / \text{SFR}_{\text{max}}$$

Food conversion efficiency (FCE; %) is based on the total feed applied (FD; kg) over a given time interval relative to the change in fish biomass (FB; kg) for this time interval. The reciprocal value, food conversion ratio (FCR), is also commonly used. FCE and FCR values are typically

calculated for fish populations, rather than individual fish, and include losses due to fish mortality and applied feed that is not consumed. FCE and FCR are calculated by:

$$FCE = 100.0 (FB_t - FB_0) / FD$$

$$FCR = FD / (FB_t - FB_0)$$

Typical moisture contents of fish and feeds (FS_{mst} and FD_{mst} ; range >0 - 1) are 0.75 for fish, 0.10 for dry prepared feeds, 0.40 for moist prepared feeds, and 0.65-0.95 for natural foods. Inter-conversion of wet weight (ww) and dry weight (dw) values is based on moisture content, where:

$$SFR_{dw} = SFR (1.0 - FD_{mst}) / (1.0 - FS_{mst})$$

$$FCR_{dw} = FCR (1.0 - FD_{mst}) / (1.0 - FS_{mst})$$

and $FCE_{dw} = FCE (1.0 - FS_{mst}) / (1.0 - FD_{mst})$

For feed rate models, natural foods are expressed in dry weight and prepared feeds are expressed in wet weight. Thus, for fish utilizing natural foods and prepared feeds:

$$FD_{mst} = FD_{PF-mst} (FGI - FGI_{NF}) / FGI$$

7.4 Fish survival

Fish survival is dependent on a complex interaction of water quality variables, fish physiological status, and presence of pathogens. However, some method to estimate fish population numbers over a culture period is required in order to generate fish biomass schedules based on fish body weights. If it is assumed that mortality losses are proportional to population levels (SMR, 1/day), predicted numbers of fish over a culture period (POP_t) can be based on the expected fish number (POP_{tp}) at the end of the total period (tp) by:

$$POP_t = POP_0 e^{(SMR \cdot t)}$$

where $SMR = \log_e (POP_{tp} / POP_0) / tp$

For simulations, once SMR is established by specified period lengths and expected percent survival, initial fish numbers are automatically adjusted so that given target fish numbers are achieved. Total fish lot mortality occurs when one or more water quality variables exceed their tolerance range.

7.5 Fish growth

Fish growth models in the aquaculture literature show varying consideration of fish size, anabolic and catabolic components of fish metabolism, food quality and quantity, and water quality (Ricker, 1979). Consequently, these models vary in their consideration of exponential, linear, and asymptotic fish growth stanzas (Figure 7.3) and profiles of predicted growth trajectories over time (Figure 7.4). The transition from exponential to asymptotic fish growth is due to constraints imposed by the fish environment and/or the maximum (maturation) fish size. Environmental constraints include water quality and feed quality and quantity. Environmental constraints are common in aquaculture, due to deteriorating water quality or food availability as fish and/or feed loading rates achieve or exceed maximum system capacities. However, under typical aquaculture conditions, fish weights are normally two-thirds or less of maximum maturation weights and are not significantly constrained by maximum fish size. For example, the maximum size of Nile tilapia is about 2.5 kg (Balarin and Hatton, 1979), where common harvest sizes are ≤ 1.25 kg, or $\leq 50\%$ of maximum size. For many other culture species, this market size to maximum size differential is even greater (e.g. channel catfish, rainbow trout, and sturgeon). The general lack of size constraints to growth in aquaculture production is also evident in the wide use of simplified growth models that do not account for the size constraint.

Reported growth models, according to the terminology used here, include (1) constant absolute weight growth rate (CAGR), (2) constant specific weight growth rate (CSGR), (3) length growth rate (LNGR), (4) double-logarithmic specific growth rate (DSGR), (5) von Bertalanffy growth function (VBGF), and (6) anabolic-catabolic bioenergetic function (BIOE). In reverse order, these models can be derived through successive simplifications of the fundamental bioenergetic equation of growth described earlier ($G = I - E - M$):

BIOE:	$dW/dt = a W^b - c W^d$	(anabolic and catabolic terms)
DSGR:	$dW/dt = a W^b$	(remove catabolic term)
LNGR:	$dW/dt = a W^k$	($b = \text{constant}$)
CSGR:	$dW/dt = a W$	($b = 1$)
CAGR:	$dW/dt = k$	(constant growth rate)

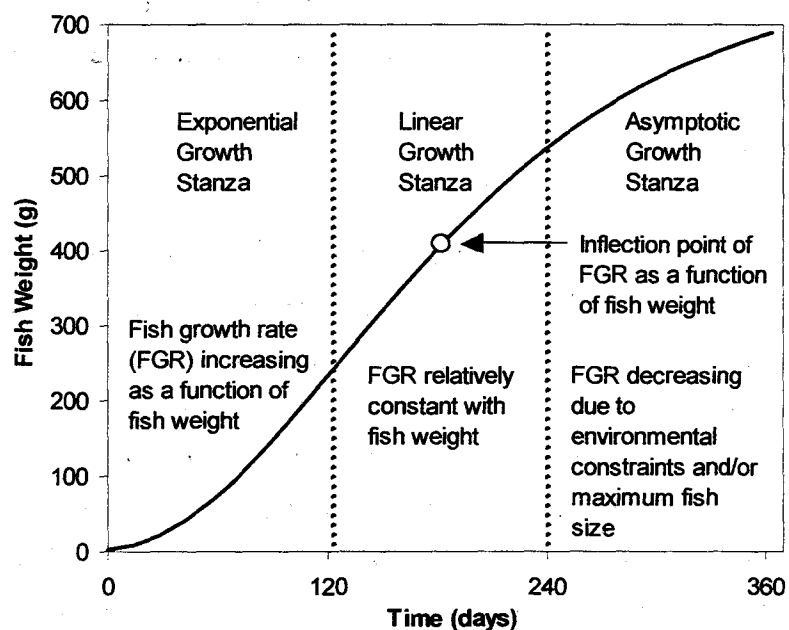


Figure 7.3. Idealized fish growth profile, including exponential, linear, and asymptotic fish growth stanzas

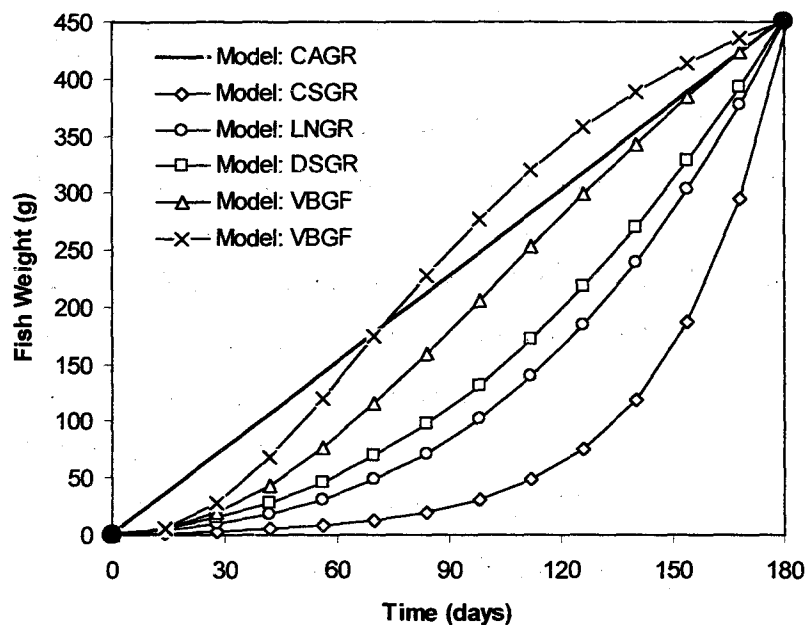


Figure 7.4. Representative fish growth profiles for each of the fish growth models identified in the text, using equivalent starting and ending weights, growth periods, and environmental conditions for each profile

The CAGR and CSGR models are only appropriate for short growth intervals. These models are not used in AquaFarm. The CAGR and CSGR models are:

$$W_t = W_o + k t$$

$$W_t = W_o e^{(t \text{ SGR}_c)} \quad (\text{where } \text{SGR}_c = 0)$$

The LNGR, DSGR, VBGF, and BIOE models are available in AquaFarm. One model is selected per fish species, depending on user preferences, availability of species-specific parameters, and appropriate uses of individual models. In their original published forms, the LNGR and DSGR models do not consider growth constraints due to maximum (asymptotic) fish size. For purposes here, a fish-size scalar term can be added to the LNGR and DSGR models. The VBGF and BIOE models both consider the fish-size constraint in their original, published form. For all four of these models, scalar terms can be added for water quality, feed quality, photoperiod, and feed availability. Water temperature is normally accounted for explicitly in growth models, but can alternatively be combined into the water quality scalar. As shown by the temperature criteria in Table 7.1 and the temperature response in Figure 7.2, fish growth declines rapidly as temperatures increase above the high optimum level, in contrast to the relatively slow rate of increase in growth rate as temperatures increase above the low tolerance level.

7.5.1 Length growth rate model

The length growth rate model (LNGR; Table 7.4) is widely used and easily calibrated by linear regression. The LNGR model is based on the simplifying assumptions that length growth rate (LGR) is constant with respect to fish length, LGR varies linearly with water temperature, and water temperatures do not rise so high that growth is reduced (Haskell, 1959; Ricker, 1975; Ricker, 1979; Piper et al., 1986; Soderberg, 1990; Soderberg, 1992). In its original form (SCL_{FS} not used), the LNGR model is well suited to fish growth in the exponential stanza and becomes increasingly less suitable as the linear stanza occupies an increasing proportion of the total growth profile. Fish lengths are converted to weights using the fish condition factor, and GR_{max} is calculated by converting L_o to W_o and L_t to W_t . The LNGR model is (same function used for regression):

$$\text{LGR}_{\text{max}} = \text{SCL}_{\text{FS}} [L_a + (L_b T)]$$

by integration $L_t = L_o + \{\text{SCL}_{\text{FS}} [L_a + (L_b T)] t / (10 \text{ mm/cm})\}$

The fish-size scalar (SCL_{FS} ; range 0 – 1) is optional and calculated by:

$$\text{If } L_0 \leq L_{inf} \text{ then: } SCL_{FS} = 1.0$$

$$\text{If } L_0 \geq L_{max}, \text{ then: } SCL_{FS} = 0$$

$$\text{If } L_0 > L_{inf} \text{ and } L_0 < L_{max}, \text{ then: } SCL_{FS} = (L_{max} - L_0) / (L_{max} - L_{inf})$$

An alternative form of the LNGR model, used for salmon hatcheries (e.g., Oregon Department of Fish and Wildlife, Portland, Oregon), accounts for the decline in growth rate at temperatures below and above the optimal temperature range (T_{mino} to T_{maxo}). If water temperature is between T_{mino} and T_{maxo} , then $LGR = LGR_{max}$. Otherwise:

$$\text{If } T < T_{mino} \text{ then } LGR_{max} = LGR_{maxo} \{ 1.0 - [(T_{mino} - T) L_f / 100] \}$$

$$\text{If } T > T_{maxo} \text{ then } LGR_{max} = LGR_{maxo} \{ 1.0 - [(T - T_{maxo}) L_f / 100] \}$$

Table 7.4. Sampling of reported parameters for the LNGR fish growth model (Soderberg, 1992; SCL_{FS} term not used) *

Fish species	Temperature range (°C)	L_a (mm/day)	L_b (mm/day/°C)
Brook trout	5 – 12	- 0.348	0.0944
Brook trout	4 – 19	+0.155	0.0355
Brook trout	7 – 19	+0.006	0.0455
Brook trout	7 – 16	- 0.068	0.0578
Rainbow trout	4 – 19	- 0.040	0.0505
Rainbow trout	7 – 19	+0.043	0.0450
Rainbow trout	7 – 16	- 0.167	0.0660
Lake trout	4 – 16	+0.176	0.0426
Lake trout	4 – 13	+0.0622	0.0588
Steelhead	4 – 19	+0.0329	0.0294
Steelhead	7 – 16	- 0.0407	0.0386
Atlantic salmon	4 – 19	+0.0043	0.0306
Atlantic salmon	7 – 16	- 0.0429	0.0371
Channel catfish	24 – 30	+0.612	0.0298
Channel catfish	24 – 28	+0.195	0.0463
Tiger muskellunge (3-4 cm)	14 – 24	- 0.0548	0.0912
Tiger muskellunge (12-13 cm)	18 – 24	+0.394	0.0471
Blue tilapia	20 – 30	- 0.853	0.0480

* Emphasis on salmonid species reflects the availability of values in the literature

7.5.2 Double-logarithmic specific growth rate model

The double-logarithmic specific growth rate model (DSGR; Table 7.5) is widely used and log-transform linear regression can be used for calibration (Parker and Larkin, 1959; Iwama and Tautz, 1981; Weatherley and Gill, 1983; Jobling, 1983a; Jobling, 1983b; Allen et al., 1984; Jensen, 1985; Hephher, 1988). The DSGR model is more generally applicable than the LNGR model, due to its better ability to consider both the exponential and linear growth stanzas. In the fundamental DSGR model (SCL_{FS} term not used), the weight exponent SGR_e is apparently based on intrinsic physiological characteristics common to all fish (Hephher, 1988). Reported values for SGR_e tend to be about 0.33 for the exponential growth stanza and increase to about 0.45 as greater proportions of the linear growth stanza are included. If SGR_e is equivalent to the reciprocal of L_e in the fish length-weight expression (e.g., $L_e = 3.0$ and $SGR_e = 0.33$), then the DSGR and LNGR models are equivalent. In contrast, the weight coefficient SGR_c is a function of fish species, environment variables, and food availability, and as evident in Table 7.5, reported values range widely. SGR_c may be represented by a constant or a function. The DSGR model is (SGR and SGR_c expressed in factor format; 1/day):

$$\begin{aligned} SGR_{max} &= SCL_{FS} SGR_c W^{-SGR_e} \\ \text{or} \quad GR_{max} &= SCL_{FS} SGR_c W^{(1.0 - SGR_e)} \\ \text{by integration} \quad W_t &= [W_0^{SGR_e} + (SCL_{FS} SGR_c SGR_e t)]^{(1.0 / SGR_e)} \end{aligned}$$

The fish-size scalar (SCL_{FS} ; range 0–1) is optional and calculated by:

$$\begin{aligned} \text{If } W_0 \leq W_{inf}, \text{ then:} \quad & SCL_{FS} = 1.0 \\ \text{If } W_0 \geq W_{max}, \text{ then:} \quad & SCL_{FS} = 0 \\ \text{If } W_0 > W_{inf} \text{ and } W_0 < W_{max}, \text{ then:} \quad & SCL_{FS} = (W_{max} - W_0) / (W_{max} - W_{inf}) \end{aligned}$$

Model parameters can be determined by log-transform linear regression. Geometric-mean fish weight (W_{gm} , g) and SGR values are calculated for each growth interval of the sample fish weights (W_0 and W_t), and their natural logs are used. In the example below, SGR_c is a function of water temperature (T ; using polynomial scalar function) and food availability (FGI ; fraction form):

Table 7.5. Sampling of reported parameters for the DSGR fish growth model *

Fish species	Temperature range (°C)	SGR _c	SGR _e	Reference
Sockeye salmon	15.0	NA	0.45	Brett, 1979
Pink salmon	15.0	NA	0.45	Brett, 1979
Coho salmon	15.5	NA	0.34	Stauffer, 1973
Salmonids	5.0 – 16.0	0.00303 T	0.33	Iwama and Tautz, 1981
Rainbow trout	12.0	0.079	0.338	Weatherley and Gill, 1983
Rainbow trout	17.0	0.0686	0.323	Jobling, 1983a
Brook trout	11.0	NA	0.333	Haskell, 1959
Brown trout	7.0 – 13.0	0.138 (-0.3474 + 0.1053 T)	0.325	Jensen, 1985
Brown trout	12.8	0.042	0.325	Elliot, 1975
Arctic char	7.0 – 13.0	0.126 (-0.0815 + 0.0917 T)	0.325	Jensen, 1985
Arctic char	4.0 – 14.0	0.075 (0.0219 + 0.0727 T)	0.325	Jobling, 1983a
Cod	NA	0.1873	0.441	Jobling, 1983b
Tarpon	NA	0.0277	0.39	Jobling, 1983b
Snakehead	NA	0.0229	0.41	Jobling, 1983b
Mosquito fish	NA	0.0342	0.44	Jobling, 1983b
Channel catfish	NA	0.086	0.326	Hepher, 1988
Common carp	NA	0.176	0.340	Hepher, 1988
Mossambic tilapia	NA	0.0390	0.41	Jobling, 1983b
Florida red tilapia	26.0 - 30.0	0.176	0.428	Ernst et al., 1989 ^a
Mixed tilapia	28.0 - 32.0	0.175	0.444	Losordo, 1997 ^b
Nile tilapia	NA	0.836	0.713	Diana, 1997 ^c

* SGR_c and SGR_e values are expressed for the calculation of SGR in units of 1/day. SGR_c may be expressed as a function of water temperature (T; °C). Emphasis on salmonid species reflects the availability of values in the literature.

^a Florida red tilapia: *Oreochromis mossambicus* x *O. hornorum* (seawater culture)

^b Mixed species: *O. niloticus* and *O. niloticus* x *O. aureus*, DSGR parameters estimated from given data

^c Marked differences from typical values reflects use of fish growth profiles consisting of linear and asymptotic growth stanzas under limited feed availability.

$$\begin{aligned}
\text{where } W_{gm} &= e^{\{ [\log_e(W_0) + \log_e(W_t)] / 2.0 \}} \\
SGR &= [(\log_e(W_t) - \log_e(W_0)) / t] \\
\text{and } \log_e(SGR) &= \log_e(SGR_c) - [SGR_e \log_e(W_{gm})] \\
\text{or } \log_e(SGR) &= \log_e(SGR_c) - \{SGR_e [(\log_e(W_0) + \log_e(W_t)) / 2.0]\} \\
\text{where } SGR_c &= k_1 + k_2 T + k_3 T^2 \\
\text{or } \log_e(SGR) &= SGR_c' - [SGR_e \log_e(W_{gm})] \\
\text{where } SGR_c' &= k_1' + k_2' T + k_3' T^2 \\
\text{and } SGR_c &= e^{SGR_c'} \\
\text{or } SGR_c' &= \log_e(SGR_c)
\end{aligned}$$

Use of SGR_c' is more convenient for regression and is the reported format in some studies. Either SGR_c (as used in Table 7.5) or SGR_c' can be used in AquaFarm. In Chapter 8, example applications of the SGR_c' regression model are provided. If the DSGR model is calibrated without temperature as an independent variable and the calibration data were generated under conditions of optimal-range water temperatures, then a temperature scalar can be applied after model calibration in the form of a water quality scalar.

7.5.3 von Bertalanffy growth function

The von Bertalanffy growth function (VBGF; Table 7.6) is widely used in fisheries and has recently shown increased application to pond-based aquaculture (Ricker, 1975; Hopkins et al., 1988; Hopkins, 1992; Prein et al., 1993; Froese and Pauly, 1996). The VBGF model, as originally formulated, accounts for asymptotic fish growth due to environmental and fish-size constraints (within one term) and is suitable for modeling fish growth over all the three growth stanzas. The VBGF model can be expanded by including water and feed quality scalars (optional), which delineates causes of asymptotic growth. The VBGF model uses fish lengths. Similar to the LNGR model, fish lengths are converted to fish weights and GR_{max} is calculated by converting L_0 to W_0 and L_t to W_t .

Table 7.6. Sampling of reported parameters for VBGF fish growth model *

Fish species	Temp. range (C)	W _{max}	L _{max}	VB _k	L _e	VB _{t0}	Reference
Silver carp	NA ^a	215	28.9	0.0281	3	-23	Hopkins, 1992
<i>O. spilurus</i> ^b	22	371	NA	0.00522	3	6.30	Hopkins et al., 1988
<i>O. spilurus</i> ^b	25	581	NA	0.00522	3	10.55	Hopkins et al., 1988
<i>O. spilurus</i> ^b	28	858	NA	0.00522	3	13.70	Hopkins et al., 1988
<i>O. aureus</i> ^c	22	208	NA	0.00260	3	-36.21	Hopkins et al., 1988
<i>O. aureus</i> ^c	25	733	NA	0.00260	3	-10.29	Hopkins et al., 1988
<i>O. aureus</i> ^c	28	1775	NA	0.00260	3	1.79	Hopkins et al., 1988
<i>O. niloticus</i>	20 - 35	100 - 4000	15- 60	0.003 - 0.05	3.0 - 3.1	0 - -200	Hopkins, p.c. ^d

* Also see ICLARM, 1996. Emphasis on tilapia species reflects availability of values in literature.

^a Not available

^b *Oreochromis spilurus*, all male, seawater culture

^c *Oreochromis aureus*, all male, seawater culture

^d Data from a wide range of extensive tilapia growout studies in Southeast Asia

In the context of a simulation, the application procedure for the VBGF model is:

- 1) Calculate the time (t) at which the current fish length (L₀) is achieved:

$$t_0 = VB_{t0} + \log_e(1.0 - L_0/L_{max}) / (-VB_k)$$

- 2) Increment time forward one time-step: $t = t_0 + \text{time-step}$

- 3) Calculate the new fish weight at the new time:

$$L_t = L_{max} \{ 1.0 - e^{[-VB_k (t - VB_{t0})]} \}$$

- 4) Calculate maximum length growth rate (LGR) as the change in length divided by the time-step:

$$LGR_{max} = (L_t - L_0) / t$$

In step 1, the VBGF is rearranged to solve for time. Water temperature is accounted for explicitly in the LNGR and DSGR models, but reported forms of the VBGF model do not include a water temperature term. For purposes here, a water temperature term is added to the VBGF model, where

SCL_{WT} is calculated at the current water temperature and SCL_{WTcal} is calculated at the model calibration mean temperature:

$$GR_{max} = [(W_t - W_0) / t] SCL_{WT} / SCL_{WTcal}$$

VBGF model parameters are best fitted by non-linear least squares, for which L_e can be included in the regression. By allowing L_e to diverge from its standard value of 3.0, and a better fit will be obtained for some datasets. A simplified, linear regression technique called the Gulland and Holt Plot (GHP) can be used (Gulland and Holt, 1959; Hopkins, 1992). The GHP requires fish size sampling data from at least four time intervals in order to provide reliable parameter estimates. The GHP is a plot of fish-length growth rate versus fish length and is fitted with a straight line:

$$(L_t - L_i) / t = b + [m (L_t + L_i) / 2.0]$$

where $L_{max} = -b / m$, $VB_k = -m$, and VB_{t0} is assigned so that the initial fish size is achieved on day zero of the growth trial.

7.5.4 Application of LNGR, DSGR, and VBGF fish growth models

Application of the LNGR, DSGR, and VBGF models assumes that these models are calibrated under conditions where fish growth is maximized, for the given temperature range of the model. These optimal conditions, with respect to fish growth, include satiation feeding, optimal feed quality, and optimal water quality other than water temperature. The maximum growth rates calculated by these models are then scaled to (1) target fish growth rate (expressed as FGI), (2) water quality (SCL_{WQ}), (3) feed quality (SCL_{FQ}), (4) photoperiod (SCL_{PP}), and (5) metabolic food processing (SCL_{FP}).

Use of SCL_{WQ} (previously described) and SCL_{FQ} is optional, and these scalars can be ignored if water and feed quality are within optimum ranges or if water and feed quality are comparable between the study used to parameterize the growth model and the study to which the model is applied. SCL_{FQ} is calculated similar to SCL_{WQ} , using given criteria and a selected scalar function. SCL_{FQ} can be based on the feed protein content (%; range >1 – 100; e.g., 35%) or the feed protein-energy ratio (mg protein/ ME kcal; range >1 – 240; e.g., 100 mg/kcal). For protein content, $C_{mint} =$

0, C_{mino} = given, C_{maxo} = given, and $C_{\text{maxt}} = 100$. For the protein-energy ratio, $C_{\text{mint}} = 0$, C_{mino} = given, C_{maxo} = given, and $C_{\text{maxt}} = 240$. Approximate default criteria (user accessible) are provided by AquaFarm and are organized according to the trophic level of the fish (herbivores/detritivores, omnivores, and carnivores).

For diurnal simulations, the photoperiod scalar (SCL_{pp}) and food processing scalar (i.e. metabolic processing; SCL_{fp}) are calculated hourly, such that fish growth, feeding, and metabolic rates vary over the 24-hr day. These scalars are applied such that time-integrated rates over a 24-hr period are equivalent to daily mean values. In other words, the mean scalar for a 24-hr period is equal to one. The sinusoid function used to calculate diurnal scalar values is (Card et al., 1976; similar to function used in Chapter 5, Facility climate):

$$\begin{aligned} SCL_{\text{pp}} &= 1.0 + [(2 \text{ PMR}_{\text{pp}}) - 2] a \{ \sin(\pi t_h / 12 - c) + b \sin[2(\pi t_h / 12 - c)] \} \\ SCL_{\text{fp}} &= 1.0 + [(2 \text{ PMR}_{\text{fp}}) - 2] a \{ \sin(\pi t_h / 12 - c) + b \sin[2(\pi t_h / 12 - c)] \} \\ af &= 2\pi / 24 \\ x &= af(t_{\text{hmid}} - t_{\text{hmin}}) \\ a &= 0.5 / [\sin(x) + b \sin(2x)] \\ b &= -\cos(x) / [2 \cos(2x)] \\ c &= t_{\text{hmid}} af \\ t_{\text{hmid}} &= (t_{\text{hmin}} + t_{\text{hmax}}) / 2 \end{aligned}$$

For SCL_{pp} , times t_{hmin} and t_{hmax} are based on times of sunrise and sunset. For SCL_{fp} , times t_{hmin} and t_{hmax} are based on given offsets from sunrise (e.g. +2.0 hr) and sunset (e.g. -2.0 hr), at which time the application of prepared feed is begun and ended, respectively. Specified feed application periods can be specific to the size-stage of the fish lot, where smaller fish are typically fed more intensively than larger fish. Daily amplitudes for SCL_{pp} and SCL_{fp} are represented by the terms containing the peak-mean ratios, PMR_{pp} and PMR_{fp} (see Fish metabolism). If the time from t_{hmin} to t_{hmax} or from t_{hmax} to t_{hmin} is less than eight hours, then the sinusoid function described above becomes unsuitable for use and linear interpolation is applied.

In the modeling approach used here, (1) fish growth rates are based on target growth rates, (2) feeding rates are a function of growth rates, and (3) metabolic rates are a function of feeding rates. For diurnal simulations, the modeling simplification is used that growth, feeding, and metabolic

rates vary together over the 24-hr day. However, this is a modeling convenience only and does not detract from the rigor of this approach. Nighttime “feeding rates” can be thought of as nighttime “food processing rates”. This simplification is invisible to the user, and reported feeding rate schedules correspond to designated, daily feeding periods. In practice, food consumption is mainly restricted to daylight hours and fish metabolism is distributed over the day in response to photoperiod, fish activity, feeding, and feed processing. These relationships are emulated in the method used here but they are not strictly modeled.

Whether the LNGR, DSGR, or VBGF method is used, fish growth rates for a fish lot are calculated at each simulation step and applied using the uniform procedure described below:

- 1) $GR_{max,calc}$ (g ww fish/fish/day) is calculated by the LNGR, DSGR, or VBGF method, as a function of fish size and water temperature. A water quality scalar (SCL_{WQ}) and a feed quality scalar (SCL_{FQ}) can be applied (optional). Water temperature is considered explicitly and not included in SCL_{WQ} . The corrected $GR_{max,calc}$ (GR_{max}) is calculated by:

$$GR_{max} = GR_{max,calc} SCL_{WQ} SCL_{FQ}$$

- 2) For daily simulations, the diurnal FGI (FGI') is not used and $FGI' = FGI$. For diurnal simulations, FGI' is calculated according to the photoperiod and feed application timing:

$$FGI' = FGI (SCL_{PP} + SCL_{FP}) / 2.0$$

$$FGI_{NF}' = FGI_{NF} (SCL_{PP} + SCL_{FP}) / 2.0$$

- 3) GR is calculated by scaling GR_{max} to FGI' ,

$$GR = (FGI' / 100) GR_{max}$$

- 4) FFI is calculated as a function of FGI' (described later). The calculated maximum feeding rate (FR_{max} ; described later) is converted to dry weight terms (FR_{dw-max} ; g dw feed/fish/day) using the weighted mean moisture content of prepared and natural foods. The actual feeding rate (FR_{dw} ; g dw feed/fish/day; total for natural and prepared foods) is calculated by:

$$FR_{dw} = (FFI / 100) FR_{dw-max}$$

- 5) If fish utilize natural food, then FR_{NF-dw} (g dw natural food/fish/day) is calculated by:

$$FR_{NF-dw} = FR_{dw} (FGI_{NF}' / FGI')$$

6) If fish utilize prepared feed, then FR_{PF-ww} (g ww prepared feed/fish/day) is calculated by:

$$FR_{PF-ww} = [FR_{dw} / (1.0 - FD_{PFmst} / 100.0)] (FGI_{PF}' / FGI')$$

$$\text{where } FGI' = FGI_{NF}' + FGI_{PF}'$$

7.5.5 Bioenergetic growth model

The bioenergetic growth model (BIOE; Table 7.7) is so named because its functional form more closely approximates fish bioenergetics than the other growth models (Ursin, 1967; Ursin, 1979; Brett and Groves, 1979; Hepher, 1988; Liu and Chang, 1992; Nath 1996). Since this model contains both anabolic and catabolic terms, it is most appropriately used when fish-size constraints to fish growth are significant. The BIOE method is identical to that used in the aquaculture software POND (Nath, 1996), except that the water and feed quality scalars (SCL_{WQ} and SCL_{FQ}) are calculated by methods described here. In addition, the function is rearranged to calculate fish growth and feeding rates based on the target growth rate. A non-linear parameter estimation method for the BIOE model described by Nath (1996) is not supported by AquaFarm. The BIOE method gives negative growth rates when feed is not available (e.g., night). Calculation methods for the water temperature scalar (SCL_{WT}) and the photoperiod scalar (SCL_{PP}) differ from those of the other growth models, and the feed availability scalar is not used. Catabolic rates are used to determine nighttime metabolic rates. Values for the feeding catabolism parameter (FC) used by Nath (1996) appear to be too high (e.g., 0.5), where this apparent error would be accounted for by the other parameters. Nath defined this parameter as the “fraction of the food assimilated that is used for feeding catabolism”. If this term does represent an apparent heat increment (assumed), then it is well above reported apparent heat increment values, which are about 0.15.

Table 7.7. Reported parameters for the bioenergetic growth model (BIOE; Nath, 1996)

Parameter	Common carp	African catfish	Nile tilapia	Channel catfish	Channel catfish	Striped bass	Hybrid bass
Anab. and catab.							
DE _{min}	0.552182	0.604677	0.613243	0.59617	0.675535	0.671377	0.714069
DE _{max}	0.863553	0.790724	0.764879	0.853442	0.825653	0.820571	0.872751
AE	0.670403	0.673948	0.686799	0.687917	0.672477	0.647159	0.66252
AC	1.12562	1.09118	1.02518	1.03377	1.00574	1.01147	0.96502
FC	0.542543	0.479202	0.552739	0.535707	0.559038	0.569673	0.586156
CE	0.718516	0.808136	0.850645	0.550478	0.64037	0.921394	0.830726
CC	0.0143931	0.0131722	0.013882	0.0457304	0.0534001	0.0274303	0.0169292
CT	0.00228105	0.00974941	0.0166826	0.0304031	0.0539144	0.0210141	0.0718164
Feed quality							
Protein criteria	31	40	26	32	31	35	35
Protein parameter	0.0780699	0.105066	0.0910785	0.0906903	0.105873	0.0958644	0.106813
Gross energy criteria	3.1	3.6	2.6	3	2.5	3	3
Gross energy param.	0.857784	0.910912	0.902036	0.940492	0.85	0.85	0.85
Water temperature							
C _{mint}	10.2565	10.9975	12.4413	12.4516	13.3341	8.40269	10.3979
C _{maxt}	35.9885	36.1834	36.2529	36.0109	34.4891	33.9478	33.2375
C _{maxo}	29.931	29.3961	31.6559	31.8324	30.9673	25.0441	24.0713

The procedure for the BIOE model is:

- 1) The maximum growth rate (GR_{max} ; g ww fish/fish/day) is calculated as the net sum of anabolism and catabolism:

$$GR_{max} = ANB - CAT$$

where $ANB = FD_{DIG} (1.0 - FC) SCL_{FQ} FR$

$$CAT = CC e^{(a CT)} W^{CE}, \text{ where } a = T - T_{min} \text{ (if } a < 0, \text{ then } a = 0)$$

$$FR_{max} = SCL_{PP} SCL_{WT} SCL_{WQ} AC W^{AE}$$

$$SCL_{WT} = \text{use exponential scalar (see Chapter 6, Environmental scalars) with single optimum (} C_{mint}, C_{maxo}, \text{ and } C_{maxt})$$

$$SCL_{PP} = \text{if daily simulation, then } SCL_{PP} = \text{photoperiod} / 24; \text{ if diurnal simulation, then } SCL_{PP} = 1 \text{ during day and } SCL_{PP} = 0 \text{ during night}$$

- 2) The fraction of ingested feed that is digested is (same as method used for metabolism):

$$FFI_{mnt} = CAT / FR_{max}$$

$$FFI = FR / FR_{max}$$

$$FD_{DIG} = DE_{max} - [(DE_{max} - DE_{min}) (FFI - FFI_{mnt}) / (FFI_{max} - FFI_{mnt})]$$

- 3) For the day light period, the target growth rate (GR ; g ww fish/fish/day) is defined by:

$$GR = (FGI / 100) GR_{max}$$

- 4) For the day light period, the method is rearranged, by use of the quadratic equation, to calculate the feeding rate (FR ; g ww fish/fish/day) that yields a given GR :

$$a = DE_{max} - (b FFI_{mnt})$$

$$b = (DE_{min} - DE_{max}) / (1.0 - FFI_{mnt})$$

$$c = (GR + CAT) / SCL_{FQ} FR_{max} (1.0 - FC)$$

$$d = a^2 - 4 b (-c)$$

$$FFI = 100 (-a + d^{1/2}) / (2 b)$$

$$FR = (FFI / 100) FR_{max}$$

- 5) The feeding rate is converted to dry weight terms (FR_{dw} ; g dw fish/fish/day):

$$FR_{dw} = FR (100 - FS_{mst}) / 100$$

6) If fish utilize natural food, then FR_{NF-dw} (g dw natural food/fish/day) is calculated by:

$$FR_{NF-dw} = FR_{dw} (FGI_{NF} / FGI)$$

7) If fish utilize prepared feed, then FR_{PF-ww} (g ww prepared feed/fish/day) is calculated by:

$$FR_{PF-ww} = [FR_{dw} / (1.0 - FD_{PF-mst} / 100.0)] (FGI_{PF} / FGI)$$

$$\text{where } FGI = FGI_{NF} + FGI_{PF}$$

7.6 Fish weight distributions

The use of mean fish weights for growout fish lots is adequate for modeling survival, growth, feed application, metabolism, and biomass support for the fish lot as a whole. However, consideration of the distribution of individual weights within a fish lot is required to model certain types of fish lot management and for predicting weight distributions at fish lot harvest or release (e.g., Watten, 1992; Summerfelt et al., 1993; Cuenco et al., 1985c). Fish weight distributions are an important aspect of aquaculture production. Whether fish are released to the wild or harvested for market, the variability in fish weight is just as important as the mean weight.

7.6.1 Basis of fish weight distributions

Growth rates of individual fish may vary due to (1) genetically based differences (including fish sex) in performance potential between fish, (2) agonistic behavior (territoriality and aggression) between fish, and (3) competition for limited food resources, resulting in disproportional food consumption rates between fish (Ricker, 1975; Cuenco, et al., 1985c; Koebele, 1985; Thorpe and Huntingford, 1992). Under these conditions, fish exist in dominance hierarchies, where larger, dominant fish occupy preferred habitat areas with respect to water quality, cover, and access to food. Genetically based differences may vary ontogenetically, due to reproductive maturation and tradeoffs between gametic and somatic growth. Agonistic behavior is density dependent, varies ontogenetically, and impacts the food assimilation efficiency (via fish activity level) and food consumption rate of individual fish. Disproportional food consumption between fish results when (1) food resources are available at less than satiation levels for the fish lot as a whole and (2) prepared food resources are applied at limited water surface areas or volumes of the rearing unit and are therefore defensible. Disproportional food consumption causes a divergence in individual fish weights over time (growth depensation) and has been reported to be the primary mechanism behind

fish size variation (Koebele, 1985). Natural food resources are normally disbursed evenly, and the lower fish densities used in such systems limits the ability of individual fish to dominate. When food resources are consumed proportionally by fish, smaller fish grow at higher specific rates than larger fish and fish size disparity decreases over time (growth compensation; Ricker, 1979).

In addition to biology and behavior based impacts on fish weight distributions, fish lot management often utilizes (1) fish lot dividing, where fish are size-graded and low or high grades removed, and (2) fish lot combining, where one fish lot is added to another. These sorting and mixing processes result from standard management practices of low grade culling, high grade harvesting and partial restocking, and control of fish weight variability within single fish lots (see Chapter 3, Fish lot handling and biomass management). As a result of these combined intrinsic and extrinsic impacts on fish, (1) fish weight variability rarely remains constant, (2) fish weight distributions may spread, contract, or become skewed or multi-modal, and (3) normal distributions often do not adequately represent fish weight distributions.

7.6.2 Modeling fish weight distributions

To support these considerations, growout fish lots may be modeled using either mean weights or weight distributions. Methods to simulate weight distributions were newly developed here, and no such models were found in the literature. Broodfish and egg lots are never modeled as distributions, but they can be represented by normal distributions of ATU and APU values (see Broodfish maturation and egg incubation), which are defined by means and coefficients of variation (%; $CV = 100 \text{ SD} / \text{mean}$; SD = standard deviation). CV values for broodfish and egg lots are assumed to remain constant over their culture periods and are carried forward to initialize the growout life-stage (broodfish → eggs → growout).

Fish weight distributions within a fish lot are represented by histograms. A histogram is composed of a given number of bins (e.g., 30; termed *bin count*), where each bin is defined by a mean weight and number of fish. The bin count remains constant unless the fish lot is divided or combined with another fish lot, in which case histograms and bin counts are also divided or combined. For new growout lots originating from facility inputs or life-stage transfers, initial weight distributions are defined by normal distributions, means, and CV values. Normal distributions are converted to histograms, using the range $\pm 3.0 \text{ SD}$ and dividing this range into same-sized, discrete increments totaling the bin count. The total number of fish in the histogram is made to equal the

original number of fish in the normal distribution. For this conversion, the normal frequency function is used (Little and Hills, 1978):

$$N_B = \{N_T / [SD (2 \pi)^{0.5}]\} \exp\{-0.5 [(W_B - W_M) / SD]^2\}$$

where N_B = number of fish in the bin defined by W_B , N_T = total number of fish in fish lot, SD = standard deviation of weights in fish lot (g), W_B = mean fish weight of given bin (g), and W_M = mean fish weight of the fish lot (g).

Bin weights (W_B) and fish numbers (N_B) change over time, and each bin of fish is individually modeled with respect to growth and feeding. Differential fish performance between bins is quantified using given values for a feed competition index (FCI; range 1 – 2; e.g., 1.3) and a fish performance index (FPI; range 1 – 2; e.g., 1.1). FCI expresses the competitive advantage of the largest fish relative to the mean fish size, with respect to the consumption of prepared (applied) feed. The FCI is used to distribute prepared feed among bins, and the given FCI value is adjusted (FCI') to account for the amount of prepared feed relative to total feed (prepared and natural). Feed availability for the fish lot as a whole is expressed as the fish lot FGI (FGI_M). FGI_M equals the mean of individual-bin FGI values (FGI_B). Feeding competition can only exist when the fish lot is fed below satiation levels ($FGI_M < 100\%$). If FCI equals 1.0, then no competition exists and all bins use FGI_M . As FCI is increased from 1.0 to 2.0, FGI_B of the largest fish (FGI_{BL}) approaches 100%, and FGI_B of the smallest fish (FGI_{BS}) approaches 0.0%:

$$\begin{aligned} FCI' &= FCI [1/FCI + (1 - 1/FCI) (FGI_{PF} / FGI_M)] \\ FGI_{BL} &= FCI' FGI_M \quad (\text{if } FGI_{BL} > 100, \text{ then } FGI_{BL} = 100) \\ FGI_{BS} &= (2 FGI_M) - FGI_{BL} \quad (\text{if } FGI_{BS} < 1.0, \text{ then } FGI_{BS} = 1.0) \end{aligned}$$

For example, if FGI_M is 100%, then all FGI_B values are 100% regardless of the FCI' value. If FGI_M is 70% and FCI' is 1.3, then FGI_{BL} is 91% and FGI_{BS} is 49%, where FGI_M remains at 70%. Following calculation of these extremes, FGI_B values of intermediate bins are determined by linear interpolation. Overall, this procedure emulates a competition hierarchy, where larger fish feed to satiation first and leave progressively less feed for smaller fish. The total amount of feed consumed by the fish lot is unchanged.

FPI expresses the genetically (physiologically) based superior performance of the largest fish relative to the mean fish size, with respect to the maximum capacity for feeding and growth. It is assumed that the fish that are largest initially have the highest physiological potential. Fish with FPI values greater than 1.0 out-perform the fish lot mean, and fish with FPI values less than 1.0 under-perform the mean. Mean growth and feeding rates for the fish lot as a whole are unchanged. FPI is applied similarly to FCI, but FPI is independent of feed availability. The mean FPI for the whole fish lot (1.0) equals the mean of individual-bin FPI values (FPI_B). As FPI is increased from 1.0 to 2.0, the FPI_B of the largest fish (FPI_{BL}) approaches 2.0, and FPI_B of the smallest fish (FPI_{BS}) approaches zero:

$$\begin{aligned} FPI_{BL} &= FPI && (\text{if } FPI_{BL} > 1.9, \text{ then } FPI_{BL} = 1.9) \\ FPI_{BS} &= 2.0 - FPI_{BL} \end{aligned}$$

Given these extremes, FPI_B values of intermediate bins are determined by linear interpolation. This procedure emulates a performance capacity hierarchy, where larger fish have a higher physiological capacity for feeding and growth. The performance of the fish lot as a whole is unchanged.

When growout fish lots are modeled using weight distributions rather than mean weights, additional management options can be applied (see Chapter 3, Fish lot handling and biomass management). The use of distributions provides a basis for the division of fish lots based on fish size range. For high-grade removal of fish, fish are counted bin by bin, in the order of the largest to smallest fish size, to determine if the required high-grade proportion of the total fish lot is available. Low-grade removal uses a similar, inverse approach. For the management of fish size ranges, fish size variability is quantified as a calculated CV, supporting decisions (1) to divide a fish lot based on a high CV or (2) to not combine two fish lots because the resulting CV would be excessive. When a fish lot is divided, the weight distribution is divided into two distributions, at the given division weight. When two fish lots are combined, the two distributions are also combined. In each case, the bin count is conserved, and thus the bin count of a divided fish lot is reduced and the bin count of a combined fish lot is increased. Alternatively, for combined fish lots, bin structures may be compressed to the original bin count of new fish lots (e.g., 30). This procedure reduces the resolution of the new distribution but also maintains bin counts and corresponding calculation intensity at reasonable levels.

7.7 Natural fish productivity

Food resources used by a given fish lot may consist of (1) natural (endogenous) food resources only, (2) natural foods plus supplemental prepared feeds, or (3) prepared (exogenous) feeds only. The contribution of natural food resources to fish feeding and growth is termed natural fish productivity (NFP; kg fish/ha/day). Background considerations and methods used to quantify and model NFP are described below.

7.7.1 Natural food resources

Natural food resources for fish include bacterial-detrital aggregate (BDA), phytoplankton, zooplankton, invertebrates, and fish prey (polyculture). BDA represents the detrital and heterotrophic bacteria based food chain (Schroeder, 1978; Opuszynski, 1981; Moriarty and Pullin, 1987). Qualitative aspects of BDA feeding have been examined for some species (e.g., Bowen, 1982), but quantitative impacts on NFP are not well understood. Phytoplankton (primary productivity) supported food chains typically dominate solar-algae fish ponds (Schroeder, et al. 1990). Phytoplankton may be (1) consumed directly from the water column (e.g., carp and tilapia), (2) consumed as settled aggregate (e.g., tilapia), (3) a major contributor of organic solids (dead phytoplankton) to the BDA food chain, and (4) consumed by zooplankton (secondary productivity) which in turn are consumed by fish. Due to the grazing pressure exerted by phytophagous fish (e.g., silver carp), it has been reported that plankton size can decline appreciably over the culture period, e.g., from $>10\text{-}30\text{ }\mu\text{m}$ to $<10\text{ }\mu\text{m}$ (nanoplankton) (Spataru, 1977; Cremer and Smitherman, 1980; Opuszynski, 1981). Feeding efficiency declines with phytoplankton size, and thus phytoplankton as a direct food resource is degraded over the culture period. It has also been demonstrated that fish grazing pressure can reduce zooplankton densities (e.g., Diana et al., 1990), again representing a degradation of natural food resources over the culture period.

The contribution of specific natural foods to NFP depends on fish species (feeding habits), fish size (when feeding habits vary ontogenetically), and the biological productivity and management of the aquaculture system. For herbivores and detritivores such as carp, tilapia, and crayfish under extensive aquaculture production (500-5000 kg fish/ha), natural foods can be a primary or sole food source. Natural foods may also be significant for fry and fingerling production of carnivorous species such as striped/hybrid bass, sea bass, and red drum, for which zooplankton food resources are utilized. Natural food resources can be indirectly managed by control of fish densities and

maintenance of nutrient levels for primary productivity. While natural food resources may exist in more intensively managed systems, their relative contribution declines with increasing management intensity until they become negligible.

7.7.2 Modeling natural fish productivity

Mechanistic models used to quantify NFP are complex and mainly used as research tools (Svirezhev et al., 1984). In the method developed here, NFP is approximated by empirically based relationships between NFP and net primary productivity (NPP) and between NFP and fish biomass density (FBD; kg/ha) (McConnell et al., 1977; Almazan and Boyd, 1978b; Colman and Edwards, 1987; Hepher, 1988; Schroeder et al., 1990; Knud-Hansen et al., 1991; Diana, 1997). This method was not previously described in the literature, but uses well known concepts and terms from the literature. The procedure accounts for trends in NFP over a fish culture period, in which endogenous food resources may be initially high or unlimited and subsequently exhausted, as a function of increasing fish density and food consumption in association with fish growth. For diurnal simulations, the daily mean NPP is used when NFP is a function of NPP. Diurnal modeling of fish catabolism of endogenous foods is by the same procedures used for exogenous feeds. Natural foods that are explicitly considered are limited to BDA and phytoplankton, with respect to their representation by state variables and mass balance modeling (including fish consumption). However, in the NFP model used here, all natural foods which contribute to the productivity of a given fish lot can be implicitly considered.

In the NFP method developed here, empirically based *critical standing crop* (FBD_{csc}) and *carrying capacity* (FBD_{cc}) fish densities are utilized (Hepher, 1988). At fish densities less than FBD_{csc} , the availability of natural food resources either exceeds maximum consumption rates by fish or, at least, these resources are not negatively impacted by fish density. As fish density increases above FBD_{csc} due to fish growth, natural food resources are utilized by fish beyond their sustainable yield and hence depleted, resulting in a decline in NFP. When fish density achieves FBD_{cc} , natural food resources are depleted to a level that no longer supports fish growth and NFP is reduced to zero. The ratio of FBD_{cc} to FBD_{csc} typically ranges from 1.5 to 3.0. Use of NFP without supplemental feeding yields sigmoidal fish growth curves, as natural food resources are initially unlimited, then overwhelmed, and finally exhausted.

The procedure and calculations of this NFP model are listed below and illustrated in Figure 7.5. This procedure is repeated for each fish lot at each simulation time step. FBD_{cc} , FBD_{csc} , and other parameters are provided as default, user accessible values. The peaked NFP profile shown in Figure 7.5 is characteristic of NFP, as reported in numerous studies (e.g., Ernst et al., 1989).

- 1) At the initial simulation step, the current mean fish weight is a given. Otherwise, a new weight is calculated from the weight and growth rate in the prior simulation step. Current FBD and NFP values are updated, using the mean fish weight, growth rate, and number of fish.
- 2) Maximum potential NFP (NFP_{max}) may be specified as annual regimes of expected monthly mean values (e.g., 20 - 60 kg/ha/day; linear interpolation used) or calculated as a function of NPP ($gC/m^2/day$; expressed per area; positive value), where:

$$NFP_{max} = a + b NPP + c NPP^2$$

- 3) GR_{max} is calculated using the selected growth model at the existing environmental conditions and unlimited feeding rate. The fish growth rate (GR_{NF} ; g ww fish/fish/day) and FGI (FGI_{NF}) supported by NFP are calculated using a fish biomass density scalar (SCL_{FBD}). If $FBD \leq FBD_{csc}$, then $SCL_{FBD} = 1.0$. If $FBD \geq FBD_{cc}$, then $SCL_{FBD} = 0.0$, and this procedure is terminated. Otherwise, for the case $FBD_{csc} < FBD < FBD_{cc}$, GR_{NF} and FGI_{NF} supported by NFP are calculated by:

$$GR_{NF} = SCL_{FBD} W NFP_{max} / FBD$$

$$\text{where } SCL_{FBD} = (FBD_{cc} - FBD) / (FBD_{cc} - FBD_{csc})$$

$$\text{If } GR_{NF} > GR_{max}, \text{ then } GR_{NF} = GR_{max}$$

$$FGI_{NF} = 100 GR_{NF} / GR_{max}$$

- 4) If supplemental feeds are used, then the FFI equivalent of NFP (FFI_{NF}) is calculated from FGI_{NF} (function described later). To achieve the target FFI, as based on the target FGI, the FFI to be supplied by prepared feeds (FFI_{PF}) is equal to the target FFI minus FFI_{NF} (Figure 7.6).

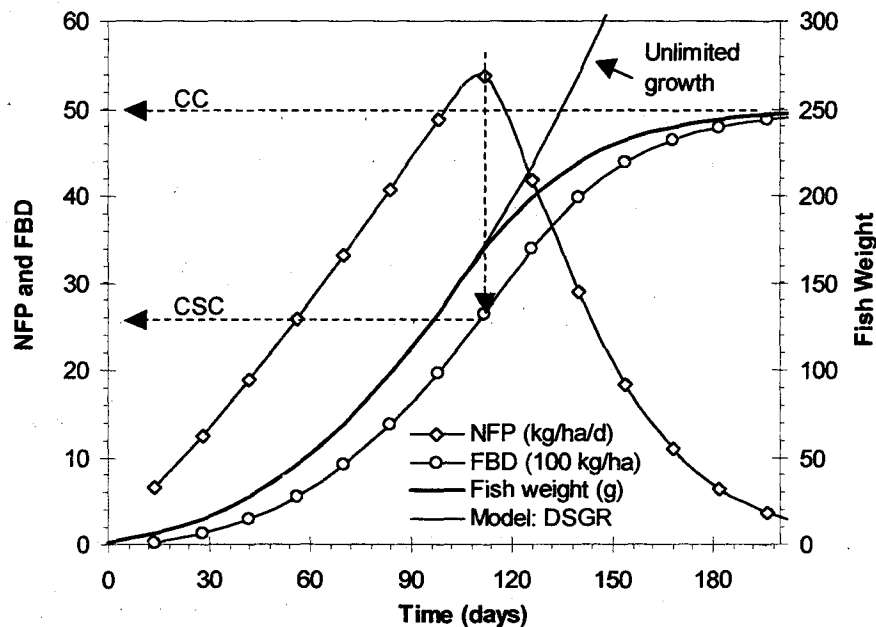


Figure 7.5. Application of the algorithm for natural fish productivity described in the text, in which supplemental feeding is not used, fish over-utilize and deplete their natural food resources, and asymptotic fish growth results

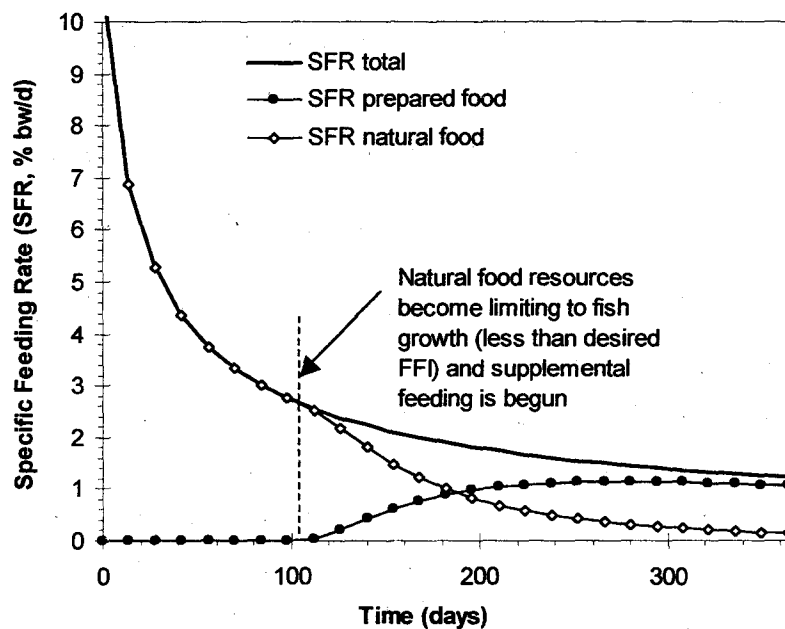


Figure 7.6. Application of the DSFR model to calculation of feeding rates, where natural fish productivity is considered and a supplemental feeding schedule is determined that maintains a specified, constant fish feeding index (FFI)

7.8 Fish feeding

If the LNGR, DSGR, or VBGF fish growth models are used, then feeding rates are determined by (1) the use of look-up tables (TABL), (2) the double-logarithmic specific feeding rate model (DSFR), or (3) the use of calculated values for food conversion efficiency (FFCE). As previously described, if the BIOE growth method is used, then fish feeding and growth rates are both calculated by the BIOE method and the methods described below are not used.

7.8.1 TABL and DSFR feeding rate methods

For the TABL and DSFR methods, maximum feeding rates (FR_{max}) are a function of water temperature and fish weight. FR_{max} is then adjusted to the fish feeding index (FFI) that yields the target fish growth index (FGI'). If SCL_{WQ} is applied to fish growth rates, then the same scalar value is applied to feeding rates. It is assumed that poor water quality decreases growth and feeding rates together. However, regardless of the use SCL_{FQ} and SCL_{FS} for growth rates, these scalars are not applied to feeding rates. Thus, food conversion efficiency (FCE) declines as feed quality declines and as growth becomes asymptotic. For diurnal simulations, the FGI' value includes SCL_{PP} and SCL_{FP} . Therefore, these scalars are accounted for in the FFI calculated from FGI' . Corrections for differences in feed moisture content between the calibration and application studies are unlikely but can be considered. After FR_{max} is calculated, feeding rate (FR) is calculated by:

$$FR = (FFI / 100) SCL_{WQ} FR_{max}$$

For the TABL method, look-up tables for feeding rates (FR_{max}) are indexed by water temperature and fish weight. Table values for specific fish species and feeds are available in the aquaculture literature and from feed manufacturers. Feeding rate tables are available as templates in AquaFarm, for which temperature and weight indices and feeding rate values are accessible to the user. Only approximate feeding rate values are provided, and feeding rate values are the user's responsibility. In the use of look-up tables, two-way linear interpolation is used to determine feeding rates, based on the current temperature and fish weight.

The DSFR model (Balarin and Haller, 1982; Ernst et al., 1989) is identical to the DSGR model in functional form and the log-transform, parameter regression procedures used. Normally, the

DSFR and DSGR models share a common calibration dataset and are applied as a paired function. The DSFR model is:

$$\begin{aligned} \text{SFR}_{\max} &= \text{SFR}_c W^{-\text{SFR}_e} \\ \text{or} \quad \text{FR}_{\max} &= \text{SFR}_c W^{(1.0 - \text{SFR}_e)} \end{aligned}$$

Parameter estimation by regression is similar to the DSGR procedure. For example, if SFR_c is a constant, SFR_c and SFR_e are determined by:

$$\begin{aligned} \log_e(\text{SFR}) &= \log_e(\text{SFR}_c) - [\text{SFR}_e \log_e(W_{gm})] \\ \text{where} \quad W_{gm} &= e^{\{[\log_e(W_o) + \log_e(W_t)] / 2.0\}} \end{aligned}$$

If, for example, SFR_c is a function of water temperature (T ; using polynomial scalar function) and feed availability (FFI; fraction form), then:

$$\begin{aligned} \log_e(\text{SFR}) &= \log_e(\text{SFR}_c) - [\text{SFR}_e \log_e(W_{gm})] \\ \text{where} \quad \text{SFR}_c &= k_1 + k_2 T + k_3 T^2 \\ \text{or} \quad \log_e(\text{SFR}) &= \text{SFR}_c' - [\text{SFR}_e \log_e(W_{gm})] \\ \text{where} \quad \text{SFR}_c' &= k_1' + k_2' T + k_3' T^2 \\ \text{and} \quad \text{SFR}_c &= e^{\text{SFR}_c'} \\ \text{or} \quad \text{SFR}_c' &= \log_e(\text{SFR}_c) \end{aligned}$$

7.8.2 FFCE feeding rate method

While feeding rate tables are readily available, feeding rate functions are poorly represented in the aquaculture literature. Often, food conversion efficiency values (FCE) are better known, and their use takes advantage of predicted growth rates. For the FFCE method, feeding rates are based on growth rates and calculated FCE values, where $\text{FR} = \text{GR} / \text{FCE}$. In contrast, for the TABL and DSFR methods, FCE is a result of calculated growth and feeding rates. FCE values can be (1) specified as a constant value, (2) determined by the use of look-up tables (similar to the use of feed tables; indexed by fish size and water temperature), or (3) calculated. Regardless of the method used, FCE values are used in conjunction with maximum growth rates (GR_{\max}) in order to calculate maximum feeding rates (FR_{\max}). Thus, table or calculated FCE values are those achieved at maximum feeding rates. SCL_{WQ} is not applied to the calculated FCE, but if SCL_{FQ} or SCL_{FS} are

used in the growth model, then they are also applied to FCE. The logical basis of this is the same as that used for the TABL and DSFR methods. The resulting FR_{max} value is then adjusted for FFI as used for the other feed models, which accounts for any use of SCL_{pp} and SCL_{fp} .

To derive a function for FCE, the DSGR model can be divided by the DSFR model to give FCE as a function of fish weight (Figure 7.7):

$$FCE = 100 FCE_c W^{FCE_e}$$

where $FCE_c = SGR_c / SFR_c$ where $FCE_c < \{100 [(1.0 - FD_{mst}) / (1.0 - FS_{mst})]\}$

and $FCE_e = SFR_e - SGR_e$ where $FCE_e < 0$

If values for SGR_c , SFR_c , SFR_e , and SGR_e are not available, then FCE_c and FCE_e can be determined by user supplied data points for FCE:

$$FCE_e = \log_e(FCE_1 / FCE_2) / \log_e(W_1 / W_2)$$

$$FCE_c = FCE_1 / (100 W_1^{FCE_e})$$

where FCE_1 and FCE_2 = FCE values at fish weights W_1 and W_2 respectively

7.8.3 FCE dependency on feeding rate

In addition to the dependency of FCE on fish size, FCE varies with fish feeding rate for a given fish size (Paloheimo and Dickie, 1966; Payne, 1979; Brett and Groves, 1979; Brett, 1979; Huisman and Valentijn, 1981). FCE first increases with increasing feeding rate above a maintenance ration (FFI_{mnt} ; e.g., 10% or 0.1), then reaches a maximum efficiency at an optimum ration (FFI_{opt} ; e.g., 50% or 0.5), and finally declines as feeding rate is increased further to a maximum ration (FFI_{max} ; 100% or 1.0). The bioenergetic mechanisms underlying the response of FCE to feeding rate are complex. The shape of the FCE-FFI curve varies to some degree with fish species, fish size, and environmental conditions.

While the concepts and complexities of the FCE-FFI relationship have been well reported (e.g., Paloheimo and Dickie, 1966; Payne, 1979; Brett and Groves, 1979; Brett, 1979), practical functional approaches for defining this relationship have not. An expression for the FCE-FFI relationship was developed here and is illustrated in Figure 7.8. FFI is calculated as a function of FGI and then FCE is calculated using this FFI value:

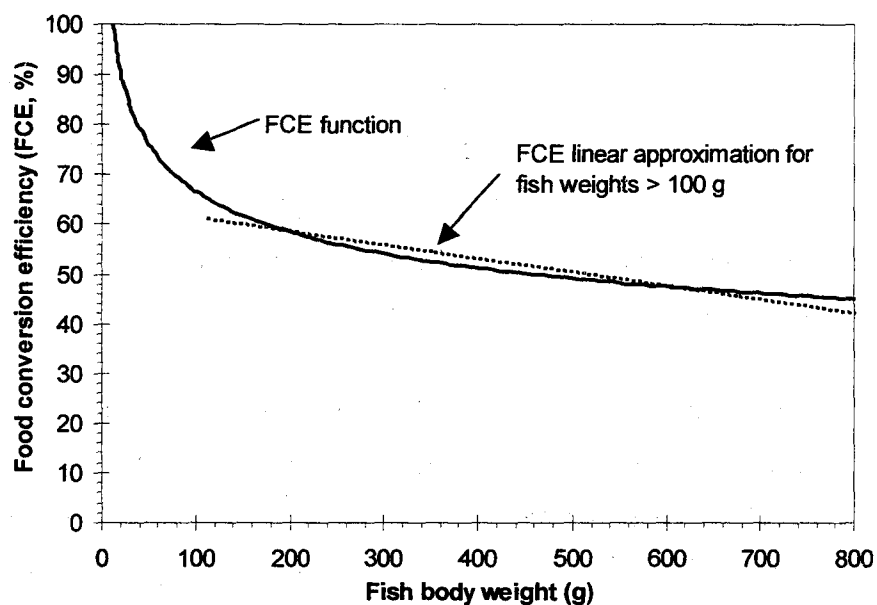


Figure 7.7. Food conversion efficiency as a function of fish weight, calculated by methods given in the text, for which it may be sufficient to represent this relationship with a straight line for larger fish sizes (i.e. $FCE = a - bW$)

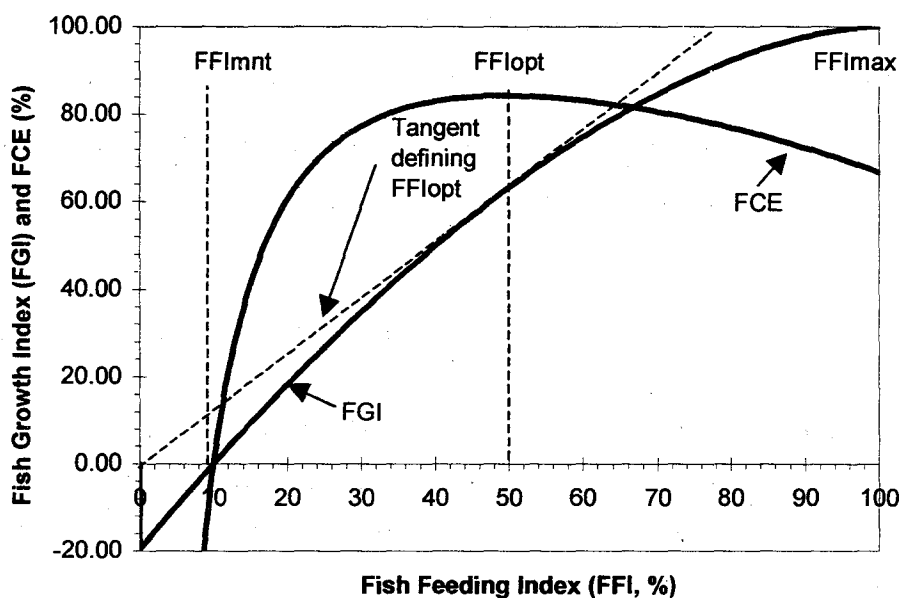


Figure 7.8. Fish growth rate (as FGI) and food conversion efficiency (FCE) as a function of fish feeding rate (as FFI) calculated by methods given in the text

$$\begin{aligned} \text{FGI} &= 1.0 - [(\text{FFI}_{\text{max}} - \text{FFI}) / (\text{FFI}_{\text{max}} - \text{FFI}_{\text{mnt}})]^k \\ \text{or} \quad \text{FGI} &= 1.0 - [(1.0 - \text{FFI}) / (1.0 - \text{FFI}_{\text{mnt}})]^k \\ \text{and} \quad \text{FFI} &= 1.0 - [(1.0 - \text{FGI})^{1/k} (1.0 - \text{FFI}_{\text{mnt}})] \\ \text{and} \quad \text{FCE} &= 100 (\text{SGR}_{\text{max}} \text{FGI}) / (\text{SFR}_{\text{max}} \text{FFI}) \\ \text{where} \quad k &= \text{used to adjust shape of FGI-FFI curve and region of optimum FCE} \\ &\quad \text{(typical range: 1.5 to 2.0; a value of 1.7 is used in Figure 7.8)} \end{aligned}$$

The optimum feeding rate with respect to FCE (FFI_{opt}) is predicted at the highest point on the FCE-FFI curve, where FCE is maximized. On the FGI-FFI curve, it is found where a tangent drawn from the origin intersects the curve. Corey and English (1985) applied principals of this concept using a relatively complex, iterative “shooting” procedure to optimize feeding rates over the rearing period as a whole. In the approach used here, however, feeding rates are used that achieve desired growth rates, and feeding rates are not managed with respect to FCE. FCE can be managed indirectly based on target growth rates, but this is under the responsibility of the user. In practice, feeding rates where FCE is maximized are typically two-thirds or less of maximum feeding rates (e.g. 50% FFI; Brett, 1979), causing significantly slower growth rates and longer growout periods. Especially for intensive aquaculture, economic considerations of facility capacity utilization, fish biomass support, and production throughput normally overwhelm economic considerations of FCE optimization. Therefore, feeding rates well above FFI_{opt} are normally used. As evident in Figure 7.8, responses of FGI and FCE to feeding rates greater than FFI_{opt} may be adequately represented with a simple linear function: i.e., $\text{FGI} = a + b \text{FFI}$ and $\text{FCE} = c - d \text{FFI}$.

7.9 Fish feed digestion and metabolism

Fish oxygen consumption, metabolite excretion, and fecal egestion occur in conjunction with food ingestion, digestion and catabolism. Excreted metabolites considered include carbon dioxide, dissolved nitrogen and phosphorous compounds, and inorganic and organic particulate solids. Fish excrete nitrogen mainly as ammonia (NH_3 ; $\geq 75\%$), with the remainder composed mainly of urea, which breaks downs to ammonia and carbon dioxide ($\text{CO}(\text{NH}_2)_2 + \text{H}_2\text{O} \rightarrow 2 \text{NH}_3 + \text{CO}_2$). Here, all excreted nitrogen is considered to be unionized ammonia (NH_3). Excreted phosphorous (P) is assumed to be in the form of ortho-phosphate (HPO_4^{-2}). Any impact of fish metabolism on

alkalinity is assumed to be negligible. Egested particulate solids (fecal material) result from undigested foods and are comprised of inorganic and organic solids, the latter containing N, P, and BOD (biochemical oxygen demand). The specific composition of fecal material is dependent on feed composition and digestion efficiency. Generally, fecal ash content (inorganic solids) is increased and organic and caloric contents are decreased relative to feed composition (Brett and Groves, 1979). The BOD content of fecal material is approximately 1.0 kg ultimate BOD per kg dry weight solids (Speece, 1973). Applied feeds that remain uneaten (waste feed) may be an additional source of particulate solids in fish rearing units. In the methods used here, however, it is assumed that all applied feed is consumed.

Fish oxygen consumption and metabolite/fecal excretion rates (g/kg fish/day or mg/kg fish/hr) are represented by terms in the mass balance equations of fish rearing units. These rates are a function of feeding rate, food digestion and conversion efficiencies, food composition, stoichiometry of food catabolism, and fish composition (Huisman, 1976; Brett, 1979; Brett and Groves, 1979; Hepher, 1988; Meyer-Burgdorff et al., 1989; Jobling, 1994). Two approaches are described here to calculate these rates. In the simpler method, reported ratios of compound consumption and excretion per unit food consumption (g compound/g feed) are used. As shown in Table 7.8, these ratios range widely. For example, reported oxygen-food ratios range from about 0.25 (salmonids; Willoughby et al., 1972) to 0.61 (sockeye salmon; Brett and Zala 1975). Discrepancies in these values are due to a variety of factors, including fish species, fish activity level, feeding rate, feed composition and digestible energy, and the empirical methods used (e.g., daily mean or shorter term rates). As an alternative to the use of reported ratios, a more robust approach is also used in which compound-food ratios are calculated as a function of food composition and digestion efficiency.

7.9.1 Calculation of compound-food ratios

The calculation of compound-food ratios is a multi-step procedure. The first task is to calculate ratios for complete food oxidation, as a function of food composition and catabolic parameters. Feed compositions for prepared feeds are available from feed manufacturers (e.g., feed bag label). Natural food resources considered here include phytoplankton, particulate organic solids in the water column, and settled organic solids. Each of these natural foods can be individually designated for use by a given fish species. The combined, weighted mean composition of natural food is based on the food components utilized and their individual compositions. Constituents considered include

protein (calculated; includes N), lipids (5% assumed), carbohydrates (calculated), fiber (10% assumed), ash (5% assumed), and P (calculated). N and P contents of solids and phytoplankton are maintained as state variables. Protein content is based on N content, assuming that protein is 16% N. All calculations for natural food are carried out in dry weight terms. For both prepared and natural foods, carbohydrates are represented as nitrogen free extract (NFE), where percent NFE = 100 - protein - lipid - fiber - ash - moisture. If both prepared and natural foods are utilized, their combined, weighted mean composition is based on their relative ingestion rates by fish. An example budget for deriving oxygen demand and carbon dioxide production values for a prepared fish feed is given in Table 7.8, assuming complete oxidation of feed. In this budget, the feed composition values are variables and the mass-energy conversion terms are parameters.

In the second step of this procedure, stoichiometric ratios of complete food oxidation are corrected for food digestion and conversion efficiencies, in order to account for the undigested and stored feed fractions that are not catabolized. An example budget for deriving fractional uses of ingested feed as a function of fish feeding rate is given in Table 7.9. In this example, FCE varies from zero to 90% (wet wt. basis) and digestion efficiency varies from 90 to 60% (dry wt. basis) as feeding rate is increased from maintenance (10% FFI) to maximum (100% FFI) levels. It is generally accepted that food digestion efficiency declines with increasing feed ingestion rate, but the magnitude of this response, as defined by DE_{max} and DE_{min} , depends on fish species and environmental conditions (Speece, 1973; Hepher 1988; Meyer-Burgdorff, 1989). For a given FFI and FCE (dw), fractional fates of ingested feed are calculated by:

$$FD_{DIG} = DE_{max} - [(DE_{max} - DE_{min}) (FFI - FFI_{mnt}) / (FFI_{max} - FFI_{mnt})]$$

$$FD_{UND} = 1.0 - FD_{DIG}$$

$$FD_{GRO} = FCE_{dw} / 100$$

$$FD_{MET} = FD_{DIG} - FD_{GRO}$$

In the third step of this procedure, feed composition values from Table 7.8 and catabolic fractions from Table 7.9 are combined to calculate compound-food ratios of food catabolism (Table 7.10). In the example exercise, the simplifying assumption is used that fish and feed material compositions are comparable (other than moisture content). This simplification is not used here, and N and P uptake and excretion for digested feed is based on a material balance considering the N and P content of the fish (Table 7.11).

Table 7.8. Budget worksheet for deriving oxygen demand and carbon dioxide production values for a fish food of given composition *

Food component	Component fraction (g cp/ g fd)	Caloric content (kcal/ g cp)	Caloric content (kcal/ g fd)	Oxycaloric equivalent (g O ₂ / kcal)	Oxygen demand (g O ₂ / g fd)	RQ (mol CO ₂ / mol O ₂)	Carbon dioxide production (g CO ₂ / g fd)
(a)	(b)	(c)	(d)	(e)	(f)	(g)	(h)
Crude protein	0.45	4.0	1.800	0.313	0.563	0.9	0.696
Crude lipid	0.15	8.0	1.200	0.305	0.366	0.7	0.352
NFE	0.15	2.0	0.300	0.283	0.085	1.0	0.117
Crude fiber	0.04	0.0	0.000	0.000	0.000	1.0	0.000
Ash	0.11	0.0	0.000	0.000	0.000	0.0	0.000
Moisture	0.10	0.0	0.000	0.000	0.000	0.0	0.000
Total	1.00	---	3.300	---	1.013	---	1.165

* Column letters used to identify columns and associated footnotes. Abbreviations: food (fd) and food component (cp).

^b Values represent a typical trout growout feed; nitrogen free extract (NFE; carbohydrates) is calculated from given values, phosphorous is contained in given components (1.7%), and protein is assumed to contain 16% nitrogen.

^c Caloric content values (metabolizable energy; kcal) of food components vary among fish species; the values here represent approximate averages of literature values (Brett and Groves, 1979; Piper et al., 1986; Hepher, 1988; Jobling, 1994).

^d Value = (b) x (c)

^e Brett and Groves, 1979

^f Value = (d) x (e)

^g Respiratory quotient (RQ; Brett and Groves, 1979)

^h Value = (f) x (g) x (44 g CO₂ / mol) / (32 g O₂ / mol)

Table 7.9. Example budget for deriving fractional uses of ingested feed as a function of fish feeding rate

Feeding rate (as FFI, %)	Food conversion efficiency (FCE, %)		Fractional uses of ingested food (g use/g food)		
FFI	FCE (ww)	FCE (dw)	Undigested ^a	Growth ^b	Catabolized ^c
10.00	0.00	0.00	0.10	0.00	0.90
20.00	60.00	20.00	0.13	0.20	0.67
40.00	75.00	25.00	0.20	0.25	0.55
60.00	90.00	30.00	0.27	0.30	0.43
80.00	75.00	25.00	0.33	0.25	0.42
100.00	60.00	20.00	0.40	0.20	0.40

^a Undigested fraction: based on linear response of digestion efficiency to feeding rate

^b Growth fraction: equivalent to dry weight food conversion efficiency expressed as fraction

^c Catabolized fraction = 1.0 - undigested fraction - growth fraction = digested fraction - growth fraction

Table 7.10. Example budget for deriving compound-food ratios of food catabolism, combining feed composition values from Table 7.8 and catabolic fractions from Table 7.9

Feeding rate	Food catabolism (g compound / g food) ^a					Total metabolism ^b
FFI	Oxygen (O ₂)	Carbon dioxide (CO ₂)	Total ammonia (N)	Phosphorous (P)	Particulate solids (dw)	(mg O ₂ /kg fish/hr)
10.00	0.912	1.049	0.065	0.0153	0.100	114
20.00	0.675	0.777	0.048	0.0113	0.133	169
40.00	0.557	0.641	0.040	0.0094	0.200	279
60.00	0.439	0.505	0.031	0.0074	0.267	329
80.00	0.422	0.485	0.030	0.0071	0.333	422
100.00	0.405	0.466	0.029	0.0068	0.400	507
Reported ^c	0.20 - 0.60	0.25 - 0.70	0.025 - 0.040	0.005 - 0.050	0.30 - 0.65	50 - 500+
Default ^d	0.35	0.48 ^e	0.03	0.005	0.3 ^f	variable

^a Expressed as g compound / g food, for wet weight food at 10% moisture content

^b Calculated at a feeding rate of 30 g feed/kg fish/day (equivalent to 3% body weight per day)

^c Reported values: ranges are based on a wide review of the aquaculture literature

^d User-accessible values provided by AquaFarm (not used if compound-food ratios are calculated)

^e Based on 1.0 mol CO₂ / 1.0 mol O₂ (0.48 = 0.35 x 44 / 32)

^f Organic solids (0.27; 90%), inorganic solids (0.03; 10%); organic solids (6% N, 2% P)

Table 7.11 Material composition of a fish (major components) ^a

Component	Wet weight fraction	Dry weight fraction ^b
Water	0.74	0.0000
Protein	0.16	0.6154
Lipid	0.07	0.2692
Ash	0.03	0.1154 ^c
Carbon	11.44	44
Nitrogen	0.0256 ^d	0.0985
Phosphorous	0.01	0.0385
Calcium	0.01352	0.052
Magnesium	0.00039	0.0015

^a Approximate consensus of reported values: Creswell, 1993 (pg. 142), Weatherly and Gill, 1987 (p. 101), Hepher, 1988 (p. 167), Boyd and Green, 1998

^b $dw = ww / (1.0 - FS_{mst} / 100)$; for dry weight components: 1.0 = protein + lipid + ash

^c Boyd and Green (1998) reported an average value 18.7 (mixed species) and 19.4 (tilapia)

^d Value = 0.16×0.16 , where 0.16 N / protein

In the final step of this procedure, daily mean oxygen consumption rates and metabolite/fecal excretion rates (g compound/kg fish/day) are calculated by multiplying compound-food ratios by the daily feed application rate (g feed/kg fish/day). The impact of fish excretory products on alkalinity is considered, including NH_3 , $H_2PO_4^{-1}$, and HPO_4^{-2} , but fish uptake and excretion of HCO_3^{-1} is ignored. The proportion of undigested food of the food consumed (FD_{UND}) is combined with food ingestion rates to calculate production rates of fecal material by fish. The composition of fecal material is assumed to be the same as that of the ingested food, including inorganic solids (ash), organic solids, and the N and P content of organic solids. This simplifying assumption may result in some degree of over estimation of the fecal organic fraction.

7.9.2 Considerations in the use of compound-food ratios

The correction of compound-food ratios from feed composition to food catabolism illustrates an important concept regarding fish utilization of feeds. Metabolizable energy contents of feeds (kcal/g) depend on feed composition and species-specific digestion capabilities. Because energy needs for maintenance and activity must be satisfied before growth can occur, dietary protein will be used for energy when the diet is deficient in non-protein calories (lipids and carbohydrates). As use of protein for energy is increased, fish nitrogen excretion and exothermic energy losses of

amino acid deamination (heat increment) also increase. Accordingly, nitrogen loading by fish on their culture system is increased and the net energy content of the feed is reduced. To minimize protein use for energy and maximize protein use for growth, fish feeds can be formulated to achieve protein to energy ratios that spare protein as an energy source. This is normally achieved by increasing the proportion of lipids.

The results of the example exercise demonstrate the pronounced impact of fish feeding rates on compound-food ratios, due to the dependency of food conversion and digestion efficiencies on fish feeding rate. Specific results of this example are dependent on the values used for food digestion efficiencies, conversion efficiencies, and energy and protein contents. For example, higher digestion efficiencies would increase oxygen-food ratios and higher conversion efficiencies would decrease oxygen-food ratios. Metabolizable energy contents of fish feeds vary from 2.0 to 3.5 kcal/g or more, compared to the 3.3 kcal/g used in the example, with a directly proportional impact on compound-food ratios for oxygen and carbon dioxide. In addition, protein contents of fish feeds vary from about 25 to 55% dry weight (dw), and fish protein contents typically range from about 50 to 70 % dw (Weatherley and Gill, 1987).

To simplify the example exercise, it was assumed that fish and feed protein contents were comparable (50% dw) and thus nitrogen-food ratios were a product of catabolized fractions and nitrogen content of the feed. Under practical aquaculture, however, feed protein levels are typically less than those of fish, and feeds are normally formulated to allow protein sparing for growth. The resulting decrease in the nitrogen-food catabolic ratio is established by considering this protein differential in the nitrogen mass balance of the fish. For example, if fish protein content is increased to 60% dw in the example exercise, then the nitrogen-food ratio at the 80% FFI feeding level is 0.027 g N/ g food (compared to 0.030). If feed protein content is reduced to 40% dw in the example exercise, then the nitrogen-food ratio at the 80% FFI feeding level is 0.021 g N/ g food (compared to 0.030), reflecting both the nitrogen content reduction of the feed and preferential nitrogen uptake by the fish. This concept of compound incorporation (for digested food) as a function of availability and body composition is also applied to phosphorous.

7.9.3 Diurnal fish metabolism

In the application of daily mean metabolic rates (based on daily feeding rates) to facility design, it is critical to consider that over a 24-hour diurnal cycle, hourly fish metabolic rates may

vary up to three fold or more due to feed application events during daylight hours, diurnal temperature oscillations, and diurnal fish activity levels (Brett and Zala, 1975; Brett and Groves, 1979; Colt and Orwicz, 1991b). Accordingly, peak biomass support demands on fish culture systems may exceed daily mean demands by a factor two or more (peak-mean ratio). Magnitudes of diurnal variations tend to decrease when the number of feedings per day is increased and the daily feeding period is lengthened, for the same total daily feed. Required peak-mean ratios for facility design also depend on management tolerance for short term, sub-optimal water quality. Depending on aquaculture management intensity, strategies used to address diurnal changes in fish metabolic loading differ on how closely hourly levels of fish biomass support capacity are matched to demand. If biomass support capacity is maintained at a constant rate that satisfies peak requirements over a whole day, then biomass support capacity is not fully utilized during periods of low demand but facility management is simplified. Indeed, many aquaculture facilities do not use diurnal management for fish biomass support, other than feeding (e.g., salmon hatcheries), and biomass support is managed on a weekly or seasonal basis such that peak diurnal demands are met.

To simulate this type of management in the context of a daily simulation, stringent water quality, fish loading, and/or feed loading criteria are used for the management of fish biomass support (see Chapter 3). This serves to amplify biomass support needs. Application of peak-mean ratios to daily mean metabolic rates is an erroneous approach, since it results in the over-estimation of daily mean metabolic rates, fish waste production, and fish impacts on water quality.

If needed, diurnal simulations provide much better resolution of fish metabolic rates. Diurnal simulations can be used to quantify the full, diurnal range of fish metabolism and simulate the use of diurnal management of biomass support. As described earlier, in the modeling approach used here, feeding rates are a function of growth rates and metabolic rates are a function of feeding rates. Therefore, diurnal metabolism is accounted for by the diurnal feed-processing rates described earlier, and only a few additional considerations need to be applied to model diurnal metabolism. By the function described earlier, diurnal metabolic rates are represented by a sinusoid function over the 24-hr day, such that the time integrated rates over the 24-hr day are equivalent to the corresponding daily mean values. Diurnal profiles of fish oxygen consumption and carbon dioxide excretion rates match the peaks and lows of diurnal feed-processing rates. However, as demonstrated by empirical studies (see Chapter 8), peaks and lows of nitrogen, phosphorous, and solid excretion lag those of oxygen consumption by a given lag period (e.g., 3 hr). This adjustment is used to account for gut passage and digestive processing times of food.

7.10 Broodfish maturation and egg incubation

The sexual maturation of broodfish is based on accumulated temperature units (ATU, degree-days) and/or photoperiod units (APU, hour-days) required to achieve spawning condition, for fish above a minimum size and within required temperature and day length ranges (Blaxter, 1969; Hoar, 1969; Piper et al., 1986). A specified female-male sex ratio is used for spawning, and egg production per female is a function of fish size (length or weight). Depending on fish species, fish can spawn once per year, repeat spawn, or die after spawning. Fish maturation rates are used to schedule broodfish holding periods and spawning events. Broodfish growth, feeding, and metabolic rates are handled similarly to growout fish, using the simplest methods.

Egg and larval development is based on accumulated temperature units (ATU, degree-days) required to achieve major development stages: eyed egg, hatched larvae, and first-feeding fry (Blaxter, 1969; Piper et al., 1986). Egg development rates are used to schedule egg incubation periods and handling events. Weights of first-feeding fry are a species-specific biological parameter and are used to define initial weights for growout fish lots that originate from egg lots. Egg metabolic rates are a function of water temperature, and only oxygen consumption is considered.

7.11 Application of fish performance engineering to facility modeling

Broodfish, egg, and growout lots are simulation objects and are updated stepwise over the course of a simulation. Simplified, analytical integration or Eulerian numerical integration is suitable for all of the methods presented in this chapter, using time steps of one day or less. The staged, iterative procedure by which AquaFarm is applied to the design and management of aquaculture facilities is described in Chapter 2. Given that fish performance is the guiding process of design and management, it is useful to review the role of fish performance in this design procedure:

- 1) Production specification. Facility production objectives are specified in terms of fish production targets (dates, numbers, and states). Fish environmental criteria are specified to define the environment that is to be maintained by fish culture systems. Management strategies are specified to define the fish culture procedures to be used. Alternative fish performance models are selected based on preferences and available parameters.

- 2) Production trajectory. The feasibility of production trajectory objectives are assessed and fish production schedules are generated. For broodfish and eggs, development trajectories are a simply function of accumulated photoperiod and temperature units. For fish growout using supplemental or complete prepared feeds, iterative simulations are normally required to determine the fish feeding schedules that achieve target growth rates. This is accomplished using the fish growth index (FGI) approach described earlier. If prepared feeds are not used, fish growth rates are based solely on NFP regimes and are not directly controllable
- 3) Production scale. The feasibility of production scale objectives are assessed by combining production trajectories and fish numbers:
 - a) Fish number schedules are based on initial numbers and estimated survival.
 - b) Fish biomass schedules are based on fish number and weight schedules.
 - c) Usage schedules for fish rearing units are based on biomass schedules (kg), desired biomass density levels (kg/m^3), and the resulting rearing volume requirements (m^3).
 - d) Water flow rate schedules for fish rearing units are based on desired water exchange rates (no./day) or biomass loading rates ($\text{kg fish/m}^3/\text{day}$).
 - e) Feed application schedules for fish rearing units (kg feed/RU/day) are based on fish feeding rate (% bw/day) and biomass schedules.
- 4) Biomass support. Mass balance analyses are applied to fish rearing units to better quantify peak and mean biomass support requirements for diurnal and seasonal periods. This includes operational requirements of influent and effluent water systems and treatment processes performed within fish rearing units (e.g. aeration).
 - a) Determine compound-food metabolic ratios based on food quality and feeding rate.
 - b) Combine fish biomass density (kg/m^3) with metabolite/fecal production rates ($\text{g compound/kg fish/day}$) to get mass sources and sinks due to fish processes ($\text{g compound/m}^3/\text{day}$). Include additional, significant, mass transfer processes of the fish rearing unit, including influent and effluent water flow rates and passive and managed, physical, chemical, and biological processes. Heat transfer between fish rearing units and their environment may also be an important consideration, especially for static ponds and lower water exchange rates, where temperatures may significantly diverge from influent temperatures.

- c) If the fish culture system is pre-defined, regarding rearing unit water flowrates, influent water quality, and in-pond treatment processes, then estimate fish impacts on water quality and determine if water quality criteria are maintained. If the fish culture system is to be designed, then determine required water flowrates, influent water quality, and/or in-pond water treatment processes required to maintain water quality criteria.
- d) Assess management risk by determining the elapsed time between system failure and fish death or high stress, due to deterioration in water quality to fish tolerance extremes. System failure includes loss of power or critical components (e.g. water pumps and aerators) and is simulated by terminating all water flow and treatment processes of the fish rearing unit.

8. AquaFarm Testing, Calibration, and Validation

Accomplishments regarding the testing, calibration, and validation of AquaFarm are presented in this chapter. These exercises are defined according to their normal usage in modeling work (Cuenco, 1989), with an end objective of determining the degree of confidence that can be placed on simulation results.

Testing (includes debugging) consisted of verifying that AquaFarm performed according to its intended functionality. Because the following procedures must conform to their given specifications, direct testing was sufficient to validate: (1) data input and output, management, and display tasks, (2) integration procedures for differential equations and simulation processing, (3) simulation of facility management, (4) simulation of actively managed, energy and mass transfer processes, and (5) achievement of correct results for all calculations. Testing was facilitated by the ability to isolate individual unit processes and groups of processes, as directed through the interface of AquaFarm. Overall, testing showed that the functionality of AquaFarm was sufficiently developed, as it was found that full ranges of reasonable results could be achieved for a variety of system types, solely by the adjustment of input parameters and variables within reasonable ranges.

Calibration consisted of determining standard values for model parameters (equation coefficients and exponents). Since the unit-process models used in AquaFarm were largely developed from the aquaculture literature and are mechanistic in nature, direct use or derivation of parameter values from the literature was utilized to a large degree and additional calibration was not attempted for most parameters. Many of these parameter values were provided in the tables accompanying Chapters 4 through 7. Together with the additional calibration exercises described below, the total set of parameter values so derived represents the standard (default) parameter set of AquaFarm. Parameter values that are not essentially known as fixed constants can be accessed and modified through the interface of AquaFarm.

The primary objective of this chapter concerns validation exercises that were used to evaluate simulation results. In addition, some preliminary sensitivity analyses and additional calibration exercises were accomplished in a few areas. First, individual unit processes were considered, paralleling their delineation in Chapters 4 through 7. Second, system-level perspectives were considered, using representative examples of aquaculture systems. Relative to the analytical capacity of AquaFarm, these validation exercises were necessarily limited in scope and resolution. It was assumed that the major burden of validation could be placed on the supporting literature. The

quantity and quality of empirical data that would be required for a comprehensive, statistically based validation of AquaFarm is considerable and beyond the scope of this dissertation.

8.1 Aquatic chemistry

8.1.1 Physical properties

Physical properties of water were verified by direct comparison of calculated values to reported values over full ranges of temperature (0 - 40 °C) and salinity (0 - 40 ppt). Simplified methods for water density, specific heat capacity, and vapor pressure were validated in Chapter 4. Since these property methods are used intensively over the course of a simulation, in order to minimize calculation intensity, simplified methods are the default methods used by AquaFarm.

8.1.2 Dissolved gases

Equilibria concentrations of dissolved gases were verified by direct comparison of calculated values to reported values over full ranges of temperature (0 - 40 °C), salinity (0 - 40 ppt), altitude, barometric pressure, water depth, and hydrostatic pressure. The simpler (shorter) literature methods for dissolved gases were found to be adequate within a context of aquaculture modeling. Simplified and rigorous methods were essentially equivalent or agreed within a few percent, the latter case found for dissolved carbon dioxide and nitrogen. Dissolved nitrogen is not normally important unless gas super saturation exists.

8.1.3 Acid-base chemistry

Derived methods for calculating equilibrium constants (pK) values were found to largely agree with literature methods but did not provide a reduction in calculation intensity. Thus, derived methods for pK values are used only when literature methods are not available. Literature methods for calculating pK values were verified by comparison of results to reported pK values.

The internal consistency of Alkalinity Model 1 (AM1) was verified by successful completion of interrelated computations, where successively different variables were made independent for the same, given acid-base system and uniform results were achieved. External validation was accomplished by (1) successful completion of example problems given in aquatic chemistry texts

and (2) construction of pC-pH (Figure 8.1) and Deffeye's diagrams (Figure 8.2) for a variety of acid-base systems (Snoeyink and Jenkins, 1980; Stumm and Morgan, 1981). The latter included water equilibrated with a carbon dioxide gas phase and/or a calcium carbonate solid phase. To achieve exact agreement with example problems given in aquatic chemistry texts, it was sometimes necessary to use pK values as given in the example problems rather than calculated pK values based on the methods here. Some variability exists in the literature for reported pK values at various temperatures and salinities. Based on the successful verification of AM1, it is assumed that AM1 can be used to accurately represent acid-base systems and therefore to evaluate Alkalinity Models 2 and 3 (AM2 and AM3). As described in Chapter 4, AM2 and AM3 are simplified models used to reduce calculation intensity.

The internal consistency of pH and alkalinity adjustments using AM1 was confirmed by (1) determining quantities of a given compound required to achieve an adjusted pH or alkalinity level and (2) independently adding this compound quantity to the original water to confirm that the specified pH or alkalinity level was achieved. External validation was accomplished by successful completion of example problems (Snoeyink and Jenkins, 1980; Stumm and Morgan, 1981).

The appropriate use of AM2 and AM3 depends on water quality conditions and the relative contributions of alkalinity compounds. AM1, AM2, and AM3 were compared by comparing their ability to generate data points for the construction of Deffeye's diagrams (Snoeyink and Jenkins, 1980). Using this approach, pH isopleths are plotted and compared as a function of $^{\text{mol}}\text{CO}$ and ALK_t (Figure 8.2). The impact of alkalinity components in addition to water and carbonates can be visualized and quantified through the vertical displacement of pH isopleths in the diagram. To compare AM1 and AM2, Figures 8.2A and 8.2B represent relatively nutrient-rich freshwater and seawater conditions, respectively. It is seen that use of AM2 can result in significant errors, especially at low carbonate and alkalinity concentrations in conjunction with pH levels above 8, and more so in seawater than in freshwater. Comparing AM2 and AM3 (Figures 8.2C and 8.2D), the impact of the simplification of AM3 may be considered negligible for the pH range 5-10 in freshwater and 5-9 in seawater. These results indicate that if AM2 can be used, then AM3 can be used.

Procedures required to determine if AM2 can be used are calculation intensive. If these procedures are repeated at every simulation step, then the purpose of using simplified models to reduce calculation intensity is defeated. However, different types of aquaculture systems can be characterized by typical water quality regimes, and tests used to select an alkalinity model can be

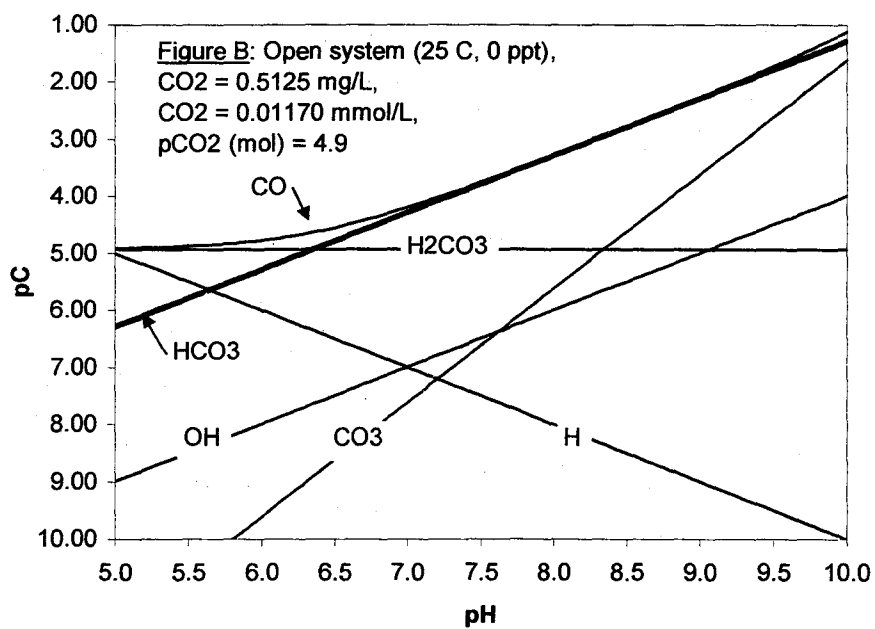
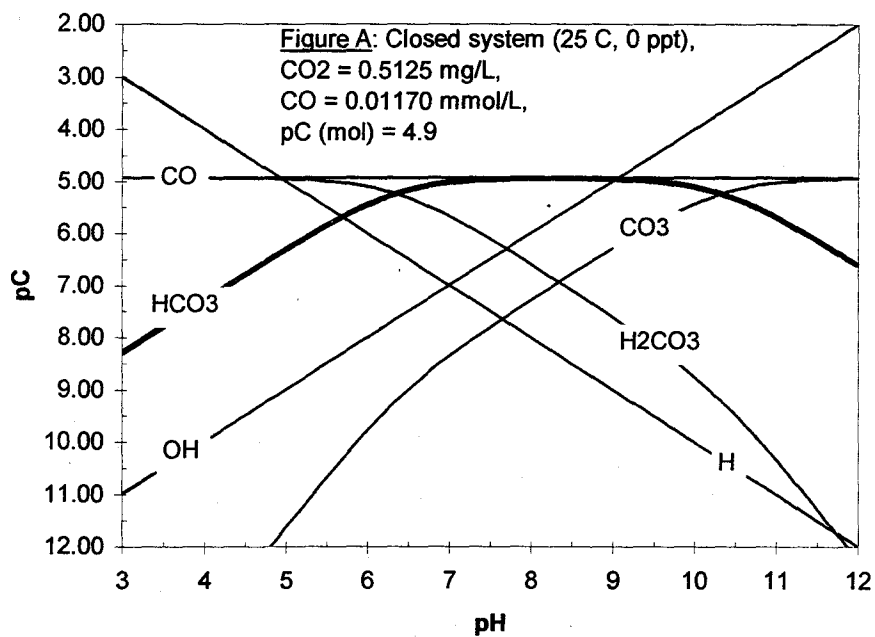


Figure 8.1. pC-pH diagrams for carbonates (25 °C, 0.0 ppt salinity) for (A) a closed system and (B) water in equilibrium with atmospheric carbon dioxide

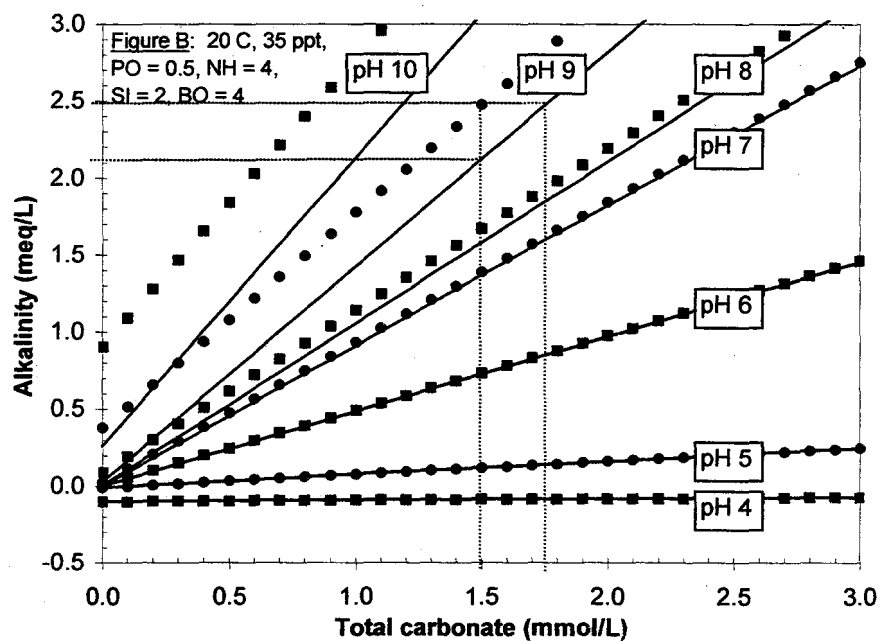
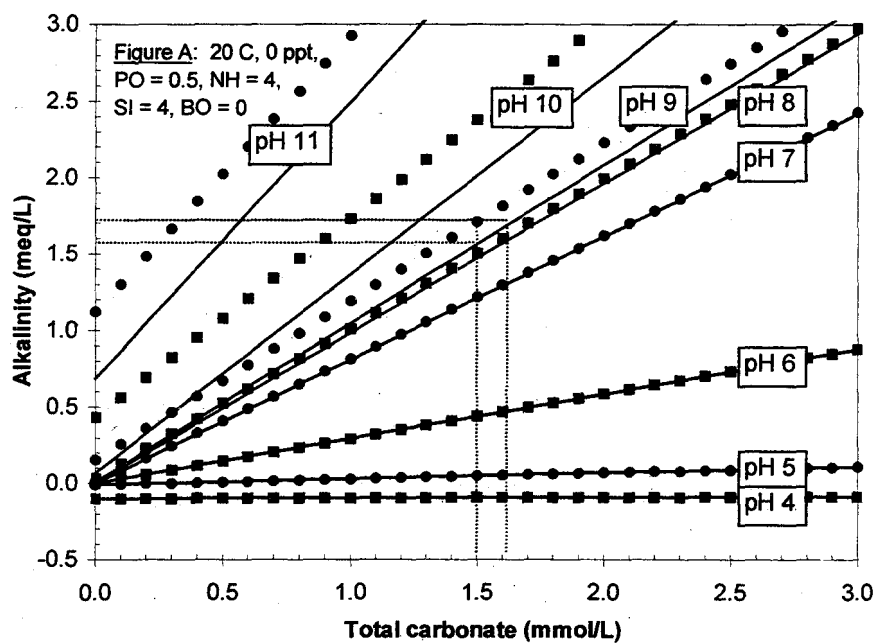


Figure 8.2. Deffeye's diagrams showing pH isopleths as a function of $^{\text{mol}}\text{CO}$ and ALK_t : (A) nutrient-rich fresh water and (B) nutrient-rich seawater, for which points were generated by Alkalinity Model 1 and lines were generated by Alkalinity Model 2

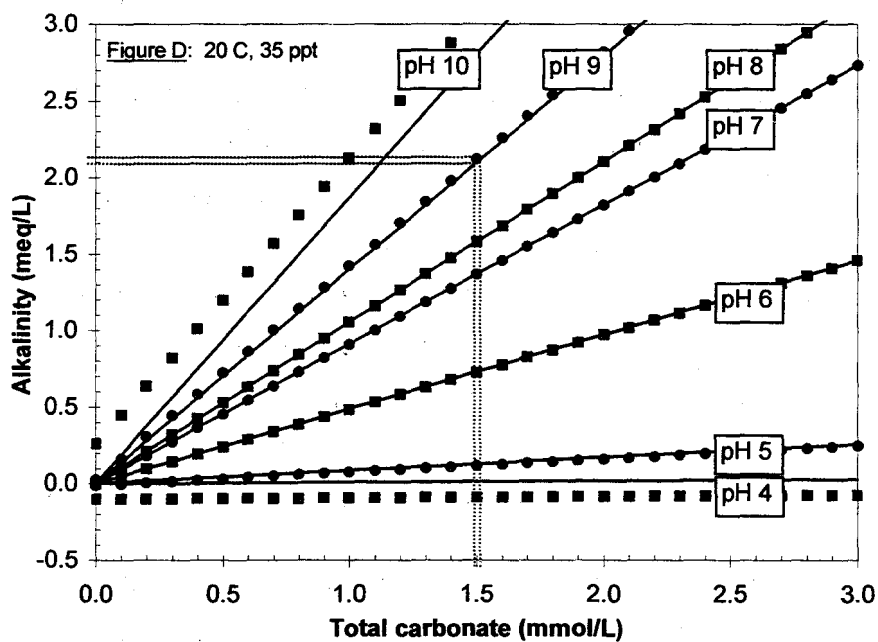
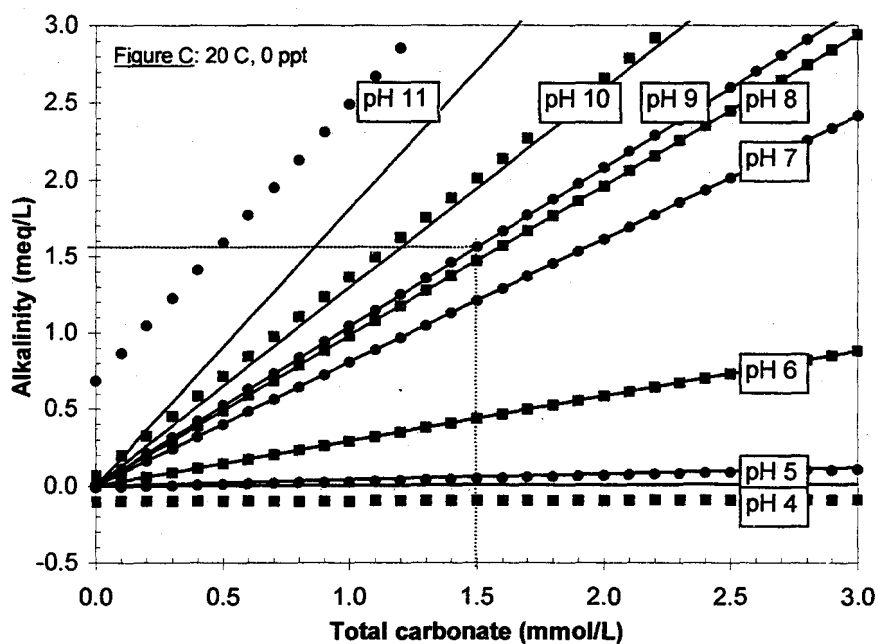


Figure 8.2 (continued). Deffeye's diagrams showing pH isopleths as a function of $^{\text{mol}}\text{CO}$ and ALK_t : (C) carbonates in fresh water and (D) carbonates in seawater, for which points were generated by Alkalinity Model 2 and lines were generated by Alkalinity Model 3

performed once, prior to a simulation. For flow-through facilities using surface waters (e.g. salmon hatcheries), ALK_{ncw} compounds (non-carbonate, non-water alkalinity; meq/L) are generally low in concentration (possible exception are silicates), carbon dioxide levels are somewhat super-saturated (due to fish respiration), and pH levels rarely exceed 8.2. For recirculating facilities, highly super saturated carbonate levels generally exist due to carbon dioxide accumulation, and pH levels are often depressed due to nitrification and carbon dioxide accumulation and rarely exceed 8.5. Thus, for flow-through and recirculating facilities, AM2 or AM3 can normally be used. For solar algae ponds, however, carbon dioxide levels may be under saturated on a diurnal basis, pH levels elevated, and ALK_{ncw} compounds at relatively high concentrations. Thus, AM1 should be used. For all types of systems, AM2 or AM3 may be used in the coarser, initial stages of a design project and AM1 for more refined, final stages.

8.2 Aquacultural engineering

8.2.1 Facility climate

Use of climate data files (historical) and controlled climates were validated by confirming that given climate data were correctly applied to simulations. Calculated times of sunrise, sunset, and daylength were equivalent to reported values for full ranges of dates and latitudes (Kreider and Kreith, 1981). For generated climates, calculated solar radiation values were comparable to reported values for full ranges of dates, latitudes, and altitudes (Kreider and Kreith, 1981) when sufficiently accurate cloud cover values were used. Solar radiation for clear skies showed good predictability. However, as illustrated in Figure 8.3, solar radiation declines from 100.0 to 35.0 percent of a given clear sky value, as cloud cover fraction is increased from 0.0 to 1.0. Therefore, accurate estimation of annual cloud cover regimes is required to accurately estimate solar radiation (Figure 8.4).

The method used to calculate diurnal solar radiation regimes with reduced calculation intensity (Monteith, 1973; Chapter 5) is illustrated in Figure 8.5 (simplified method). It was found that the use of adjusted times for sunrise and sunset was required to best represent diurnal radiation profiles (improved simplified method). These required adjustments and additional calculations detracted from the simplification intent, and therefore this method was dropped from consideration.

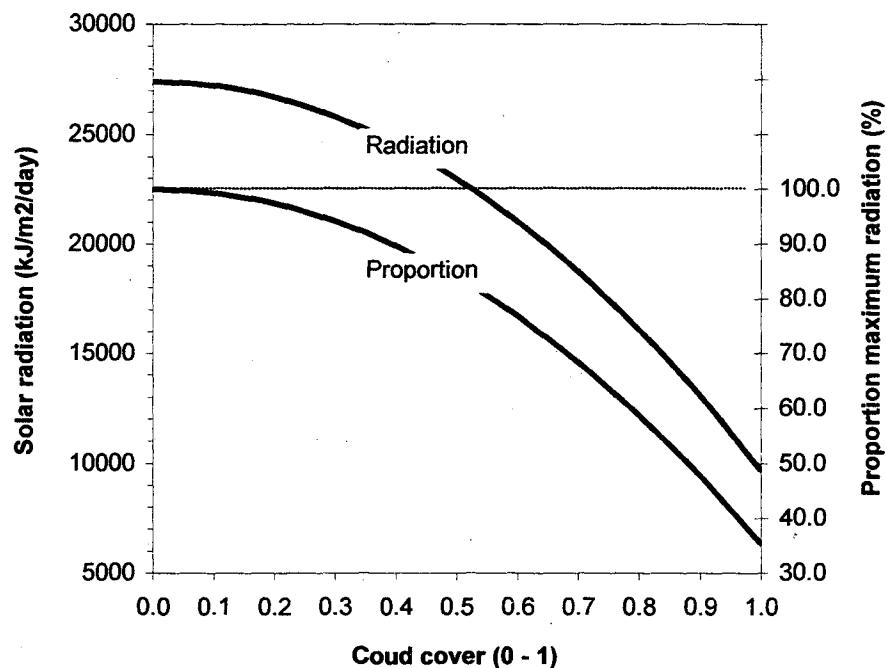


Figure 8.3. Simulated response of solar radiation to cloud cover fraction, using an example clear-sky solar radiation value of 27500 kJ/m²/day

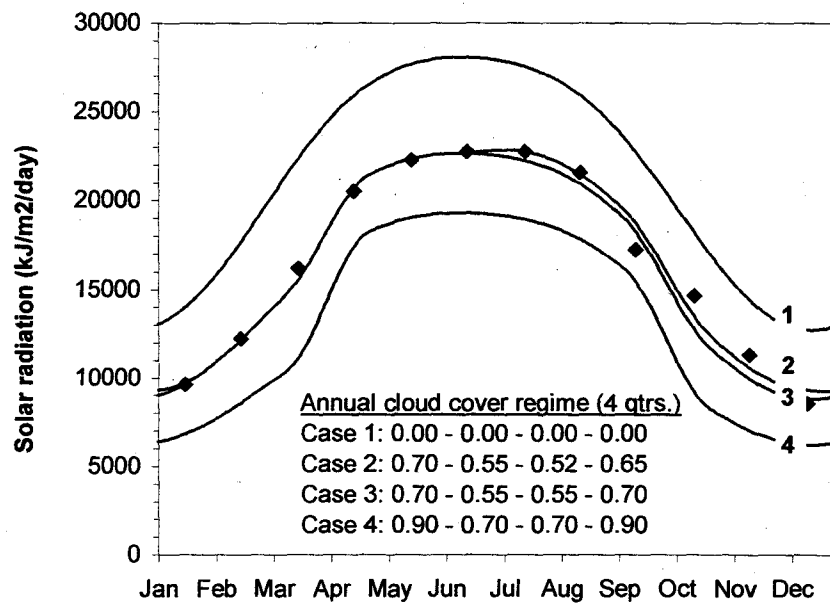


Figure 8.4. Simulated (lines) and reported (points) annual solar radiation regimes, using four different cloud cover regimes (application conditions: Table 8.1, catfish pond)

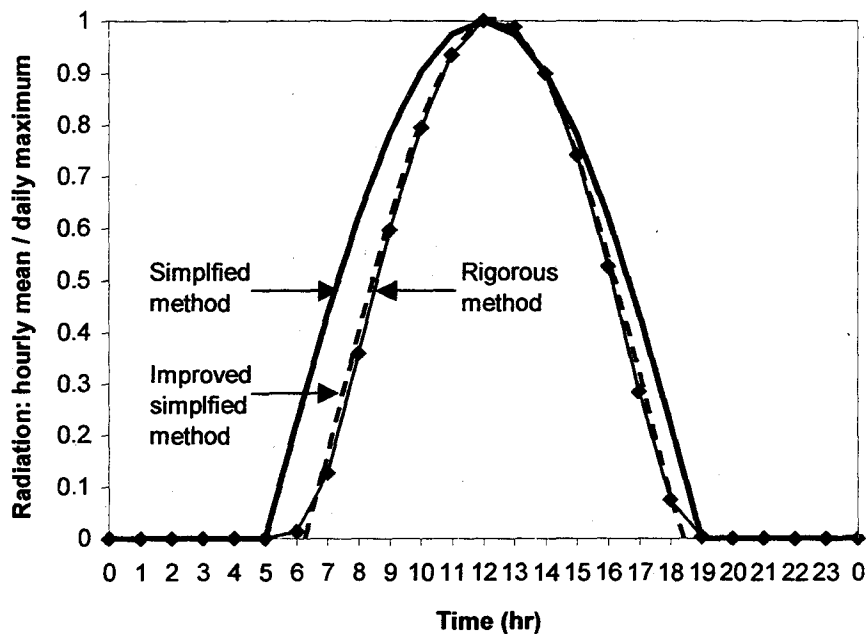


Figure 8.5. Comparison of rigorous, simplified, and improved simplified methods for calculating diurnal solar radiation regimes

The method used to approximate annual, minimum and maximum, daily mean air temperatures as a function of latitude and altitude (Chapter 5) was found to provide variable accuracy, mainly regarding poor results for annual minimum temperatures for latitudes between about 20 and 40° (both hemispheres). Given that this method is intended for rough approximations at best, AquaFarm users would be better served by the use of regionally based lookup tables or links to such data on the Internet. Once minimum and maximum annual temperatures have been established, however, the sinusoid function used to interpolate daily mean temperatures appears to be adequate (Figure 8.6). For diurnal air temperature profiles, Figure 8.7 illustrates the use of various offset times between the time of the daily maximum temperature and sunset (see diurnal sinusoid function; Chapter 5). Additional climate variables are defined by annual regimes of seasonal mean values, as illustrated in Figure 8.8.

The importance of climate variables regards their role in passive heat and gas transfer, water stratification, water mass balances (water budgets), primary productivity, and fish culture daylength (photoperiod). Therefore, the importance of accurate weather prediction depends on the type of facility and analysis resolution level of a design project. For rigorous design work, the use of historical climate data to predict future mean conditions is likely preferred. However, it is apparent that generated climates can provide adequate accuracy, while reducing user responsibilities.

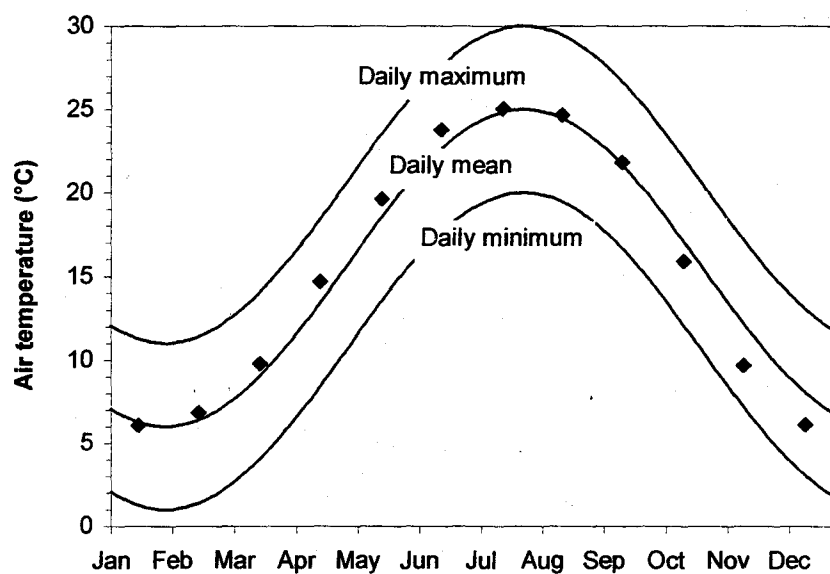


Figure 8.6. Simulated (lines) and reported (points) annual air temperature regimes (application conditions: Table 8.1, catfish pond)

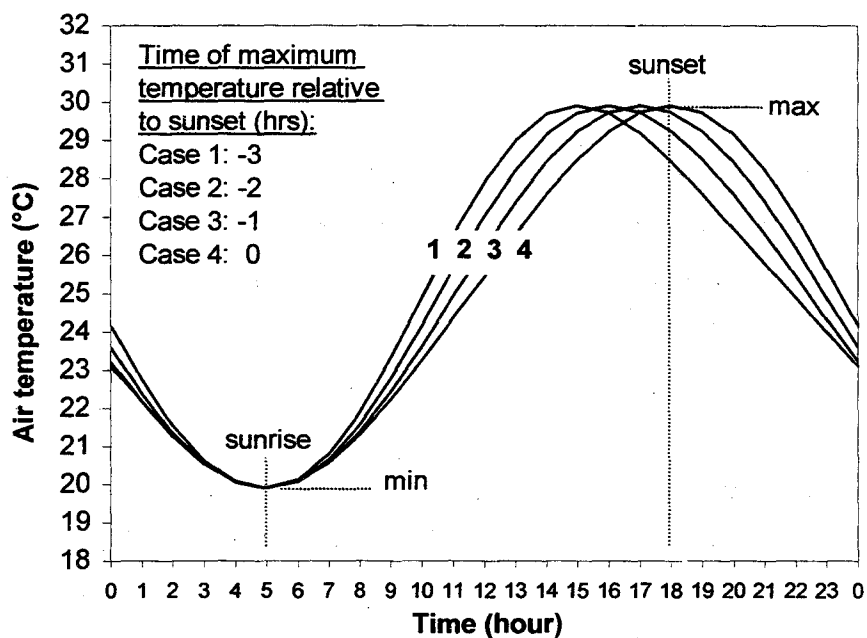


Figure 8.7. Simulated diurnal regimes for air temperature, demonstrating the ability to consider various times for the daily maximum temperature (time of daily minimum temperature may also be varied)

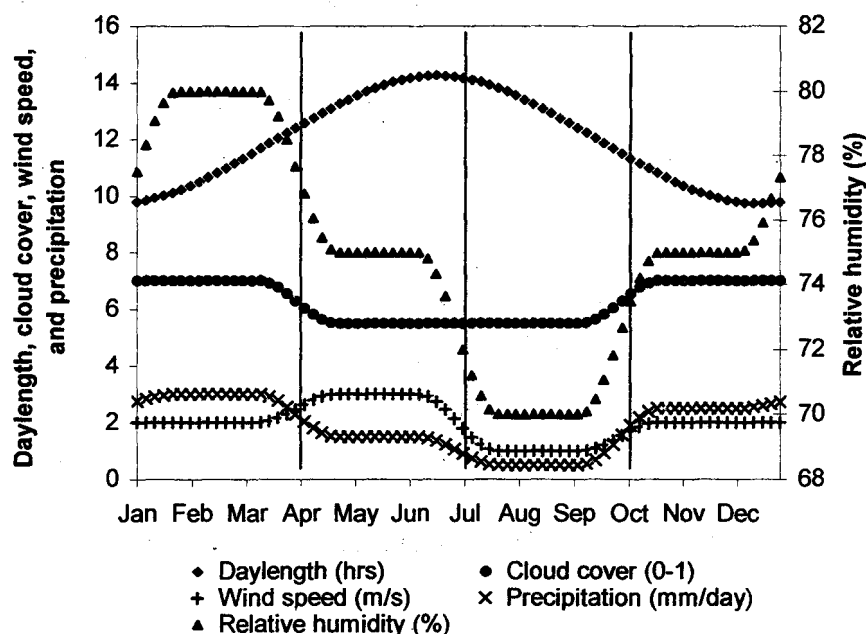


Figure 8.8. Simulated annual regimes for daylength, cloud cover, wind speed, precipitation, and relative humidity, for which regimes (other than daylength) correspond to given seasonal values

8.2.2 Heat transfer

Water temperature is a fundamental driving and limiting variable of aquaculture systems, and accurate prediction of passive heat transfer (PHT) and associated temperatures is of primary importance. Example applications of PHT for exposed and housed systems are provided below.

8.2.2.1 Exposed ponds

For applications to outdoor ponds, methods used to model PHT are similar to those described by Nath (1996). For outdoor ponds in tropical regions, Nath et al. (1994) and Nath (1996) showed that predicted water temperatures were comparable to empirical values, typically within 1.0 °C and with poorest fits within about 2.0 °C. As expected, these studies found that the use of historical weather datasets yielded the best match between predicted temperatures and the observed water temperatures concurrent with these weather datasets.

Application of the PHT model to commercial catfish ponds in northwest Mississippi, using generated weather variables, showed good agreement with reported, annual temperature regimes (Figure 8.9, A-D; application conditions: Table 8.1, catfish pond). To determine the impact of individual climate variables on PHT, climate variables were varied over their reasonable ranges, such that the given base scenario was bracketed by the values used. Results of this exercise showed (1) the greatest impact by relative humidity (e.g., 6.5 °C per 30% change in RH), (2) moderate impact by wind speed (e.g., 4.8 °C per 3.0 m/s change in WS) and air temperature (e.g., 4.6 °C per 6.0 °C change in air temperature), and (3) the lowest impact by cloud cover (2.4 °C per 0.4 change in cloud cover). These results demonstrated that all climate variables had a significant impact on PHT, and that accurate estimation of relative humidity was especially critical.

In Figures 8.10 and 8.11 (application conditions: Table 8.1, catfish pond), the same conditions used for Figure 8.9 were applied to a diurnal simulation with annually and diurnally varying water stratification. Since temperatures are oscillating diurnally, temperature regimes are represented by bands rather than lines at the resolution of Figure 8.10. Increasing this resolution, Figure 8.11 illustrates a few days of this temperature regime. These results demonstrate the compatibility of daily and diurnal simulations, for which the water temperature profile generated by a daily simulation lies along the center of the temperature band generated by a diurnal simulation for the same conditions. In Figure 8.12, a predicted heat budget for this example shows the dominance of PHT by radiation and evaporation. In summary, this exercise illustrates the simulation-generated data (as graphs and tables) that are available to AquaFarm users and demonstrates that sufficient estimation of annual water temperature regimes is possible using generated climate variables.

Table 8.1. Application conditions for example simulations of heat transfer

Mississippi catfish pond (base scenario)
<ul style="list-style-type: none"> • Location: NW Mississippi, latitude = 34° N, and altitude = 300 m • System: earthen catfish pond with 1.0-m water depth • Climate: relative humidity = 75%, annual cloud cover regime (4 quarters) = 0.70, 0.55, 0.55, and 0.70, wind speed = 2.0 m/s, annual min-max air temperature = 6 – 25 °C, and diurnal temperature amplitude = 10 °C • Annual water mixing index regime (12 months, Jan. to Dec.): 24, 24, 12, 6, 4, 2, 2, 4, 6, 12, 24, and 24 per day • Reported data: Solar data are from Kreider and Kreith (1981) for Atlanta, GA (latitude 34° N; elevation 300 m). Air temperature data are from Kreider and Kreith (1981) for Atlanta, GA, minus 1.0 °C for correction to application location. Water temperature data are from Tucker and van der Plough (1993), for surface water temperatures for commercial catfish ponds with on-demand aeration. • Simulation: PHT was simulated, ignoring the impact of evaporation on water mass balances and requirements for makeup water. Figure 8.9: 1-day time-step, water stratification is ignored. Figures 8.10 and 8.11: 1-hr time-step, water stratification is considered.
Honduras tilapia pond
<ul style="list-style-type: none"> • Location: El Carao, Honduras; latitude = 14°26' N; altitude = 583 m • System: earthen tilapia pond with 0.9-m water depth • Climate conditions on August 15: relative humidity = 75%, cloud cover = 0.50, wind speed = 3.0 m/s, and daily minimum and maximum air temperature = 20 – 35 °C (diurnal temperature amplitude = 15 °C) • Water mixing index: 2.0/day
Intensive system
<ul style="list-style-type: none"> • Location: latitude = 45° N, altitude = 300 m, and system housed in a passive greenhouse • System: volume = 1000 m³, ratio of air-wall-water to air-water surface area = 3.0, mean wall material is equivalent to 0.5-cm thick PVC, water exchange rate = 5%/ week, and influent water temperature = 10 °C • Controlled climate: wind speed = 0.1 m/s, relative humidity = 90%, cloud cover = 0.80 (includes housing), annual min-max air temperature = 10 – 30 °C, and day of annual maximum air temperature = Julian day 210 • Water heating: applied to maintain minimum temperature of 20 °C and control of water temperatures is not possible when temperatures exceed 20 °C

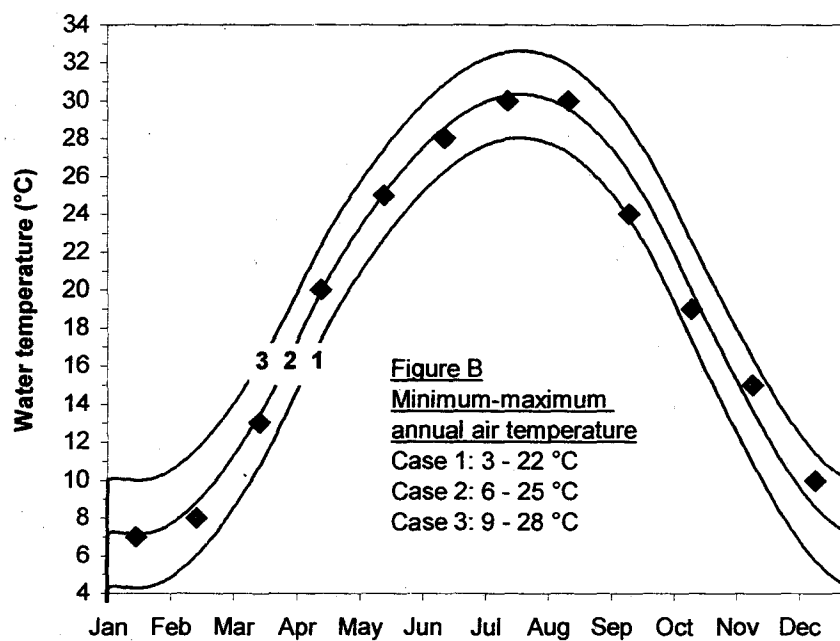
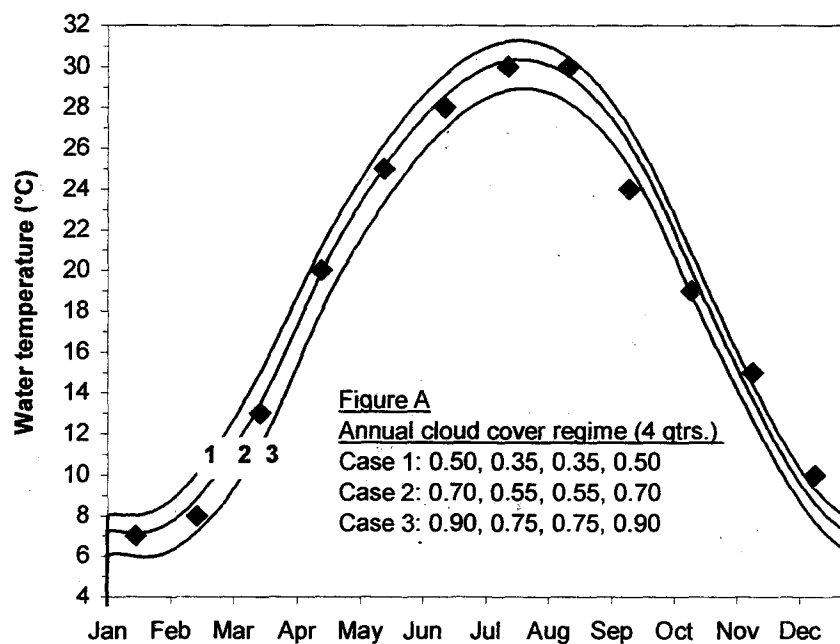


Figure 8.9. Simulated (lines) and reported (points) annual water temperature regimes for an exposed pond, using various cases for (A) cloud cover and (B) minimum-maximum annual air temperature (application conditions: Table 8.1, catfish pond; Case 2 is base scenario)

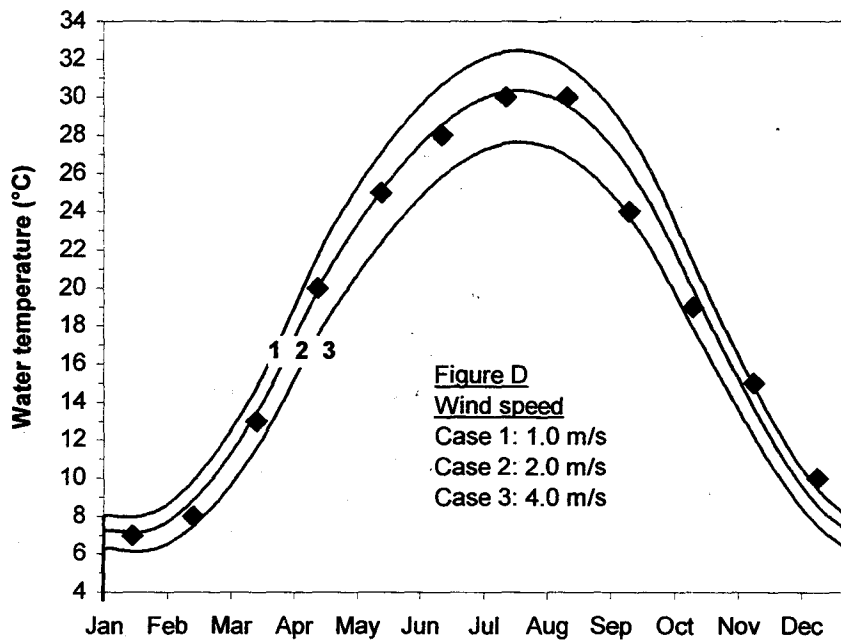
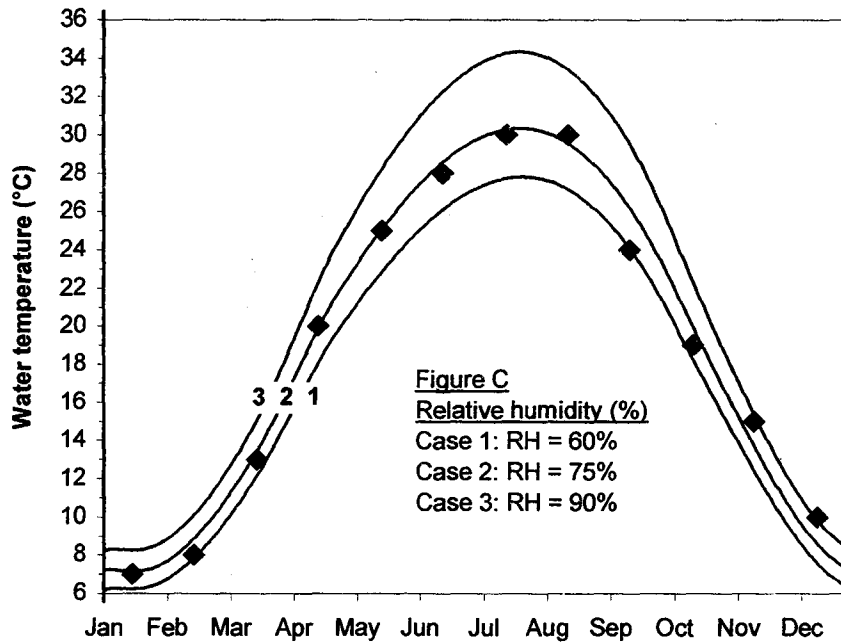


Figure 8.9 (continued). Simulated (lines) and reported (points) annual water temperature regimes for an exposed pond, using various cases for (C) relative humidity and (D) wind speed (application conditions: Table 8.1, catfish pond; Case 2 is base scenario)

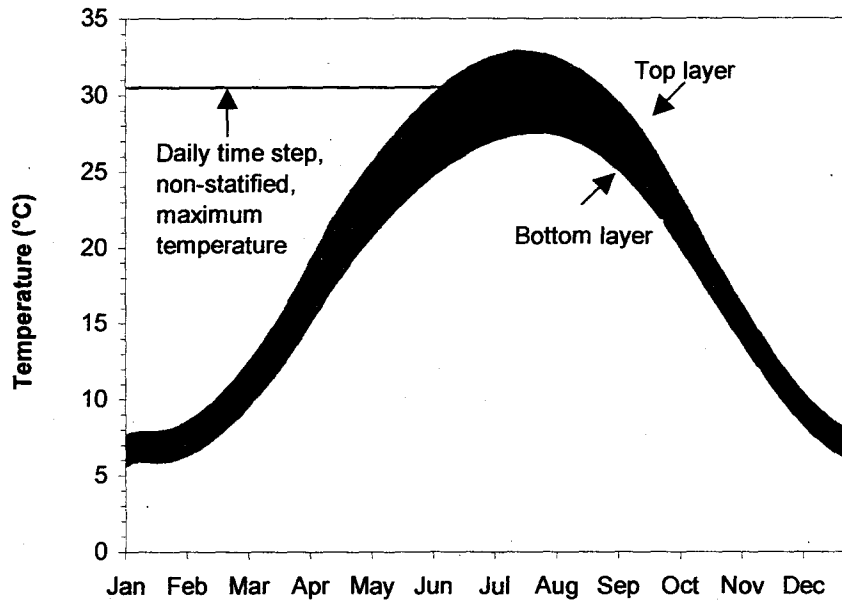


Figure 8.10. Simulated annual water temperature regime for an exposed pond, including water stratification and diurnal simulation (1-hr time step; application conditions: Table 8.1, catfish pond)

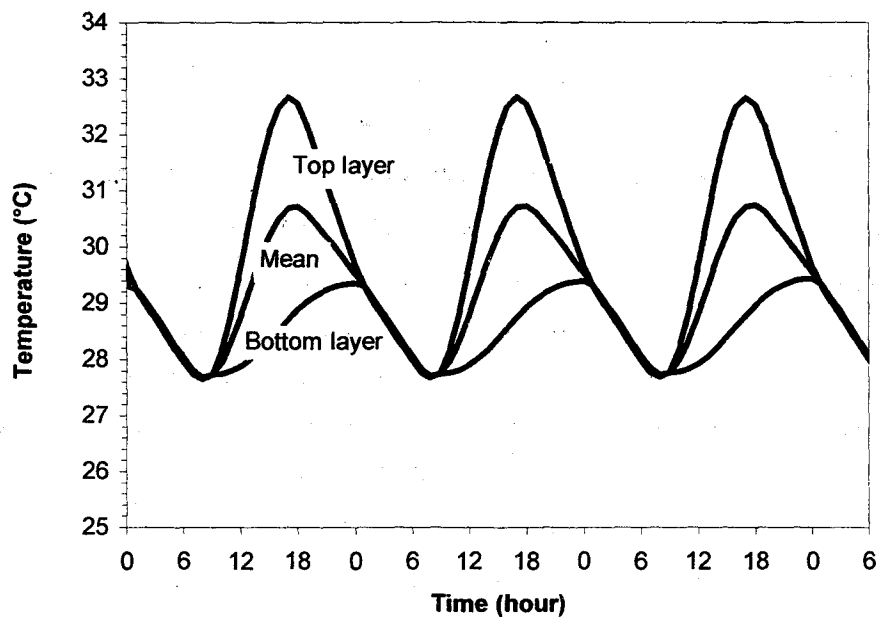


Figure 8.11. Simulated water temperatures for an exposed pond with a diurnally stratified water column, showing the water column top, bottom, and mean temperatures (1-hr time step; data represent July 19-21 from Figure 8.10)

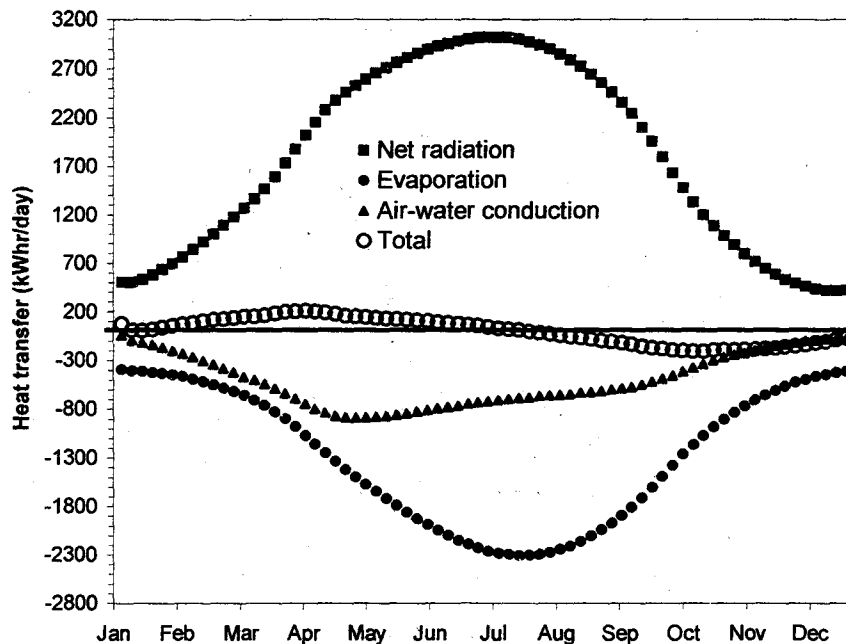


Figure 8.12. Simulated annual heat budget for an exposed pond (application conditions: Table 8.1, catfish pond)

8.2.2.2 Water thermal stratification

The thermal stratification model developed for AquaFarm uses a given annual regime for the daily “water mixing index” of the water column (WMI, 1/day; see Chapter 3). Application of the stratified-PHT model to tilapia ponds in Honduras, using generated weather variables, showed that WMI values could be calibrated to yield predicted temperatures that were comparable to observed depth-time profiles (Figure 8.13; see Table 8.1 for application conditions). Simulation results were particularly good with respect to (1) the timing of stratification initiation, (2) the timing and period of water column turnover, and (3) the maximum daily difference between the top and bottom layers. In some application trials, two areas of apparent error in predicted temperatures were (1) delayed timing of the daily temperature peak and (2) over estimation of the temperature amplitude of the bottom layer. This lack of correspondence with observed values was apparently due to an insufficient proportion of PHT by solar radiation relative to total PHT. As the relative proportion of PHT by solar radiation is increased, the timing of the peak daily temperature converges to the time of maximum solar radiation (solar noon).

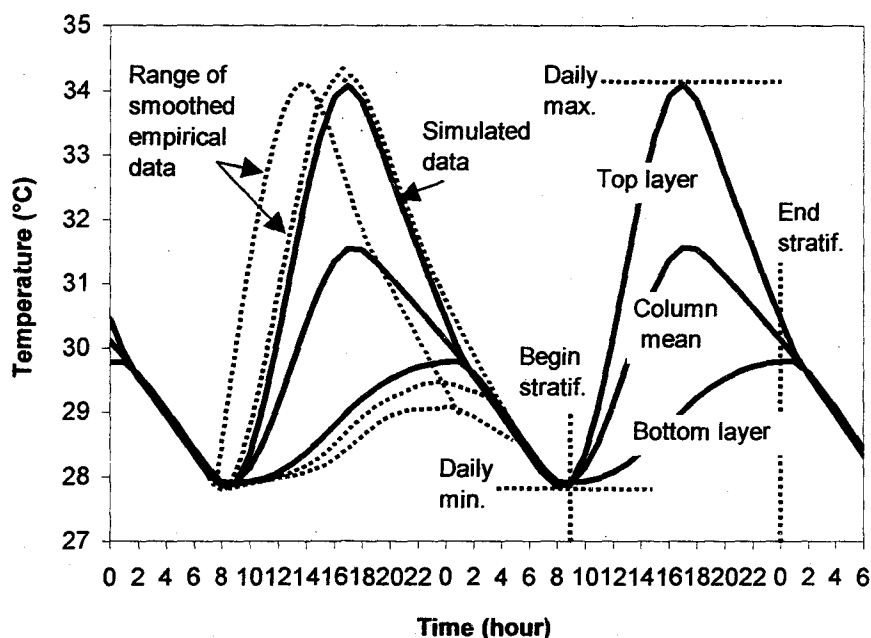


Figure 8.13. Simulated and reported water temperatures for an exposed pond with a diurnally stratified water column, showing the water column top, bottom, and mean temperatures (1-hr time step simulation; application conditions: Table 8.1, Honduras, Aug 15)

Validation of the stratified-PHT model remains to be completed, and a generally applicable method to generate WMI regimes from climate variables has not been developed. On a site-specific basis, WMI regimes can be developed from knowledge of typical, monthly temperature differences between the top and bottom layers of the water column. To demonstrate this task, WMI was varied across its full range (1.0 to 48.0) for the same pond and climate conditions used in Figure 8.13. Figure 8.14 shows the six simulations used for this exercise. Figure 8.15 provides a summary of the derived relationship between top-bottom temperature differences and WMI values. This summary figure can be used to establish monthly WMI values given an expected monthly mean temperature differential, at least for the site for which the figure was developed. For example, a typical annual WMI regime for a semi-tropical pond in the northern hemisphere is (12 months, Jan. to Dec.): 48, 36, 24, 12, 8, 4, 2, 2, 8, 16, 32, and 48 per day. Results of this exercise demonstrated the ability of the stratified-PHT model to account for a full range of stratification conditions, from completely mixed to highly stratified. As WMI was decreased from high to low values (i.e., stratification increased), the mean and bottom pond temperatures declined by about 1.5 and 4.0 °C, respectively. This was an expected impact of the insulating effect of thermal stratification.

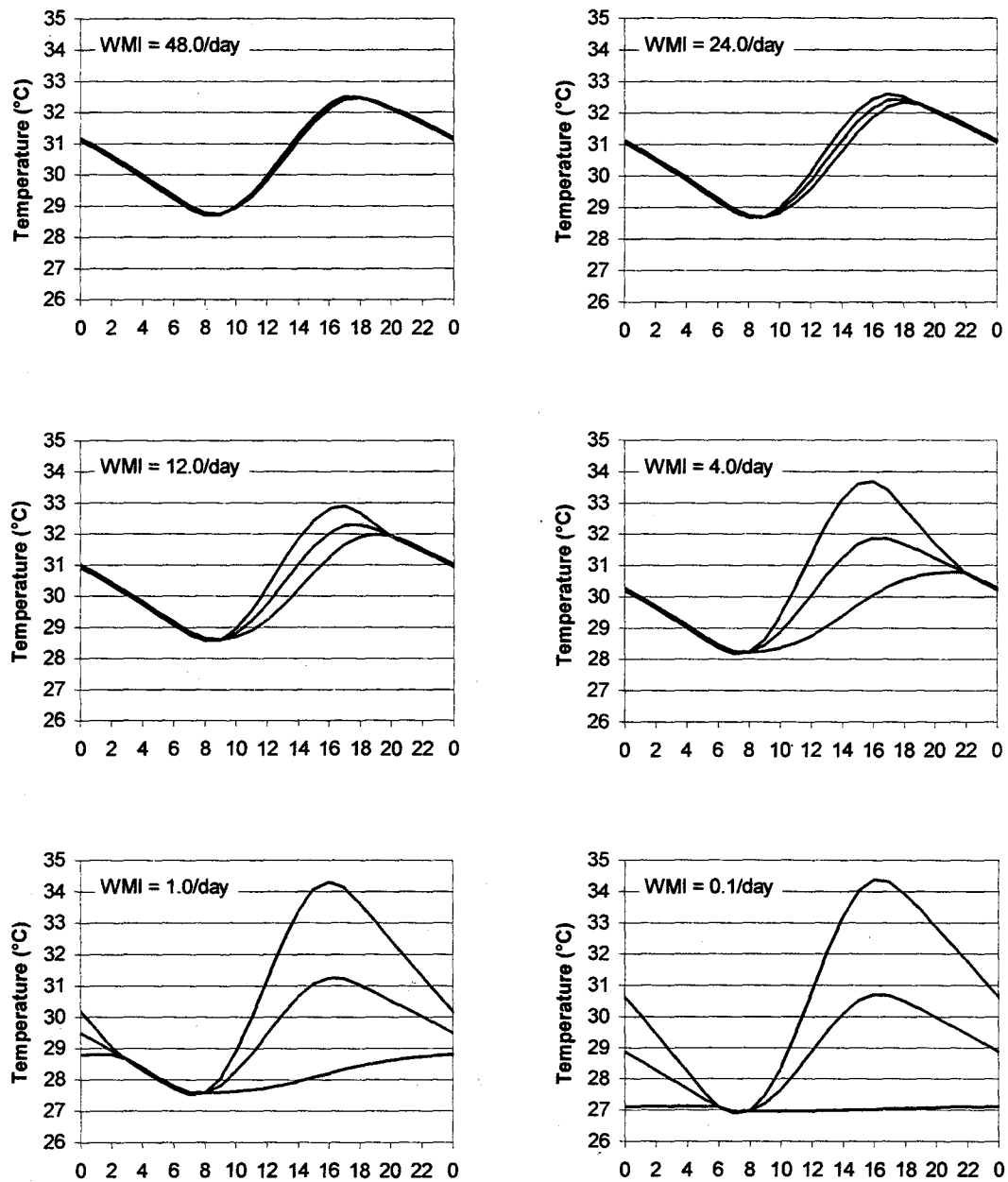


Figure 8.14. Simulated water temperatures for an exposed pond with a diurnally stratified water column and WMI values ranging from 0.1 to 48.0/day, showing the water column top, bottom, and mean temperatures (1-hr time step; application conditions: Table 8.1, Honduras, Aug 15)

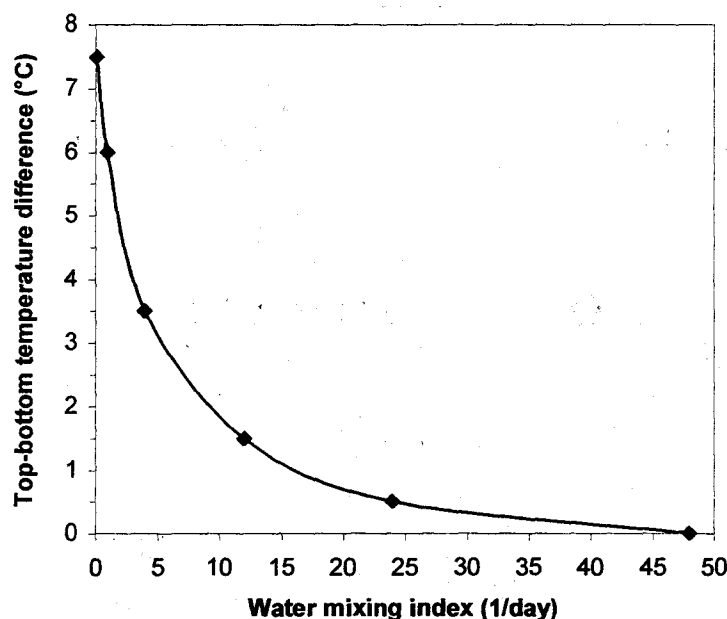


Figure 8.15. Top-bottom temperature difference as a function of water mixing index, as achieved by the series of simulations shown in Figure 8.14

8.2.2.3 Intensive aquaculture systems

The accuracy of predicted water temperatures for intensive aquaculture systems is mainly determined by the accuracy and detail of system specifications, including facility unit dimensions, construction materials, and controlled climates. Solar radiation is dropped from consideration for systems housed in buildings that block radiation, and the use of controlled climates enhances the accuracy of PHT modeling. For PHT by advection and convection-conduction, example problems for tanks and pipes provided in various texts were successfully completed (e.g. Welty et al., 1976; Henderson and Perry, 1976). Components such as in-tank aeration, gas exchangers, and trickling biofilters, as typically found in intensive systems, complicate PHT modeling. Such components greatly enhance air-water interface areas and contact (mixing) conditions. Adequate supporting studies to assess the simulation of PHT for these components were not found. An example heat budget for an intensive system, including active heat transfer (heating) to maintain a minimum temperature of 20 °C, is given in Figure 8.16 (see Table 8.1 for application conditions). This budget shows that air-water conduction, air-wall-water conduction, evaporation, solar radiation (if exposed), and long-wave radiation are all potentially significant modes of PHT. Such budgets provide useful design information that can be used to assess the utility of climate control, thermal insulation, and heat capture from effluent water.

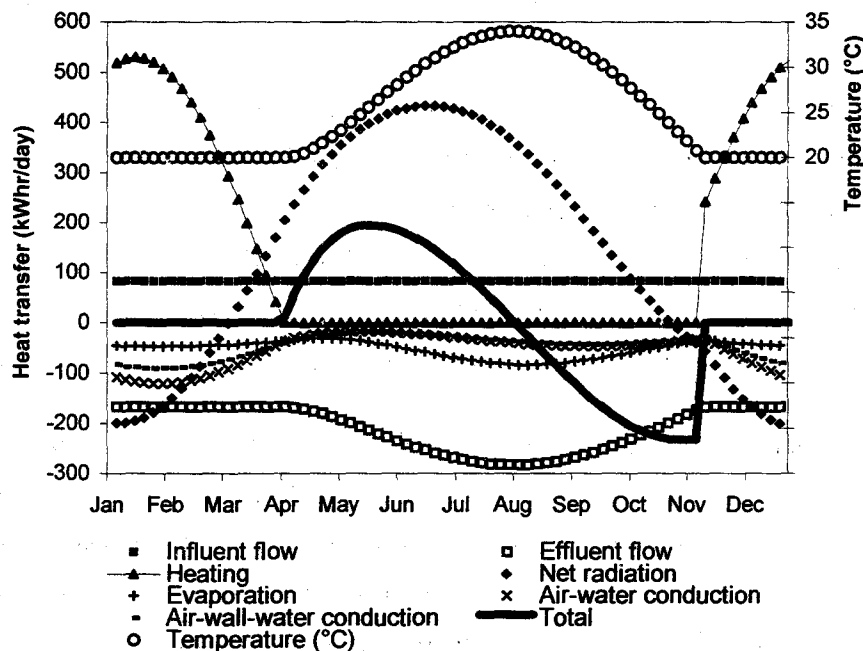


Figure 8.16. Simulated annual heat budget for an intensive, housed (passive greenhouse) system (application conditions: Table 8.1, intensive system)

8.2.3 Water flow mechanics and budgets

Simulation of gravity and pressurized water flow was validated by successful completion of example problems given in the supporting references for these methods (see Chapter 5). The scope of this validation corresponded to the stated objectives of water mechanics modeling. In general, the accuracy of simulation results is mainly dependent on the degree of detail used in specifying pumps, pipes, channels, and other facility units. When known, total dynamic head values at water pumps can be specified directly, which alleviates the need to completely specify associated water systems.

For tank-based systems, system water budgets are limited to evaporation, but this water loss can become considerable as relative humidity levels fall below 90%. Losses due to splashing and leaks are not considered. For pond-based systems, predicted water budgets for outdoor ponds in tropical regions compared well to empirical budget data given that historical weather data and sufficiently accurate seepage estimates were used (Nath and Bolte, 1998). Additional simulation trials (results not shown) demonstrated that the accuracy of predicted water budgets was directly proportional the accuracy of given water seepage rates, predicted relative humidity and evaporation, and predicted precipitation.

8.2.4 Passive and active gas transfer

Ideally, validation of passive gas transfer (PGT) would be performed in isolation, independent of other processes (e.g., oxygen diffusion without additional oxygen sources and sinks). However, such data were not found in the literature, other than those that were used to develop the methods for calculating diffusion coefficients. Therefore, PGT modeling is assessed later in this chapter, in a context of system modeling. In summary, trial applications with exposed water bodies gave results comparable to reported dissolved oxygen and carbon dioxide regimes.

The response of calculated oxygen diffusion coefficients to water velocity (Figure 8.17) and wind speed (Figure 8.18) shows that values based on wind speed will normally be used (the maximum of the two values is used; Chapter 5) except when high water velocities (e.g., fish raceways) exist in conjunction with low wind speeds. In Figure 8.18, the significant difference between the two wind speed methods is apparent. For example, at a wind speed of 4.0 m/s, the small-pond coefficient is 1.7 times the large-pond coefficient. This disparity represents a potential source of error, but its significance depends on the proportion of PGT in total gas budgets. It should also be noted that the water body area of 10-ha that serves to partition the use of the two wind speed methods is somewhat arbitrary. By either method, it is clear that diffusion coefficients are highly sensitive to wind speed. For example, values increase by a factor of 4.6 as wind speeds are increased from 1.0 to 3.0 m/s (small-pond method). Complicating this issue is that wind speeds typically vary diurnally as well as seasonally. These results indicate that daily wind speeds should be allowed to vary diurnally in AquaFarm, as done for air temperature.

For active gas transfer, by all types of water aerators, exchange columns, and cascades, the validity of gas transfer modeling is dependent on the accuracy of given physical and management specifications. The accuracy of oxygen transfer efficiencies ($\text{kg O}_2/\text{kWhr}$) is critical, since aeration is managed (i.e. energy is applied) such that given dissolved oxygen set-points are achieved, and the energy requirements so calculated are then used in resource and economic budgets.

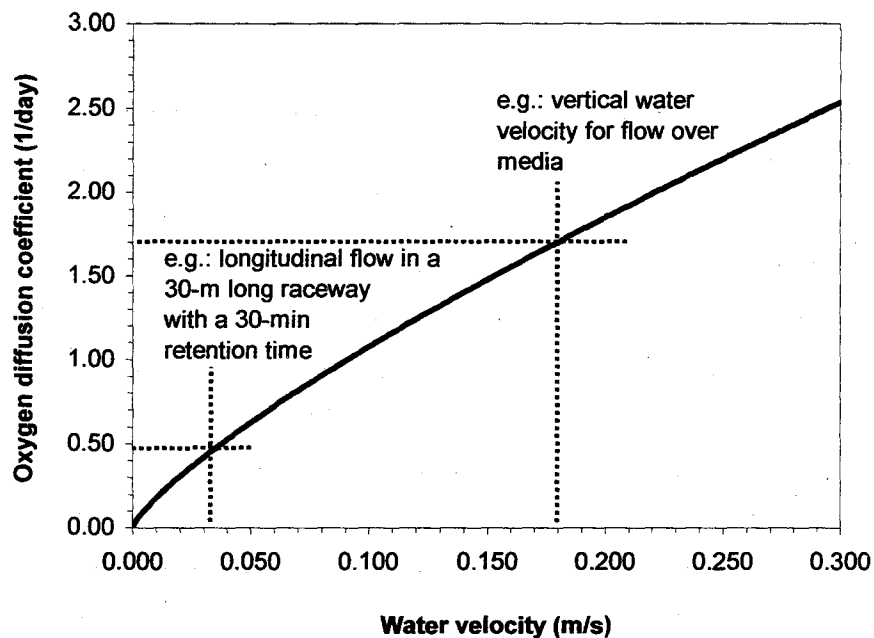


Figure 8.17. Response of the oxygen diffusion coefficient to water velocity

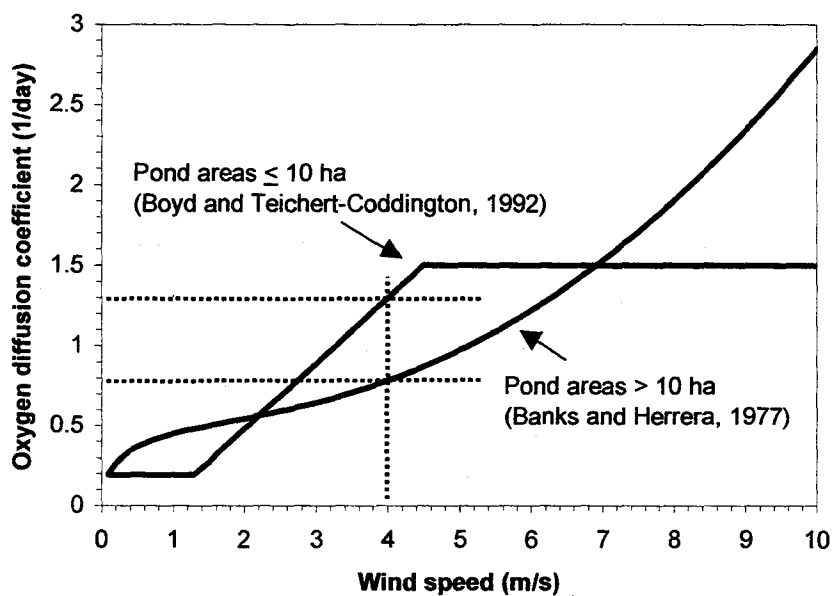


Figure 8.18. Response of the oxygen diffusion coefficient to wind speed

8.2.5 Additional methods

The use of reported settling velocities (cm/s) for particulate solids was assumed sufficient. Resulting solid sedimentation rates (1/day) were not directly validated, but trial simulations for fish ponds and tanks containing solids of fish and phytoplankton origin gave reasonable results (see system simulations later in this chapter). The complicating issues described in Chapter 5 make the interpretation of reported data and the validation of solid sedimentation rates a difficult task. For solids filtration and fractionation (managed processes), method validity depends on the accuracy of given solid removal efficiencies, which are highly specific to filter design and operation. Similarly, for chemical filtration, method validity depends on the accuracy of given compound removal efficiencies. For compound addition and the application of active heat transfer, method validity was confirmed by the achievement of specified set-point concentrations (or temperatures), under a variety of water quality conditions and static and flowing water (see process control later in this chapter). Compound addition include pH and alkalinity adjustment, for which methods of aquatic chemistry, in addition to mass transfer, are employed to determine required quantities.

8.3 Aquatic biology

8.3.1 Soil processes

Uptake and release rates of compounds across the water-soil interface are established by given annual regimes (Chapter 6). The validity of soil process modeling depends on the accuracy of these regimes. Oxygen consumption rates show a reasonable level of agreement in the literature, but alkalinity, nitrogen, and phosphorous uptake and release are more site-specific (Chapter 6, Table 6.2). In trial applications to solar algae ponds presented later in this chapter, soil processes were used in conjunction with benthic bacterial processes (sediment oxidation and nitrate denitrification).

8.3.2 Bacterial processes

Bacterial processes occurring in aquaculture systems are typically associated with a host of additional processes, and their separate study, calibration, and validation is not well represented in the aquaculture literature. A coarse level of method validation for heterotrophic, nitrifying, and denitrifying bacterial processes in solar algae ponds was accomplished within a context of pond

ecosystem modeling, as described later in this chapter. Similarly, for flow-through and recirculating tank-based systems, preliminary validation of solid oxidation and passive ammonia nitrification was performed within a whole-system context, as described later in this chapter. Generally, the use of reported model parameters for bacterial processes was assumed sufficient. For all passive bacterial processes, the required accuracy of given parameters depends on the proportions of bacterial compound consumption and production within total compound budgets. For typical intensive, flowing water systems, suspended and settled solids are usually not allowed to accumulate beyond low levels, except in filters and sedimentation traps from which they are regularly removed. While solid oxidation remains significant, its role is diminished and the accuracy of associated parameters is less important. In contrast, oxidation of organic solids is normally a major component of oxygen and nutrient budgets in pond-based systems. Additional bacterial processes likely to be important include passive and active nitrification for intensive systems and passive nitrification and denitrification for pond based systems.

Processes of nitrifying bacteria in ammonia biofilters (active nitrification) are relatively isolated and can be separately evaluated. Studies of active nitrification were well represented in the aquaculture literature and provided a basis for assessing model performance. Trial applications of biofilters using various hydraulic loading and influent water quality conditions gave results comparable to reported nitrification rates and demonstrated that expected filter behavior was achieved (Brune and Gunther, 1981; Malone et al., 1993; Zhu and Chen, 1999). Areas of validation included (1) responses to hydraulic loading (Figure 8.19), (2) responses to ammonia concentration (Figure 8.20), and (3) impacts of filter backwashing (Figure 8.21) (see Table 8.2 for application conditions). The accuracy of predicted nitrification rates primarily depends on given filter specifications, which are highly specific to filter design and management. Simulation results for a biofilter undergoing frequent solids cleaning (Figure 8.21) showed a decrease in nitrification that was comparable to reported declines (Malone et al., 1993), due mainly to the concurrent removal of nitrifying bacteria. Simulation results adequately accounted for the oxidation of accumulated organic solids in biofilters as an additional ammonia source and oxygen demand.

Table 8.2. Conditions for simulation trials of an ammonia biofilter

Variable hydraulic loading rate (Figure 8.19)
<ul style="list-style-type: none"> • System: fully conditioned biofilter, media surface area to volume ratio = 500 m²/m³, media surface area = 4000 m², total media volume = 8 m³, and media void volume = 50% • Biofilter parameters: TAN_{std} = 1.0 mg N/L, TAN_{min} = 0.07 mg N/L, R_{TAN-max} = 3.0 g N/m²/day, R_{TAN-std} = 0.5 g N/m²/day, K_{TAN-ANB} = 4.7 mg N/L, and oxygen limits to nitrification ignored • Conditions: influent TAN = 3.0 mg N/L, temperature = 20 °C, influent nitrate = 0.0 mg/L, and variable water exchange rate
Variable ammonia concentration (Figure 8.20)
<ul style="list-style-type: none"> • System: as above • Case 1: biofilter parameters as above • Case 2: biofilter parameters from Zhu and Chen (1999): TAN_{std} = 2.25 mg N/L, TAN_{min} = 0.07 mg N/L, R_{TAN-max} = 1.87 g N/m²/day, R_{TAN-std} = 1.0 g N/m²/day, K_{TAN-ANB} = 1.9 mg N/L, and oxygen limits to nitrification ignored • Conditions: as above, for which variable biofilter TAN concentrations (internal) were achieved by varying the filter water exchange rate
Daily removal of accumulated solids (Figure 8.21)
<ul style="list-style-type: none"> • System: as above • Biofilter parameters: as above for typical biofilter. Reduction in nitrification rate immediately following a cleaning event is 50%, with nitrification rates increasing to fully conditioned levels over a period of 5 days. All solids in the influent water are removed by biofilter. Biofilter cleaned when accumulated solids achieve 10% of total solids capacity. The resulting filter cleaning frequency is about once per day. • Conditions: influent TAN = 2.0 mg N/L, influent particulate organic solids = 20 mg dw/L, temperature = 20 °C, and water exchange rate = 1.0/min.

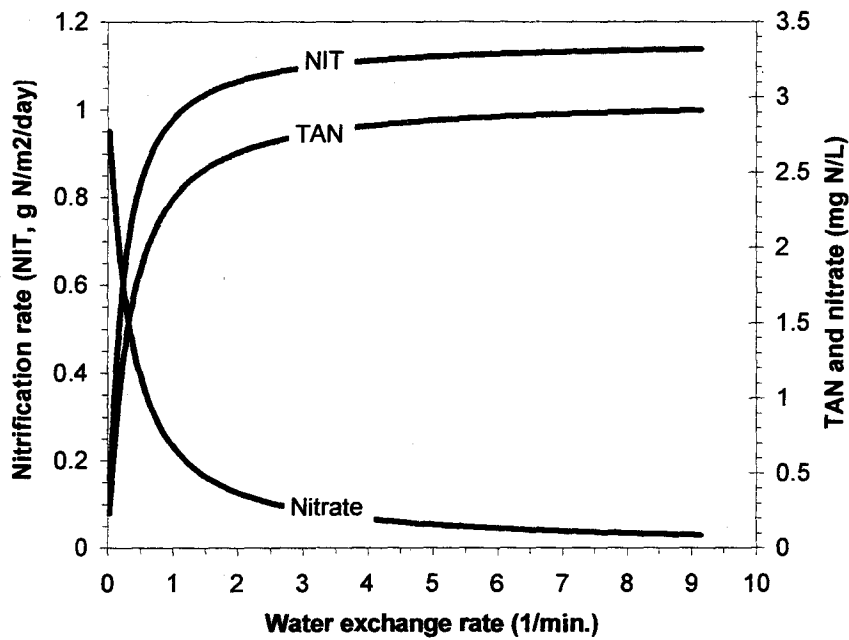


Figure 8.19. Response of nitrification rate and effluent ammonia and nitrate concentrations to hydraulic loading for an ammonia biofilter

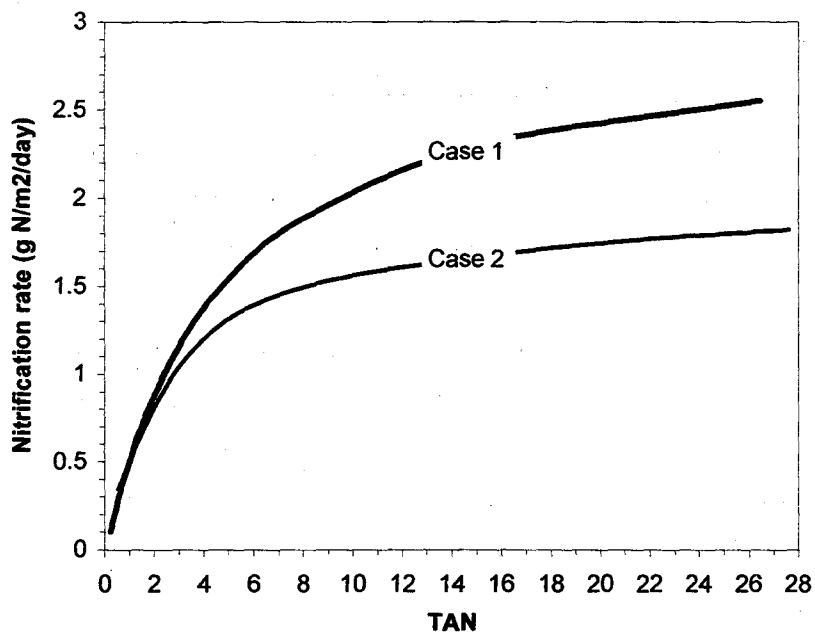


Figure 8.20. Response of nitrification rate to total ammonia nitrogen (TAN) concentration (within biofilter) for two different sets of typical ammonia biofilter parameters (cases 1 and 2)

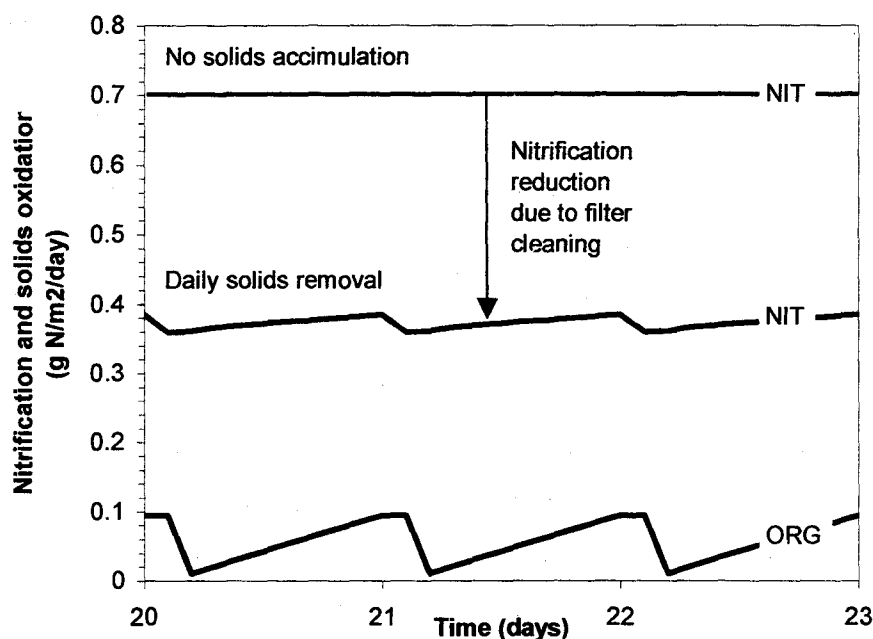


Figure 8.21. Rates of nitrification (NIT) and oxidation of organic solids (ORG; expressed as nitrogen release) in a biofilter undergoing daily solids removal (see Table 8.2 for application conditions)

8.3.3 Phytoplankton processes

Phytoplankton processes typically represent a major component of compound mass transfer in outdoor aquaculture systems and require a corresponding level of attention for system modeling. Phytoplankton processes are relatively complex and highly interactive with other unit processes. Factors that can influence primary productivity include (1) solar radiation, (2) water stratification, (3) water turbidity (inert and organic particulate solids), (4) water temperature, (5) nutrient availability, and (6) species composition and periodicity (succession) including green and blue-green algal species (Colman and Edwards, 1987). All of these influencing factors can vary temporally, spatially, and stochastically. Given the large number of parameters and variables used in the phytoplankton model and the corresponding requirements for empirical data, rigorous validation of phytoplankton processes is a considerable task. Contributions to this area of the literature are needed, but extended analyses were not accomplished here. It was assumed that the major burden of validation could be placed on the literature.

Validation exercises completed here were concerned with verifying achievement of (1) expected behavior of the phytoplankton model and (2) adequate prediction of typical diurnal and

annual regimes for phytoplankton concentrations (PC; g C/m^3) and net primary productivity (NPP; $\text{g C/m}^3/\text{day}$). Simulations for these exercises included passive gas transfer, sedimentation and oxidation of organic solids (from dead phytoplankton), and other processes in addition to primary productivity, as needed to represent static and flowing water systems. Consideration of these simultaneous processes complicated the validation of phytoplankton as an individual unit process but was required due to the nature of the available validation data.

Theoretical maximum NPP rates are about 15 to 20 $\text{g C/m}^2/\text{day}$ (areal basis), and maximum practical yields range from 5 to 10 $\text{g C/m}^2/\text{day}$ (Goldman, 1979). Values above 5.0 $\text{g C/m}^2/\text{day}$ are more typical of intensively managed algal culture systems, which are normally shallower than aquaculture ponds (e.g., 0.2 – 0.5 m depth). Typical, empirically based estimates of maximum NPP rates in fertilized fish ponds (e.g., 0.7 – 1.0 m depth) are in the vicinity of 4.0 $\text{g C/m}^3/\text{day}$ (Hepher, 1962; Colman and Edwards, 1987). These and other NPP rates reported here are based on a 24-hour period (combined light and dark periods), unless values are explicitly noted as short-term diurnal values. Unfortunately, the literature does not always clearly state the time basis of reported NPP rates (i.e., short term, light period, or 24 hour), requiring the use of assumptions to interpret some reported rates. Based on the literature, a reasonable, maximum, 24-hour mean NPP level for a water column of 1.0-m depth is considered to be about 4.0 $\text{g C/m}^3/\text{day}$, under conditions of non-limiting nutrient levels, optimum temperatures, and equatorial (12-hr photoperiod), clear sky, solar radiation levels. When an algal population is at equilibrium, the rate of cell addition (specific NPP, 1/day) equals the rate of cell loss (mortality rate, 1/day; additional losses may exist). Therefore, corresponding to a maximum NPP of 4 $\text{g C/m}^3/\text{day}$ and assuming a phytoplankton mortality rate of 10 %/day, the maximum reasonable PC is about 40 g C/m^3 .

Following the establishment of reasonable limits to PC and NPP, the logical flow of the procedure used to calibrate and validate the phytoplankton model consisted of the following steps: (1) establish the minimum phytoplankton light saturation level, (2) demonstrate saturation kinetics for light utilization and verify expected behavior for the NPP light scalar term, (3) establish achievement of reasonable NPP-PC profiles for static and flowing water conditions, (5) demonstrate saturation kinetics for nutrient utilization and compare predicted NPP rates to empirical data, and (6) verify achievement of NPP rates and PC levels for some representative case studies of aquaculture systems. Results of these exercises are described below and in system studies presented later in this chapter. Table 8.3 provides application conditions for these exercises.

8.3.3.1 Response of phytoplankton to light

Utilization of light by phytoplankton and light availability in the water column as a function of phytoplankton density (Chapter 6) are relatively complex, interactive components of the phytoplankton model. Algae show both short and long term adaptation to available light levels, but functionality for predicting adaptation and resulting light saturation levels have only received preliminary attention in the aquaculture literature (e.g., Piedrahita et al., 1993). Water turbidity is the basis of light attenuation in the water column, and yet it is typically quantified (as here) by the somewhat subjective measure of Secchi disk visibility (SDV; cm). Measurement of SDV is subject to the observer's visual acuity, sun angle and water surface glare, and judgment of the Secchi disk's disappearance and reappearance in the water column. Empirically derived and predicted relationships between SDV and phytoplankton concentration (PC) must account for any suspended solids in addition to phytoplankton, but reported data are typically weak or non-existent in this regard. These areas of concern were analyzed by placing phytoplankton in an environment where water temperature and nutrient levels were non-limiting and only available light and phytoplankton response to light impacted phytoplankton performance.

Of the parameters used in the phytoplankton model, light saturation (I_S) was the most poorly represented in the literature. Therefore, I_S was established last, after other parameters values were set, so that a maximum NPP of about $4 \text{ g C/m}^3/\text{day}$ was achieved for equatorial, maximum radiation levels (see Table 8.3 for application conditions). Simulation results showed that an I_S of about 50 Einsteins/ m^2/day ($25,284 \text{ kJ/m}^2/\text{day}$) was suitable and that NPP was highly sensitive to the I_S value used (Figure 8.22). To put this value in perspective, maximum, equatorial solar radiation levels (I_0 , incident radiation at water surface; see Chapter 6) are about $30,000 \text{ kJ/m}^2/\text{day}$ on a daily basis and $100,000 \text{ kJ/m}^2/\text{day}$ on an hourly basis. At the high algal densities attained in solar-algae fish ponds (e.g., $\text{SDV} \leq 30 \text{ cm}$, water depth 1.0-m), mean light levels integrated over the water column are only about 15% of surface light levels. Thus, 15% of maximum diurnal radiation levels ($15,000 \text{ kJ/m}^2/\text{day}$) is equivalent to $30 \text{ Einsteins/m}^2/\text{day}$ and well below the I_S level of $50 \text{ Einsteins/m}^2/\text{day}$.

Following establishment of I_S , the expected behavior of saturation kinetics for light utilization by phytoplankton was demonstrated (Figures 8.23, 8.24, and 8.25). This was accomplished by placing phytoplankton under a full range of solar radiation intensities (achieved by varying altitude

Table 8.3. Application conditions for phytoplankton simulation exercises (Figures 8.22 – 8.35)

Exercise conditions	Specifications
Phytoplankton model parameters	Table 6.7, Chapter 6: including phytoplankton mortality rate of 0.1/day, unless noted otherwise
Equatorial, maximum radiation levels	Latitude = 0°, altitude = 0 m, Julian day = 35, cloud cover = 0, and resulting solar radiation = 29670 kJ/m ² /day
Water depth	1.0 m unless otherwise noted
Particulate solids	Live and dead phytoplankton only
Non-limiting temperature	Temperature = 25 °C, using liberal temperature scalar parameters of 3, 25, 35, and 45 °C
Non-limiting nutrients	Nutrients maintained at levels to give nutrient scalars ≥ 0.98
Variable latitudes	Generated climate (including annual radiation regimes), altitude = 0 m, cloud cover = 0.5, wind speed = 2 m/s, relative humidity = 75%, and typical annual min-max air temperatures specific to each latitude
Flowing water, limited nutrients	Influent DIC (as alkalinity) = 36 mg CaCO ₃ /L, DIN = 7.0 mg N/L, DIP = 1.0 mg P/L, water depths = 0.5 and 1.0 m, and solar radiation as used for prior exercises at equatorial conditions
Static water, limited nutrients	Application site is Bang Sai, Thailand (PD/A CRSP Aquaculture Database, 1998), latitude = 14°11', altitude = 5.0 m, water depth = 0.9 m, temperature = 25 °C, cloud cover = 0.5, Julian day = 90, and resulting (generated) solar radiation = 22850 kJ/m ² /day

and latitude), using non-limiting temperature and nutrient conditions. Using a constant algal density of 7.0 g C/m³ (moderate bloom), predicted light scalar values on the order of 0.2 (24-hour basis) showed that only 20% of the maximum potential specific NPP rate (μ_{\max}) was achieved, due to light scaling alone (Figure 8.23). As light availability was increased, an expected decrease in the rate of increase for NPP was also found, for which Figure 8.24 shows the combined effect of light saturation kinetics and declining light availability with increasing algal density. As shown by the overlay of NPP and PC values in Figure 8.24, under conditions of population equilibrium and cell losses due to death only, specific NPP equaled the mortality rate and the relationship between NPP and PC was constant (specific NPP = NPP / PC).

As shown in Figure 8.25, light scalar values as a function of algal density conformed to expected exponential-decay profiles. As is evident in Figure 8.25, the negative impact of excessive light levels may be considerable but only at relatively low algal densities and high light intensities. For most conditions, the light scalar is depressed due to insufficient light levels. However, this

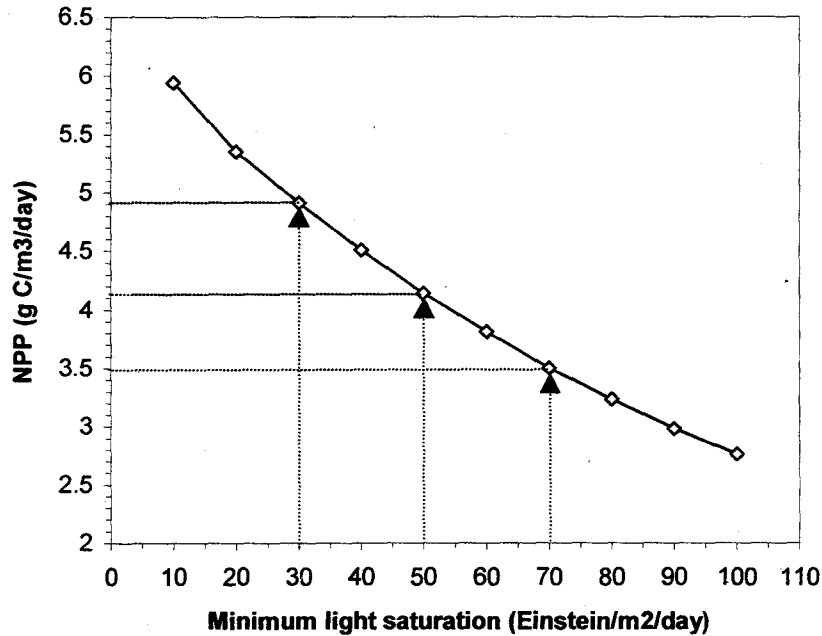


Figure 8.22. Response of NPP to the minimum light saturation of phytoplankton, for which 50 Einstein/m²/day (25,284 kJ/m²/day) is used in AquaFarm (non-limiting temperature and nutrient conditions)

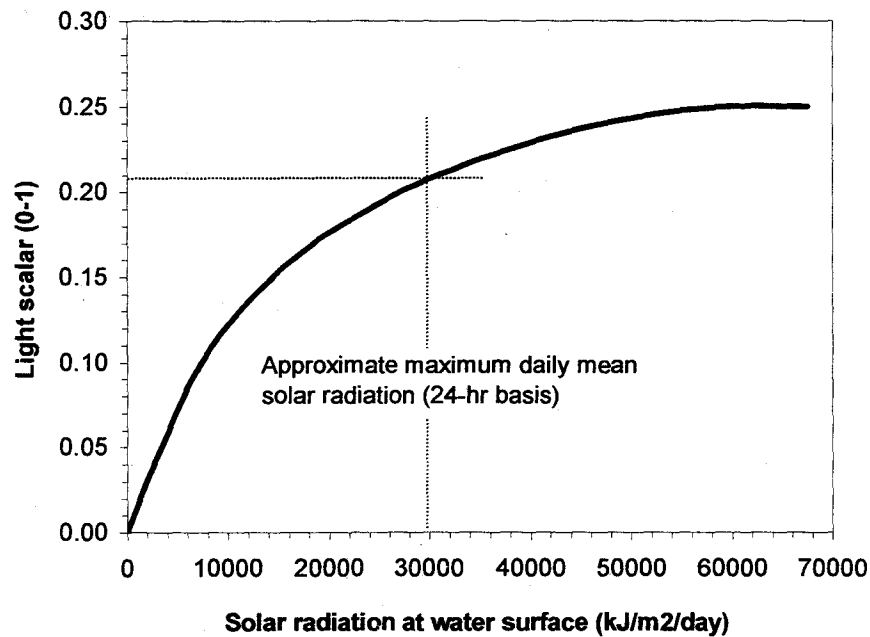


Figure 8.23. Relationship between the light scalar term (24-hr basis) of the phytoplankton model and incident solar radiation at the water surface (constant PC at 7.0 g C/m³)

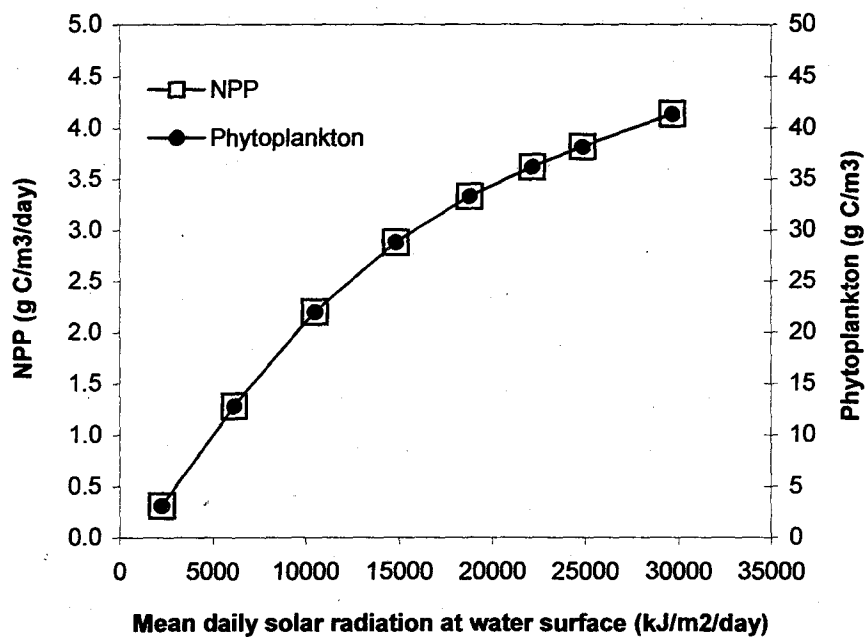


Figure 8.24. Response of NPP to incident solar radiation at the water surface, where NPP and phytoplankton values are related by a constant ratio (non-limiting temperature and nutrient conditions)

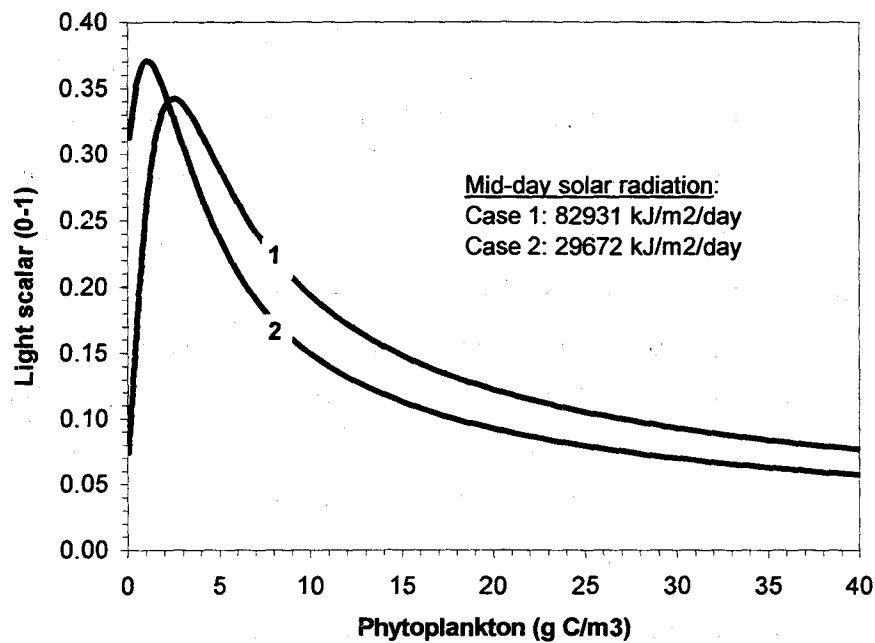


Figure 8.25. Relationship between light scalar term of phytoplankton model and phytoplankton density, for low and high mid-day solar radiation levels

conclusion is based on the daily simulations used to generate Figure 8.25 and does not necessarily apply to diurnal simulations (provided below). Overall, these results show that the light scalar term for eutrophic waters (e.g., fertilized or fed fish ponds) has a dominate impact on predicted NPP rates and has the potential to be a major source of error in phytoplankton modeling.

The next series of exercises demonstrated the critical relationship between SDV and PC. Simulation results showed that the relative slopes of (1) the light availability function and (2) the light response function had a major impact on the ability of simulations to generate expected phytoplankton behavior. Specifically, it was found that rate of descent of SDV (as a measure of light availability) in response to increasing PC (Figure 8.26) must be of adequate magnitude in order to achieve expected relationships between NPP and PC. When previously reported SDV parameters (α and β) were used, the increase in NPP with increasing PC did not display the expected asymptotic behavior (Figure 8.27), and PC levels and NPP rates reached unrealistically high values (Figure 8.28). With newly derived SDV parameters (see Chapter 6), reasonable NPP-PC profiles and reasonable maximum NPP and PC levels were achieved. Case 1 in Figure 8.26, cases 1 and 2 in Figure 8.27, and case 1 in Figure 8.28 were based on standard parameter values developed for AquaFarm. Other cases were based on reported parameters, using Secchi constant (SC) values as originally reported or that yielded maximum NPP rates close to $4.0 \text{ g C/m}^3/\text{day}$ (SC adjusted to nearest 0.1 increment; applies to SC values in the 2.5 – 2.6 range for Figures 8.27 and 8.28). Non-limiting temperature and nutrient conditions were used for Figures 8.27 and 8.28.

The phytoplankton ranges shown in Figure 8.26, expressed as carbon, chlorophyll-a, and dry weight solids, up to levels of 40 g C/m^3 , represent approximate maximum ranges for these variables according to the supporting literature. Comparing cases 1 and 2 in Figure 8.27, the maximum NPP increased from about 4.0 g C/m^3 to over 6.0 g C/m^3 when water depth was decreased from 1.0 to 0.75 m. The large impact of water depth on NPP (volumetric basis) shows that the accuracy of pond specifications and water budget modeling (for water depths) is highly critical to the accuracy of NPP modeling. Results shown in Figure 8.28 were achieved by reducing phytoplankton mortality rates to 0.001/day. While this was not intended to be realistic, it was a suitable mechanism to achieve high PC values for the purposes of this exercise.

For equilibrium (PC at steady state), non-limiting conditions (except light), using standard parameter values developed for AquaFarm, Figure 8.29 provides simulated responses of PC and NPP to increasing levels of cell removal. The latter was achieved by increasing mortality rates from

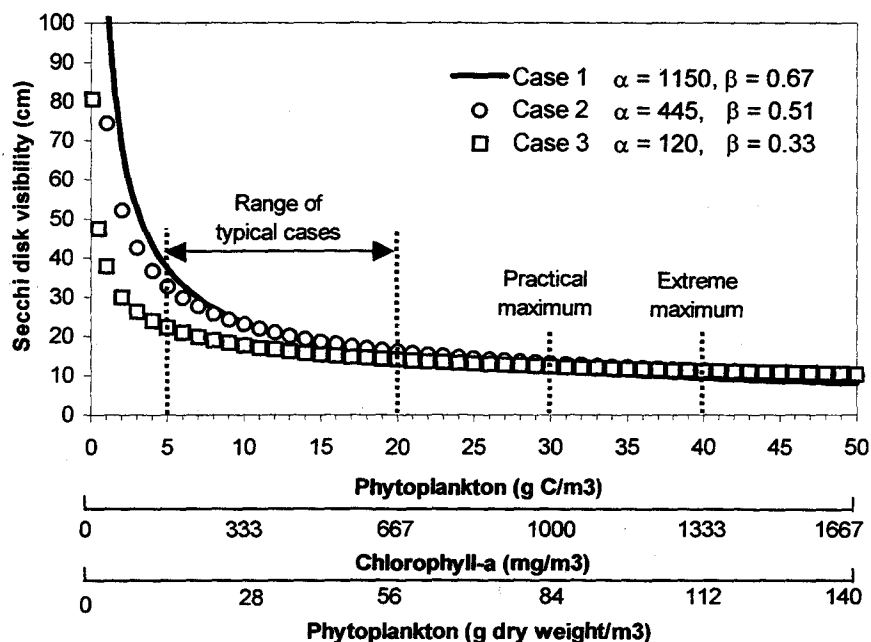


Figure 8.26. Relationship between Secchi disk visibility and phytoplankton concentration (in terms of carbon, chlorophyll, and dry weight solids), for case 1 (standard parameters), case 2 (Almazan and Boyd, 1978), and case 3 (Nath, 1996)

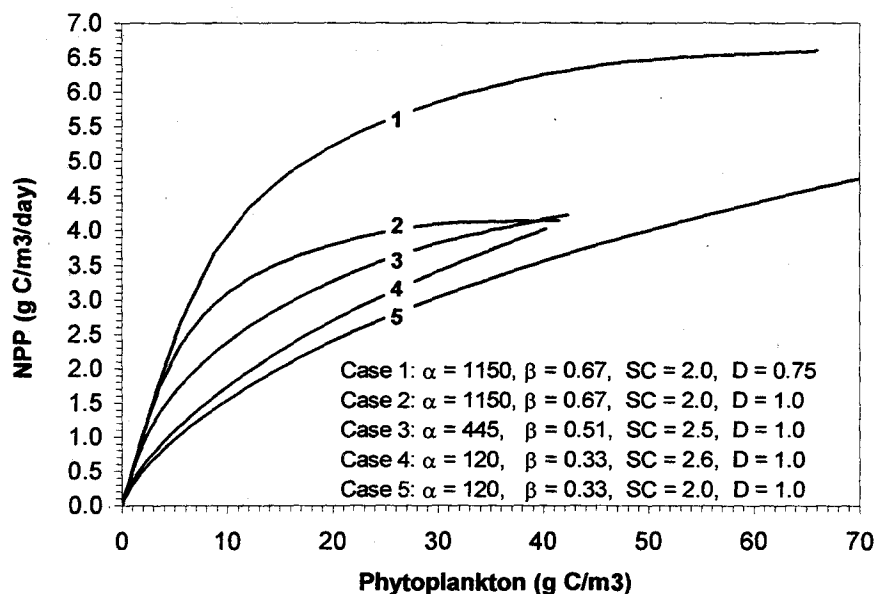


Figure 8.27. Response of NPP to phytoplankton concentration, at a phytoplankton mortality rate of 0.1/day, for cases 1 and 2 (standard parameters; depth = 0.75 and 1.0 m), case 3 (Almazan and Boyd, 1978a), case 4 (Nath, 1996; reported/adjusted parameters: $K_{DIC} = 1.0$ g C/m³, $\mu_{max} = 3.0$), and case 5 (Nath, 1996; reported parameters: $K_{DIC} = 5.0$ g C/m³, $\mu_{max} = 2.25$)

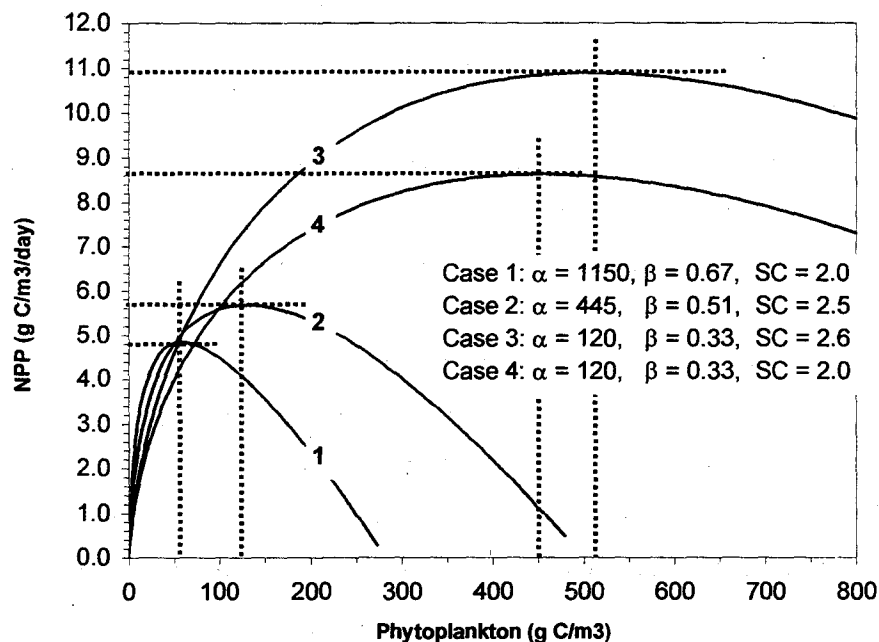


Figure 8.28. Response of NPP to phytoplankton concentration showing typical concave-down profiles, for which high phytoplankton concentrations were achieved by the use of a low phytoplankton mortality rate (0.001/day; cases 1-4 correspond to cases 2-5 in Figure 8.27)

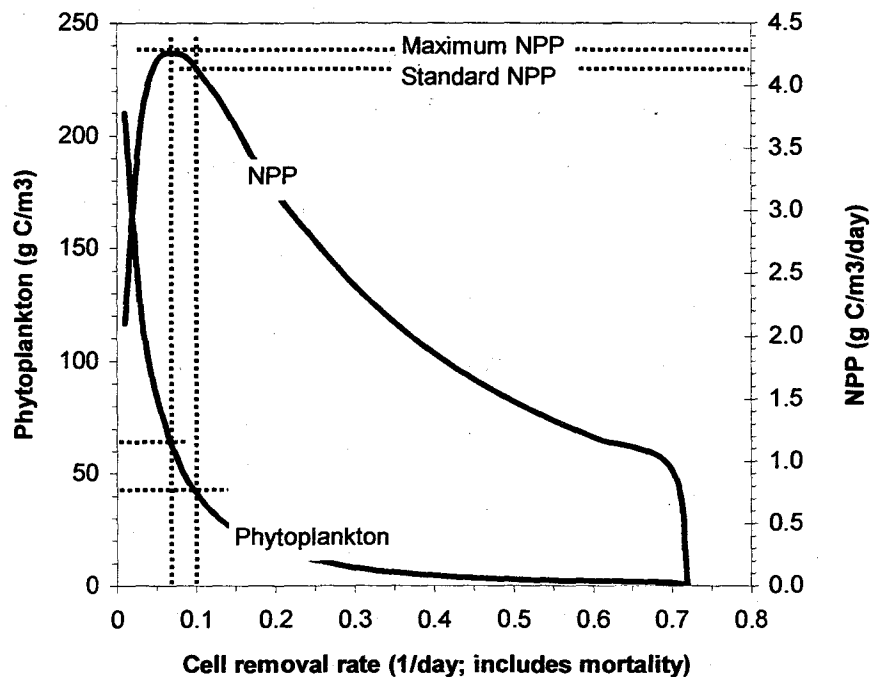


Figure 8.29. Response of phytoplankton concentration and NPP to cell removal rate (mortality and other losses), showing a typical concave-down profile of NPP and sudden decline in NPP at high cell removal rates (e.g., advective cell washout)

0.01 to 0.1/day and then increasing advection rates from 0.0 to 1.0 water exchanges per day (influent water contained no algae). The concave-down shape of the resulting NPP curve and non-concurrence of maximum NPP and PC levels have been previously reported, both in terms of empirical data and developed models (Colman and Edwards, 1987). Maximum NPP occurs when the rate of algal loss (death, sedimentation, grazing, and advection) equals the maximum possible rate of algal productivity. Algal population stability is greatest when PC levels exceed that at the maximum NPP, as increases in cropping rate cause an offsetting increase in NPP. When PC levels fall below that at the maximum NPP, increases in cropping (or death) are reinforced by a decline in NPP, leading to a population crash. Simulation exercises predicted this behavior, as illustrated in Figures 8.28 and 8.29. It is emphasized that (1) phytoplankton mortality is not included in NPP values ($\text{NPP} = \text{GPP} - \text{respiration}$), (2) phytoplankton losses may include algal grazing and advection in addition to death, and (3) algal sedimentation is included in the mortality rate.

Using the conditions of Figure 8.29 at a mortality rate of 0.1/day, no additional cell losses, and non-limiting temperature and nutrient conditions, the diurnal simulation illustrated in Figure 8.30 provides a new perspective to this discussion. While maximum NPP and PC values averaged about $4 \text{ g C/m}^3/\text{day}$ and 40 g C/m^3 over a 24-hour period, diurnal NPP rates varied from about -2 to $13 \text{ g C/m}^3/\text{day}$ (Figure 8.30, case 1). Good compatibility between diurnal and daily phytoplankton simulations was demonstrated, as daily mean PC and NPP rates generated by daily simulations were essentially equal to the 24-hr means of the diurnal profiles generated by diurnal simulations. The negative impact of high, midday, light levels on photosynthesis is clearly evident in the concave depression at the top of the NPP profile.

As described earlier, using a maximum specific NPP rate (μ_{max}) of 3.0/day, the value of 50 Einsteins/ m^2/day for I_S was established so that a maximum 24-hr NPP of about $4 \text{ g C/m}^3/\text{day}$ was achieved. Reported values for μ_{max} range from about 2.2 to 3.0/day (see Chapter 6). If a μ_{max} of 2.5/day is used, then I_S must be reduced to about 15 Einsteins/ m^2/day in order to achieve a maximum NPP in the vicinity of $4 \text{ g C/m}^3/\text{day}$. Use of these adjusted parameters is illustrated in case 2 of Figure 8.30 and resulted in a greater midday depression of NPP. A 30% depression of NPP at midday relative to diurnal peaks appears to be excessive, based on reported diurnal oxygen profiles. In concurrence, an I_S value of 15 Einsteins/ m^2/day does not in itself appear reasonable (Piedrahita et al., 1993). The use of 3.0/day for μ_{max} is supported by these results.

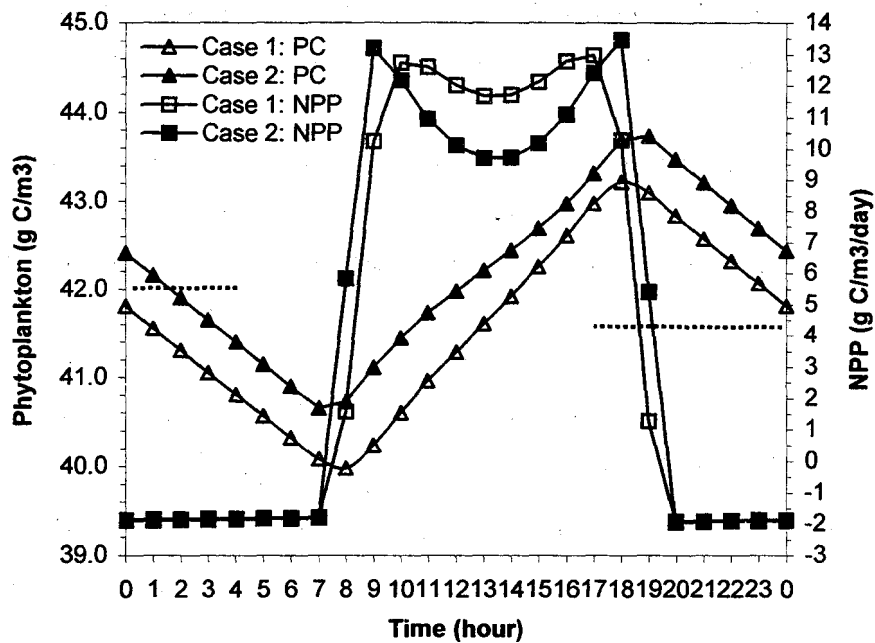


Figure 8.30. Diurnal, 24 hour, phytoplankton and NPP regimes, for case 1 (standard parameters: $I_S = 50$ Einsteins/m²/day, $\mu_{\max} = 3.0$ /day) and case 2 (test parameters: $I_S = 15$ Einsteins/m²/day, $\mu_{\max} = 2.5$ /day), where daily mean values predicted by simulation using a 1-day time-step are shown for case 1 as dotted lines

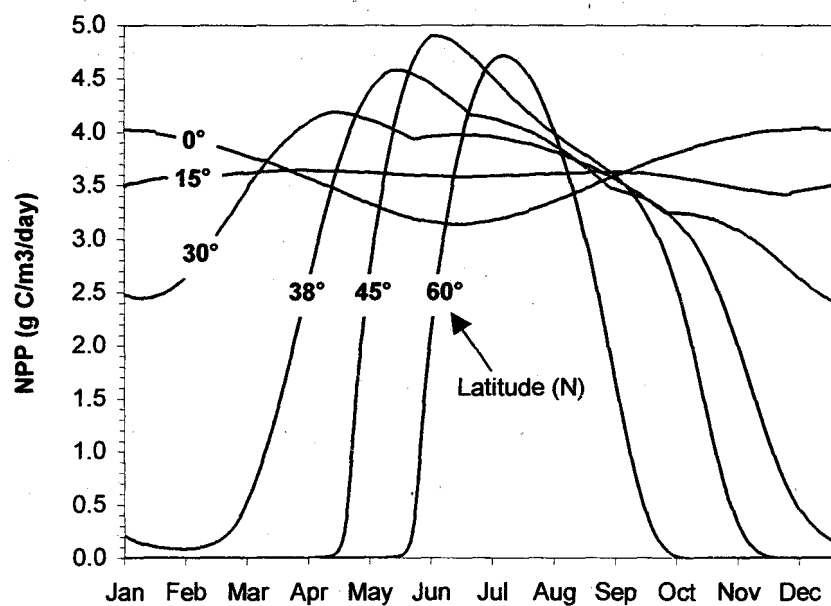


Figure 8.31. Annual NPP regimes for latitudes varying from the equator to 60° N, using generated climatic regimes, passive heat transfer, and non-limiting nutrients

The combined impacts of temperature, daylength, and solar radiation on NPP are illustrated in Figure 8.31. These simulation trials were performed for latitudes ranging from the equator to 60° North, using generated climatic regimes, passive heat transfer and predicted water temperatures, and maintenance of nutrient levels at non-limiting levels. Results showed that the reduction in NPP rates due to colder, seasonal water temperatures became an increasingly major influence at latitudes of 30° N and greater. The parameter values used for the temperature scalar clearly impacted results under colder conditions. However, only rough estimates of these parameters were available in the literature (see Chapter 6). As latitude was increased from zero to 60° N, the maximum summer daylength increased from 12 to 18.5 hours, which accounts for the high, mid summer, NPP rates at higher latitudes. At a latitude of 45° N, maximum water temperature and daylength levels combined to yield a summer peak in NPP rates of $4.9 \text{ g C/m}^3/\text{day}$ (24-hr basis), surpassing the equatorial maximum achieved earlier of about $4.2 \text{ g C/m}^3/\text{day}$. Relative trends in these profiles among latitudes and over annual periods appear to be reasonable, but empirical data adequate for the validation of these rates was not found in the literature.

In summary, simulation of light utilization by phytoplankton and light availability in the water column displayed expected behavior, in terms of predicted PC and NPP levels relative to maximum standing crops and productivity levels. Simulation results demonstrated the considerable sensitivity of predicted NPP and PC levels to the underlying relationships between phytoplankton density, water turbidity, and light availability. Given the potential dominance of the light scalar term, additional applied research and modeling work in this area would be useful.

8.3.3.2 Response of phytoplankton to nutrients

Parameters for phytoplankton nutrient kinetics (DIC, DIN, and DIP) were largely taken from the literature. Some questions remained regarding DIC kinetics, as described below. In addition, delineation of the utilization of DIN components (TAN, NO_3 , and N_2), by the use of half-saturation constants (substrate preference factors), was not well established in the available literature. Simulated and empirical data describing the response of NPP to DIC, DIN, and DIP are provided in Figures 8.31, 8.32, and 8.33 (see Table 8.3 for application conditions). For each nutrient, a series of simulations were performed using a series of concentrations for the limiting nutrient, while the remaining two nutrients and temperature were maintained at non-limiting levels (empirical data from Nath, 1996).

Simulation results for DIN and DIP showed good agreement with empirical data. Simulation results for DIC, using the parameter values derived for AquaFarm (Chapter 6), showed significant disparity with empirical data. Alternatively, if K_{DIC} was 6.0 g mg/L (versus 1.0 mg/L) and the minimum threshold DIC was 4.0 mg/L (versus 0.0 mg/L), as used by Nath (1996), simulation results showed improved fit. However, if these alternative parameters are used, DIC remains limiting even at very high DIC concentrations. For example, at a DIC of 40 mg C/L, a nutrient scalar value of 0.86 is calculated, which requires a value of 3.5/day for μ_{max} to attain an NPP of 4 g C/m³/day under the non-limiting conditions described earlier. In addition, other reported values for K_{DIC} near 1.0 g C/m³ suggest that 6.0 g C/m³ is too high (Chapter 6). Since carbon limitations to photosynthesis are known to occur in aquaculture systems, additional applied research and modeling work in this area would be useful.

For another perspective on phytoplankton nutrient response, a flowing water system was simulated for which limiting nutrient levels were provided by the influent water (Figure 8.34; see Table 8.3 for application conditions; non-limiting temperature). For cases 2-4 in Figure 8.34 (water depth 1.0 m), results supported the expected trend of a consistent quantity of total cell loss (mortality and advection; about 0.2/day) at the points where NPP levels were maximized. Similar to Figure 8.29, maximum NPP levels occurred when the rate of algal loss equaled the maximum possible rate of algal productivity. Results of case 1 in Figure 8.34 showed the pronounced impact of a decrease in water depth on NPP (volumetric basis), similar to that found for static systems.

For nutrient-limited growth of algae under flowing water (continuous culture) conditions, it is known that NPP increases and PC decreases with decreasing cell retention time (i.e., increasing water exchange rate), until an optimum retention time is reached (Drapcho and Brune, 2000). Further decreases in retention time result in a decrease in both NPP and PC until complete cell washout occurs. This expected behavior was achieved by simulations, as illustrated in Figure 8.35. Drapcho and Brune (2000) achieved NPP values exceeding 3.0 g C/m³/day (24-hr basis assumed) at a water exchange rate of 0.8/day. Trial simulations used to mimic the conditions of this study (latitude 34°; summer; water depth 0.66 m) required that μ_{max} be increased from 3.0 to 3.7/day, in order to achieve reported NPP rates. While inconclusive, these results suggest that for continuous culture conditions, where mean cell age is reduced, the potential growth capacity (vigor) of the phytoplankton population is increased on the order of 20%.

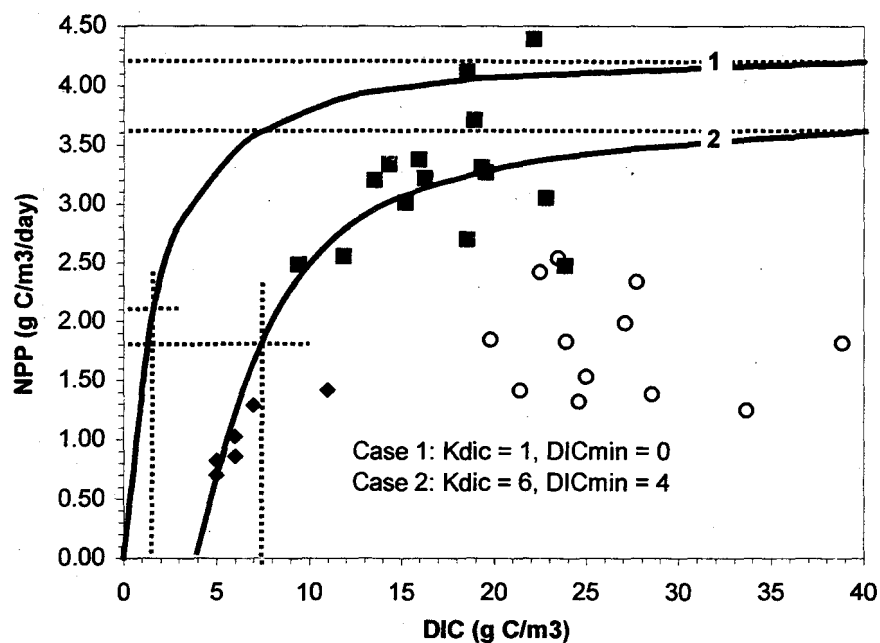


Figure 8.32. Response of NPP (lines) to dissolved inorganic carbon (DIC), for case 1 (standard parameters) and case 2 (adjusted K_{DIC} and DIC_{min}), with empirical data shown (points)

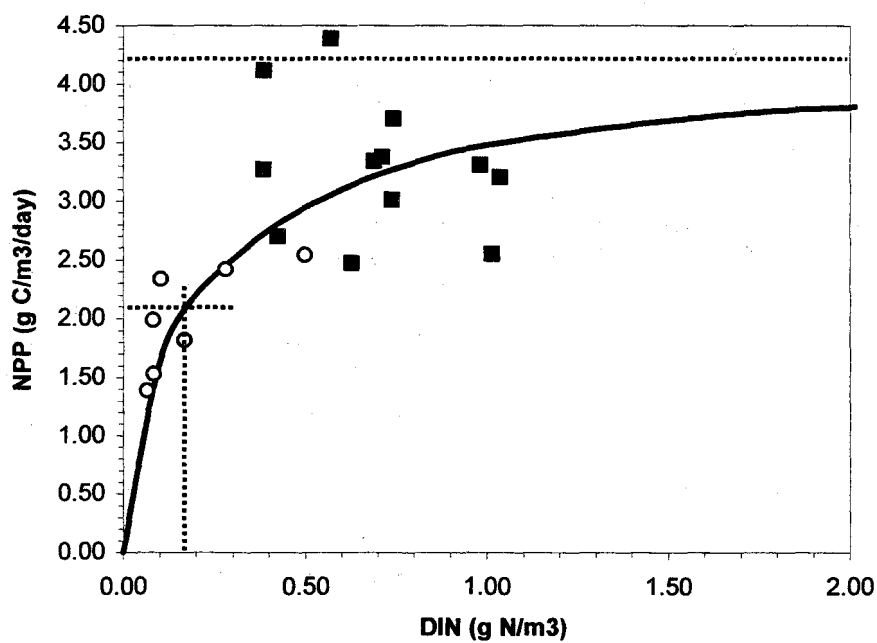


Figure 8.33. Response of NPP (lines) to dissolved inorganic nitrogen (DIN), with empirical data shown (points)

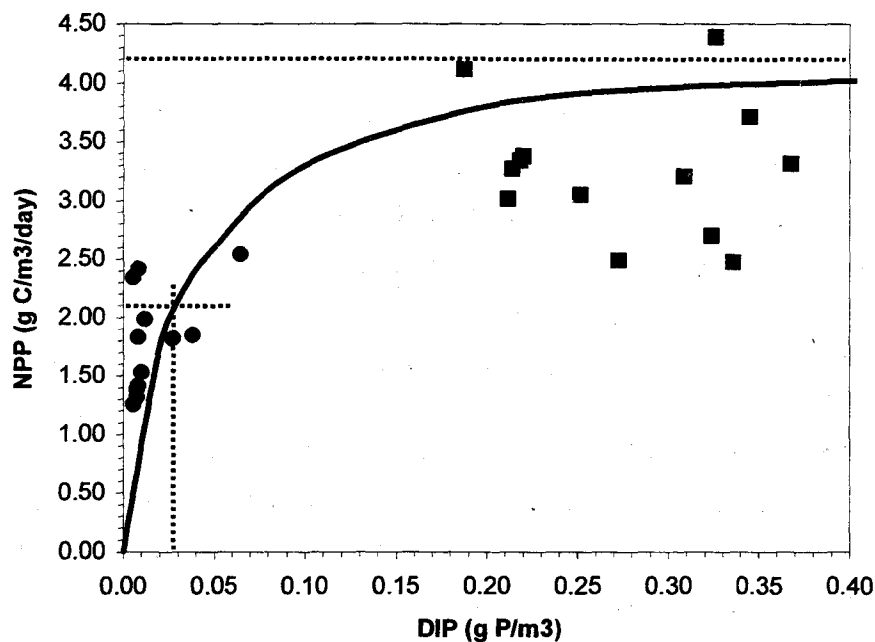


Figure 8.34. Response of NPP (lines) to dissolved inorganic phosphorous (DIP), with empirical data shown (points)

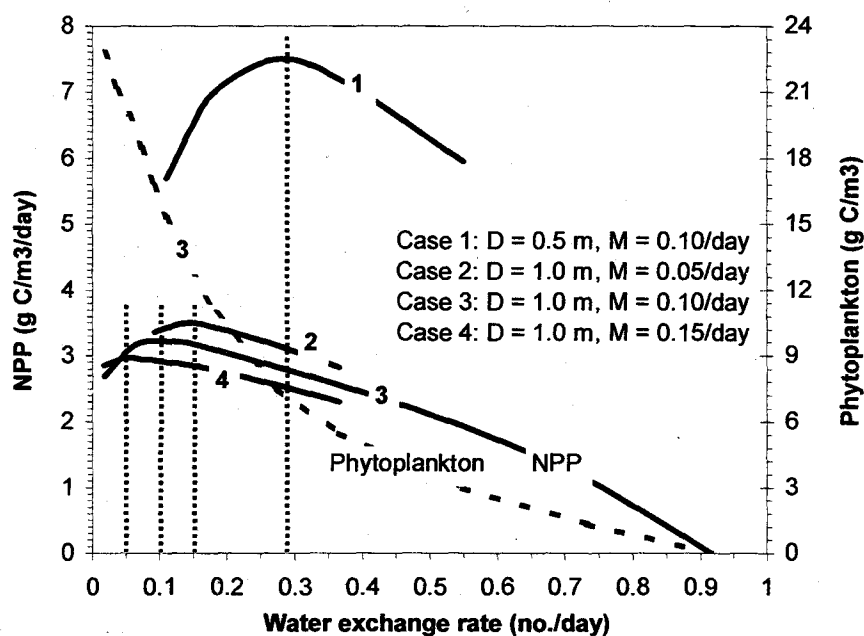


Figure 8.35. Response of NPP and PC to water exchange rate under limiting nutrient conditions for four different combinations of water depth (D) and phytoplankton mortality rate (M) (abbreviated curves shown for cases other than case 3), with maximum NPP points with respect to water exchange rate shown as dotted lines

8.4 Fish biology

Methods and models of fish biology used in AquaFarm were mainly based in the literature and a corresponding burden of validation was placed on this literature. A summary of considerations and accomplishments regarding the validation of fish biology methods is provided in Table 8.4. Parameters values for various fish species for the four, alternative growth models (LNGR, DSGR, VBGF, and BIOE) were provided in Chapter 7. Additional calibration and validation exercises were undertaken regarding fish growth and feeding (described below).

Fish oxygen consumption and metabolite/fecal excretion rates represent terms in the mass balance equations used to model fish rearing units. Validation of fish metabolic processes is considered later in this chapter, in a context of system-level simulations using various fish species. Overall, two general cases were apparent in these exercises regarding the role of fish metabolic processes. For extensive fish culture practices with no or low application rates of prepared feeds (gross fish yields ≤ 3000 kg/ha or 0.3 kg/m^2 ; solar-algae ponds), the direct impact of fish metabolism on water quality was typically overwhelmed by other processes, such as passive gas transfer and phytoplankton and bacterial processes. Under these conditions, fish were found to exert an indirect impact on water quality by providing nutrients for primary productivity (DIC, DIN, and DIP), but this was apparent only when fish were supplied with supplemental feed. The impact of fish consumption of natural foods on bacterial-detrital aggregate and phytoplankton standing crops depended on natural fish productivity levels, but major shifts in associated water quality regimes were not found. In contrast, for semi-intensive practices (gross fish yields $3000 - 20,000$ kg/ha) and intensive practices (gross fish yields $> 20,000 - 1,000,000+$ kg/ha), which relied predominately or wholly on prepared feeds, fish metabolic processes had a direct and major impact on water quality and compound budgets for fish rearing units. In summary, the required accuracy of fish metabolic modeling depended on the intensity of the aquaculture practice.

Validation and application exercises for fish growth focused on use of the double-logarithmic specific growth rate model (DSGR). When fish growth is not constrained by maximum (maturation) fish size, as is typically the case in aquaculture production, the DSGR model provides ease of calibration, an analytical solution, and good predictive power. In general, simulation exercises showed that the DSGR model was able to match results of the more comprehensive bioenergetic growth model (BIOE) under various application conditions. For cases where fish growth was constrained by the availability of natural or prepared foods, expansion of the DSGR model to

include natural fish productivity or system capacity scalars also yielded good results. In assessing the results presented below, it should be realized that inaccuracies in long-term fish weight predictions on the order of 5 to 10% are relatively minor distractions in the context of overall system design and management planning. The potential for inaccuracy in fish weight predictions increases with the length of the fish culture period. Because each simulation step uses an initial weight based on the final weight of the prior step, inaccuracies in predicted fish weights compound over time.

Table 8.4. Summary of validation accomplishments for fish biology methods

Modeling area	Validation considerations and accomplishments
Fish response to water quality	Method validity depends on the accuracy of given, species-specific water quality criteria, and linear scalar functions appear to be sufficient
Fish survival	Method validity depends on the accuracy of given, site-specific mortality rates
Fish maturation and spawning	Method validity depends on the accuracy of given, species-specific maturation and fecundity parameters
Egg incubation	Method validity depends on the accuracy of given, species-specific temperature-unit requirements
Fish growth	The LNGR, DSGR, VBGF, and BIOE growth models have been calibrated and validated for various fish species, as based on a review of the literature and additional exercises described here.
Fish weight distributions	Trial simulations demonstrated the qualitative validity of the newly developed model for fish growth variability. Quantitative calibration and validation of the parameters FPI and FCI remain to be completed.
Natural fish productivity	Method validity depends on the accuracy of given, site-specific parameters used to relate primary productivity, fish density, and natural fish productivity. Trial simulations for pond-based fish production gave seasonal regimes of fish productivity that were comparable to reported values and characteristic profiles of fish productivity were achieved.
Fish feeding (prepared feeds)	The TABL, DSFR, and FFCE feeding models have been calibrated and validated for various fish species, as based on a review of the literature and additional exercises described here.
Feed digestion and metabolism	Method validity depends on the accuracy of given, site-specific compositions of prepared feeds, known intensity of feeding rates with respect to appetite satiation, and lack of special circumstances impacting metabolism (e.g. fish stress). Trial applications with various fish species gave results that were comparable to reported metabolic rates.

8.4.1 Channel catfish growout

Calibration of the DSGR model to channel catfish growth data was performed for three datasets: (1) Figure 8.36 (Robinson and Li, 1995), (2) Figure 8.37 (Lovell, 1977), and (3) Figure 8.38 (Jensen, 1989) (see Table 8.5 for application conditions). Variables included water temperature, fish weight, and feeding and growth rates. Calibration results showed good fits for all three datasets and demonstrated that the DSGR model was capable of fitting empirical data as well as the more complex BIOE model (calibrated by Nath, 1996). Using the DSGR calibration based on Robinson and Li (1995) (Figure 8.36), validation of the DSGR model with respect to the remaining datasets showed adequate results (Figures 8.37 and 8.38). Application of this DSGR model to the validation conditions of Figure 8.38 demonstrated that calibration based on an intra-year dataset could be applied to a multi-year growout period. Validation results showed that the DSGR model was capable of predicting fish weights as well as the BIOE model (Figure 8.37), when the same calibration dataset was used for each model.

In fish growth modeling, it is difficult to avoid (1) periods of relatively poor calibration fit and (2) the dependency of validation results on the specific calibration dataset used (e.g., Figure 8.38). A wide range of variables may impact fish growth, including the specific stock used (intra-specie, genetically distinct stocks), environmental quality, feed quality, and fish handling practices. In addition, the existence of fish weight sampling error in aquaculture research is often understated (Hopkins and Yakupitiyage, 1991). Since the DSGR model can be easily calibrated by linear regression methods available on computer spreadsheets, the best approach for AquaFarm users is to use the DSGR model in conjunction with site-specific calibration datasets where available. Methods to support these regression procedures within AquaFarm are under development.

Table 8.5. Calibration and validation data sources and culture conditions for the production of channel catfish (*Ictalurus punctatus*)

Robinson and Li (1995): Figure 8.36	
Data (time series)	Fish weights, feed application rates, and water temperatures
Location	Stoneville Research Station, Mississippi, USA
System	Earthen, commercial catfish ponds
Fish culture	Fish stocked at 50 g/fish mean weight and 2.47 fish/m ² density. Fish fed to satiation (28 – 32% protein).
Production period	May 1 to October 1 (JD 121 – 274; 153 days)
Fish modeling	DSGR model: $\log_e(\text{SGR}) = [k_1 + k_2 T + k_3 T^2] - [\text{SGR}_e \log_e(W_{gm})]$ $k_1 = -7.24589, k_2 = 0.327159, k_3 = -0.00563, \text{SGR}_e = -0.33193$

Table 8.5. Continued

Lovell (1977): Figure 8.37	
Data (time series)	Fish weights, feed application rates, and water temperatures (feeding tables were developed from this study)
Location	Auburn, Alabama, USA
System	Earthen, commercial catfish ponds
Fish culture	Fish stocked at 30 g/fish mean weight and 0.59 to 0.74 fish/m density. Fish fed to satiation (36% protein).
Production period	April 15 to October 12 (JD 105 – 285; 180 days)
Fish modeling	DSGR model: $\log_e(\text{SGR}) = [k_1 + k_2 T + k_3 T^2] - [\text{SGR}_e \log_e(W_{gm})]$ $k_1 = -7.85879, k_2 = 0.342576, k_3 = -0.00435, \text{SGR}_e = -0.49098$
Jensen (1989): Figure 8.38	
Data (time series)	Fish weights, feed application rates, and water temperatures (approximate production data were derived from management charts)
Location	Louisiana, USA
System	Earthen, commercial catfish ponds
Fish culture	Fish stocked at 1.0 g/fish mean weight and 1.0 fish/m ² density. Fish fed to satiation (32% protein). Included over-wintering of fingerlings.
Production period	July 1 (year one) to October 1 (year two) (JD 182 – 639; 457 days)
Fish modeling	DSGR model: $\log_e(\text{SGR}) = [k_1 + k_2 T + k_3 T^2] - [\text{SGR}_e \log_e(W_{gm})]$ $k_1 = -5.05889, k_2 = 0.109639, k_3 = -0.00056, \text{SGR}_e = -0.37598$

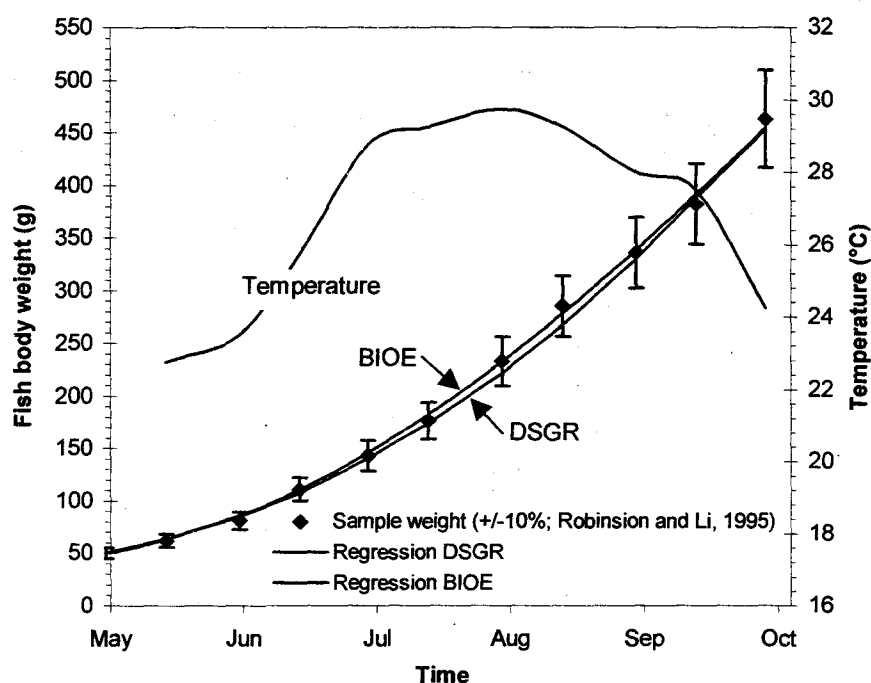


Figure 8.36. Calibration of the DSGR fish growth model (channel catfish) with data from Robinson and Li (1995), also showing the fitted calibration for the BIOE model (Nath, 1996)

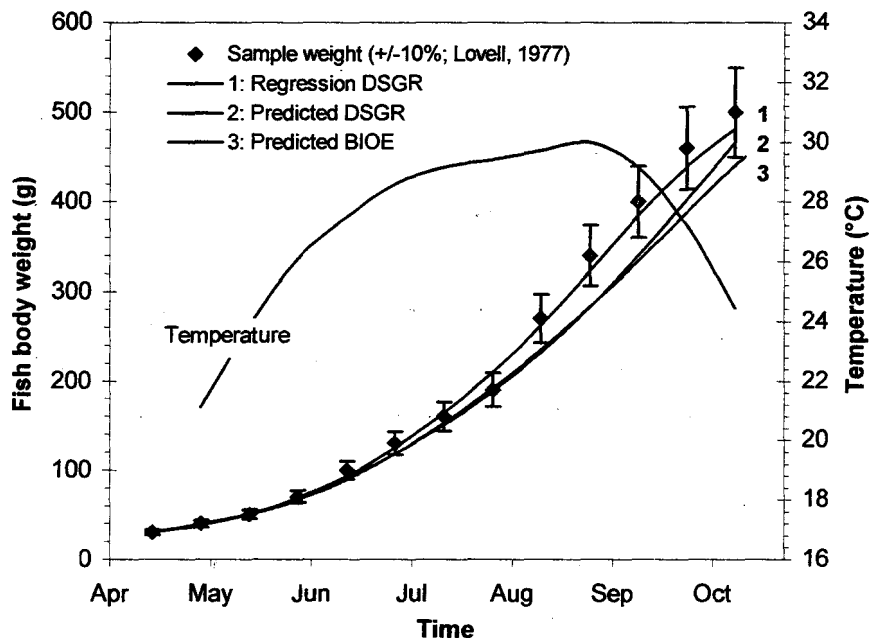


Figure 8.37. (1) Calibration of the DSGR fish growth model (channel catfish) with data from Lovell (1977; channel catfish), (2) predicted weights by the DSGR model calibrated with data from Robinson and Li (1995), and (3) predicted weights by the BIOE model calibrated with data from Robinson and Li (1995) by Nath (1996)

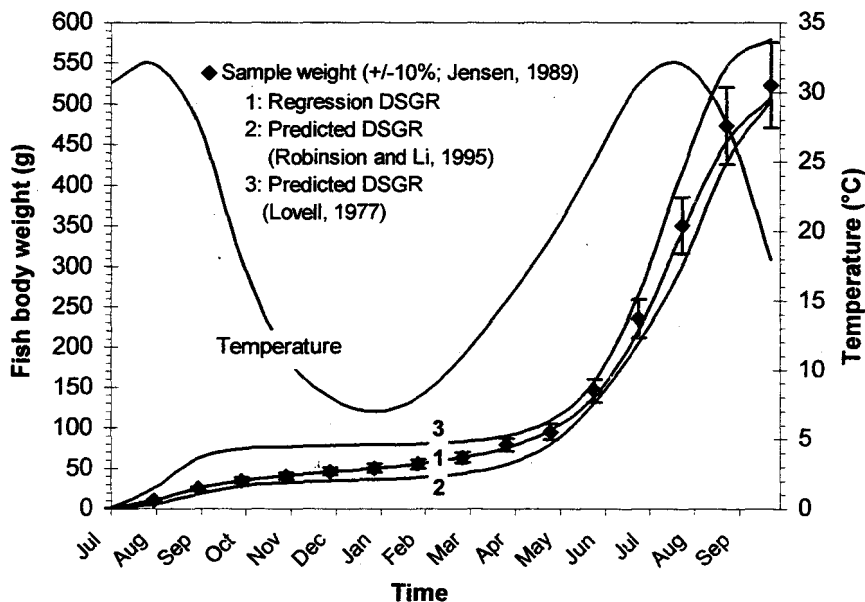


Figure 8.38. (1) Calibration of the DSGR fish growth model (channel catfish) with data from Jensen (1989), (2) predicted weights by the DSGR model calibrated with data from Robinson and Li (1995), and (3) predicted weights by the DSGR model calibrated with data from Lovell (1977)

8.4.2 Common carp growout

For the production of common carp in earthen ponds, the DSGR model provided good calibration fits to empirical data (Figure 8.39) (see Table 8.6 for application conditions). Terminal weight samples showing slight weight losses were ignored in these calibrations, as the DSGR model cannot yield negative growth rates. The DSGR model calibrated for 1-2 year old fish was applied to growth prediction for 2-3 year old fish. The predictive accuracy of the DSGR model was fair and apparently exceeded that of the BIOE model. This exercise demonstrated the capacity to apply calibration data from smaller fish to predictive applications for larger fish. The maximum fish size of about 900-g is well below the maximum weight for this species, and therefore the DSGR model was correctly applied over this weight range. The terminal, asymptotic growth regions (Sept. - Oct.) of these fish were due to declining water temperatures, not a maximum fish size constraint. Validation results indicate that additional, complicating environmental and/or feeding variables were differentially impacting the two fish populations of this exercise to some degree.

Table 8.6. Calibration and validation data sources and culture conditions for the production of common carp (*Cyprinus carpio*)

Szumiec and Szumiec (1985): Figure 8.39	
Data (time series)	Fish weights (Szumiec and Szumiec, 1985), feeding rates (Szumiec, 1979b), and monthly mean water temperatures (Szumiec, 1979a)
Location	Golysz experimental station, Poland (1969 - 1974)
System	Earthen, research carp ponds: 1500m ² , 1.5m depth
Fish culture	YC 1-2: Fish stocked at 90 g/fish mean weight YC 2-3: Fish stocked at 272 g/fish mean weight Comparable feeding intensities (as percent of maximum ration) were assumed for the two fish populations.
Production period	YC 1-2: June 9 – Oct. 9 (JD 160 – 282; 122 days) YC 2-3: June 15 – Oct. 7 (JD 166 – 280; 114 days)
Fish modeling	DSGR model: $\log_e(\text{SGR}) = [k_1 + k_2 T + k_3 T^2] - [\text{SGR}_e \log_e(W_{gm})]$ YC 1-2: $k_1 = -18.3836$, $k_2 = 1.522321$, $k_3 = -0.03755$, $\text{SGR}_e = -0.17697$ YC 2-3: $k_1 = -5.47294$, $k_2 = 0.546189$, $k_3 = -0.01115$, $\text{SGR}_e = -0.83762$

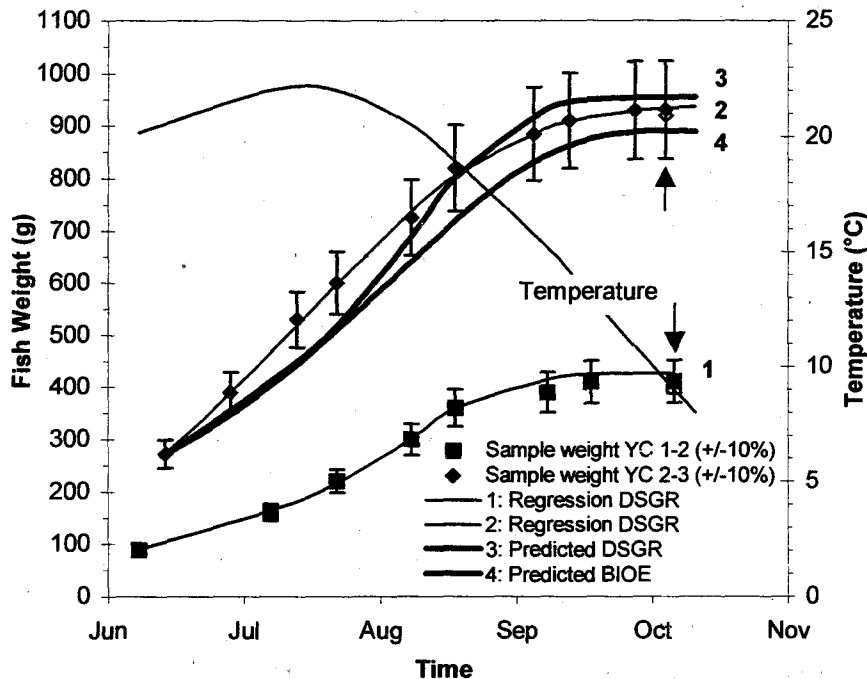


Figure 8.39. (1 and 2) Calibration of the DSGR fish growth model (common carp) with data from Szumiec and Szumiec (1985) for two fish year classes, (3) predicted fish weights by the DSGR model calibrated with data from the younger age class, and (4) predicted fish weights by the BIOE model calibrated with data from the younger age class (Nath, 1996; hollow data points indicated by arrows represent differences in the dataset as used by Nath)

8.4.3 Tilapia growout

The DSGR model was applied to tilapia growout under intensive culture (water recirculation system), for which fish growth rate was limited at fish weights greater than 400-g due to the reduction of feed application to fish tanks (Figure 8.40) (see Table 8.7 for application conditions). Feed application was reduced in response to degraded water quality, due to the maximum feed-loading capacity of the particular system under study being reached (Losordo, 1997). A case of improper application of the DSGR model is illustrated by the poor calibration fit achieved when the DSGR was applied to the entire sigmoidal curve without the use of a feed availability scalar (Figure 8.40, case 3; note that the SGR_e value of -0.77 exceeds its normal range). An improved calibration fit was achieved by (1) using data through day 150 to calibrate the DSGR model (satiation feeding) and (2) then applying the DSGR model to the entire growth period using a feed application limit (kg feed/m³/day). The feed application limit, if applicable, is based on the water treatment capacity of the fish culture system and is highly site-specific (e.g., 1 – 3 kg feed/m³/day for intensive systems).

Table 8.7. Calibration and validation data sources and culture conditions for the production of Nile and hybrid tilapia (*Oreochromis* spp.)

Losordo (1997; <i>O. niloticus</i> and <i>O. niloticus</i> x <i>O. aureus</i>): Figure 8.40				
Data (time series)	Fish weights			
Location	Fish Barn, North Carolina State University, Raleigh, North Carolina, USA			
System	Intensive recirculation system, 21 m ³ tanks, water temperature 28 – 32 °C, whole system water exchange 5-7 %/day			
Fish culture	Prepared feed applied at satiation feeding rates (assumed) up to a maximum system capacity			
Production period	240 days			
Fish modeling	DSGR model: $\log_e(\text{SGR}) = \text{SGR}_c - [\text{SGR}_e \log_e(W_{gm})]$, where water temperature considered to be in optimal range: Use of data to day 150: $\text{SGR}_c = -1.741000$, $\text{SGR}_e = -0.44861$ Use of data to day 240: $\text{SGR}_c = -0.749991$, $\text{SGR}_e = -0.77072$			
Diana et al. (1993; <i>O. niloticus</i>): Figures 8.41 and 8.42				
Data (time series)	Fish weights, feed application rates, water temperatures, and water quality			
Location	Bang Sai, Thailand: latitude = 14°11', altitude = 5.0 m			
System	Earthen ponds (250 m ²) with static water with loss makeup			
Fish culture	Fish stocked at 25.7 g/fish mean weight and 2 fish/m ² , fish harvested at 326 g/fish mean weight, satiation feeding with high quality feed, fish survival was 95%, and fish density declined from 2 to 1.9 fish/m ²			
Production period	Nov. 18 year one to Mar. 19 year two, (JD 322 – 443; 122 days)			
Fish modeling	<ul style="list-style-type: none">• DSGR model: $\log_e(\text{SGR}) = \text{SGR}_c - [\text{SGR}_e \log_e(W_{gm})]$, generic Nile tilapia model separately calibrated, where water temperature considered to be in optimal range, $\text{SGR}_c = -1.7$, and $\text{SGR}_e = -0.43$• Feed model: FCE = 70%• NFP model: 35 kg/ha/d available, 733 kg/ha CSC, 2200 kg/ha CC• Dissolved oxygen scalar: minimum optimum and tolerance DO = 50 and 10 % saturation (applied to daily mean DO)			
Diana et al. (1990; <i>O. niloticus</i>): Figure 8.43 and 8.44				
Data (time series)	Fish weights, water temperatures, and water quality			
Location	Bang Sai, Thailand: latitude = 14°11', altitude = 5.0 m			
System	Earthen ponds (250 m ²) with static water with loss makeup			
Fish culture	Fish stocked at 33-34 g/fish mean weight and 1, 2, and 3 fish/m ² , fish survival was 90%, and chicken manure was applied at 500 kg/ha/wk			
Production period	Feb. 2 to July 2, (JD 33 – 183; 151 days)			
Fish modeling	DSGR model: $\log_e(\text{SGR}) = \text{SGR}_c - [\text{SGR}_e \log_e(W_{gm})]$, generic Nile tilapia model separately calibrated, where water temperature considered to be in optimal range, $\text{SGR}_c = -1.7$, and $\text{SGR}_e = -0.43$			
NFP parameters	Fish density (fish/m ²)	Maximum potential FBP (kg/ha/day)	CSC fish density (kg/ha)	CC fish density (kg/ha)
	1	35	600	x 3 = 1800
	2	35	733	x 3 = 2200
	3	35	867	x 3 = 2600

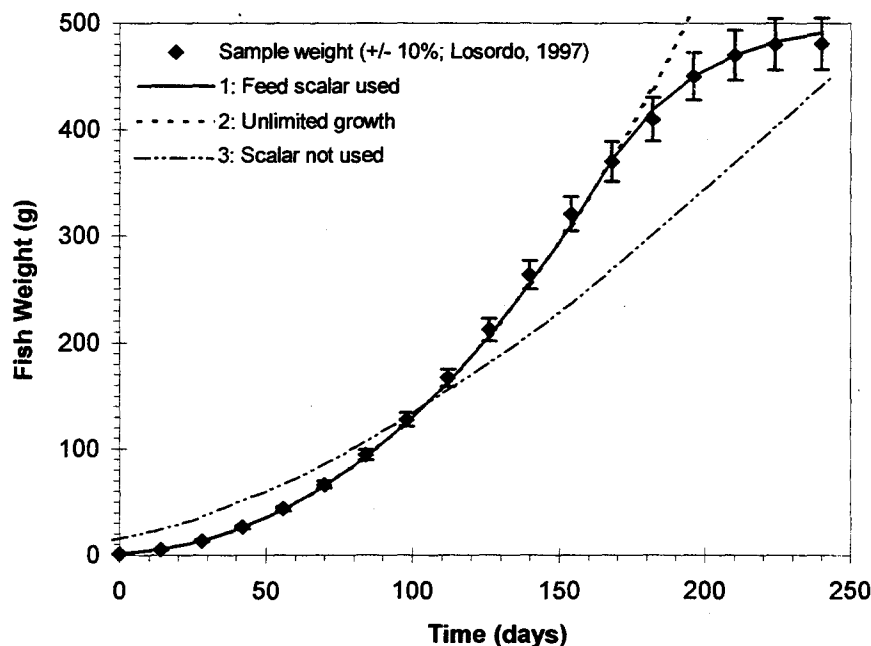


Figure 8.40. Calibration of the DSGR fish growth model (Nile and hybrid tilapia) with data from Losordo (1997) using (1) feed application rate scalar, (2) data to day 150 only, and (3) all data and no scalar terms

Whether or not a given limit is reached depends on fish biomass density and feeding rates (% fish body weight per day). A terminal, asymptotic growth stanza results when a feed application limit is reached, because as fish weight continues to increase, the reduction in feed availability represents an increasingly greater proportion of the satiation feeding level. A model calibrated for satiation feeding can be generally applied to feed-limited systems by setting the maximum feeding rate to the site-specific level. Alternatively, fish biomass density or water quality scalars can be used to limit fish growth, depending on the analysis resolution level in use. A maximum fish-size scalar could be used to give the terminal asymptotic stanza, but it would not represent the maximum maturation size under the conditions of this exercise.

A second validation exercise concerned tilapia growout in static-water ponds using application of prepared feeds to appetite satiation levels (Figures 8.41 and 8.42) (see Table 8.7 for application conditions). In this study, Diana et al. (1993) reported that fish growth was limited due to periods of low dissolved oxygen concentration (DO) when feeding rates reached higher levels. This study was simulated using a solar-algae pond ecosystem model, with DO modeling (daily, water column mean DO) and inclusion of DO in the DSGR model as a water quality scalar. Predicted results compared well to empirical observations when the minimum optimum DO level for fish was set to 50%

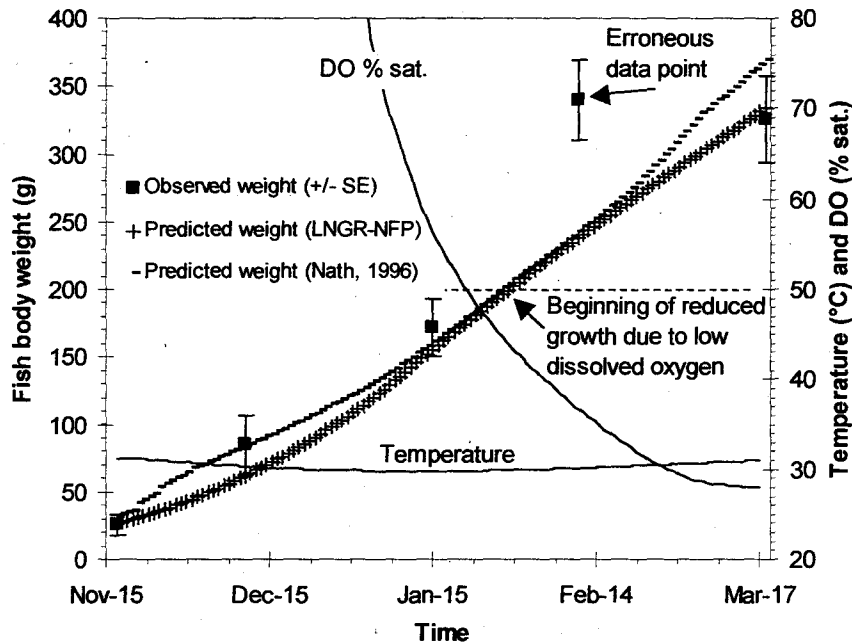


Figure 8.41. Predicted fish weights by the DSGR model (Nile tilapia), for which growth rates were scaled at sub-optimal dissolved oxygen concentrations (predicted fish weights by the BIOE model also shown; Nath, 1996)

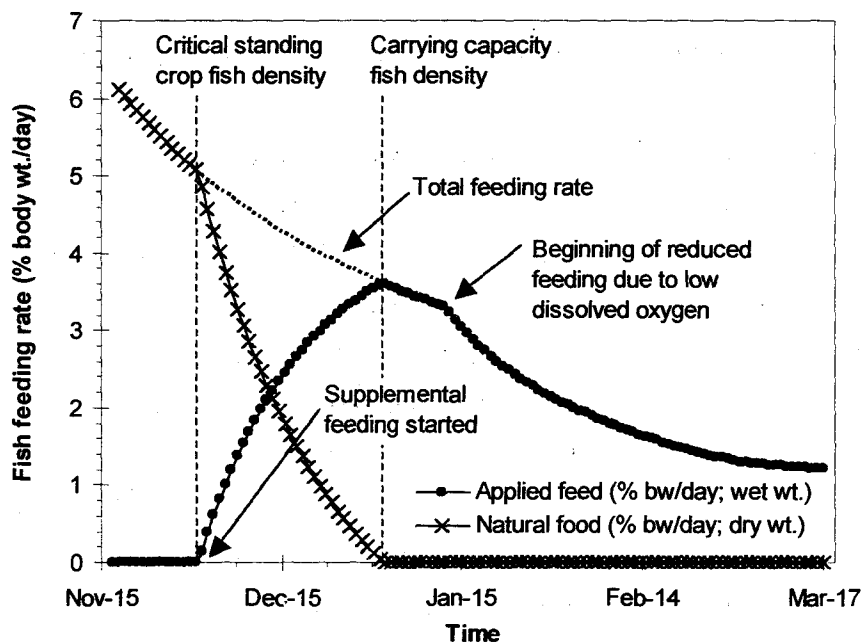


Figure 8.42. Predicted fish feeding rates by the DSGR model and 70% FCE, for which feeding rates were scaled at sub-optimal dissolved oxygen concentrations

saturation (applied to daily mean DO). Predicted daily mean DO levels declined to 28 % saturation (about 2.0 mg/L) under these conditions.

Figure 8.42 shows the predicted fish feeding regimes for this exercise, illustrating the decline in natural food and increasing requirement for supplemental, prepared feed as fish density increased over time. Simulation results showed a peak rate of 3.6 % bw/day for prepared feed, a maximum feed application rate of 93 kg/ha/day, and a food conversion efficiency for prepared feed of 78%. Diana et al. (1993) reported that feeding rates were set such that they declined from 5 to 2 % bw/day over the culture period. It is not clear if the predicted feeding rates were too low or if the supporting study did not account for the initial contribution of natural foods.

The erroneous data point identified in Figure 8.41 is typical of pond production studies for tilapia (Hopkins and Yakupitiyage, 1991) and likely for other fish as well, where smaller fish can more easily escape weight-sampling procedures using pond seining. Final samples of fish production studies (end of culture period) are often determined by complete pond inventories (e.g., harvests) and therefore provide definitive data points. The potential for this observational error in empirical study data must be kept in mind when calibrating growth models, as it incorrectly implies a final asymptotic growth stanza.

A final exercise for tilapia production concerned tilapia growout in static-water ponds, for which simulation conditions were matched to the experimental conditions used by Diana et al. (1990) (see Table 8.7 for application conditions). These conditions included fertilization (chicken manure) for enhancement of primary productivity, no use of prepared feeds, and three stocking densities of one, two, and three fish/m². This study was simulated using natural fish productivity (NFP) in conjunction with the DSGR model, as described in Chapter 7 (see Figure 7.5). Values for carrying capacity fish densities (CC) were set to approximate the asymptotic fish density and values for critical standing crop fish densities (CSC) were set at one-third of CC values (Figure 8.44). Results showed that the combined DSGR-NFP growth model could be calibrated to give reported results and that the derived CSC and CC values exhibited a functional progression with respect to fish density. Apparently, as fish stocking density was increased, the availability of natural foods on a per volume basis also increased. This implies that higher numbers of smaller fish are more efficient at ingesting and/or digesting natural foods than an equivalent biomass of larger fish. An expanded scope of calibration is needed to derive mean and standard deviation statistics for CSC and CC values across a range of fish species and densities.

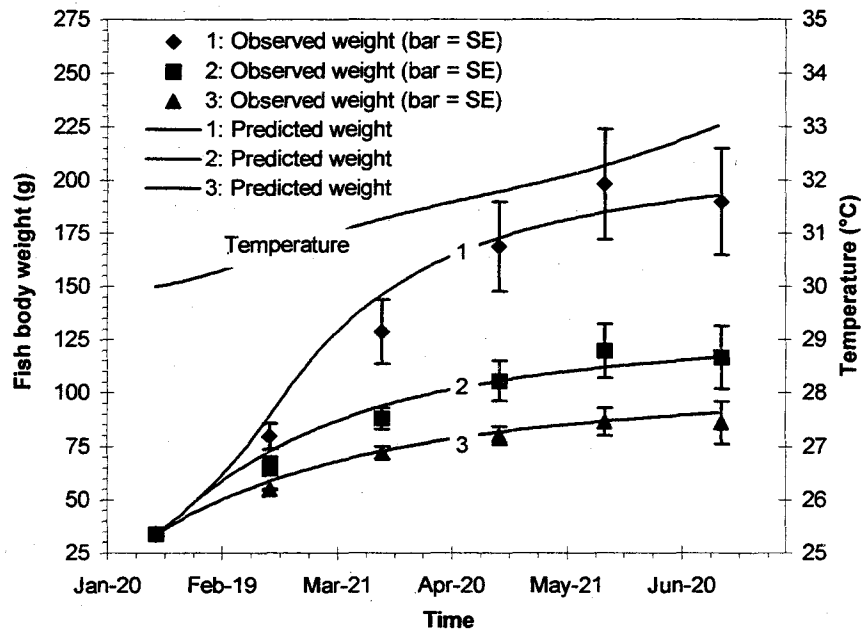


Figure 8.43. Predicted fish weights by the DSGR-NFP model (Nile tilapia), for three fish stocking densities: (1) 1.0 fish/m², (2) 2.0 fish/m², and (3) 3.0 fish/m²

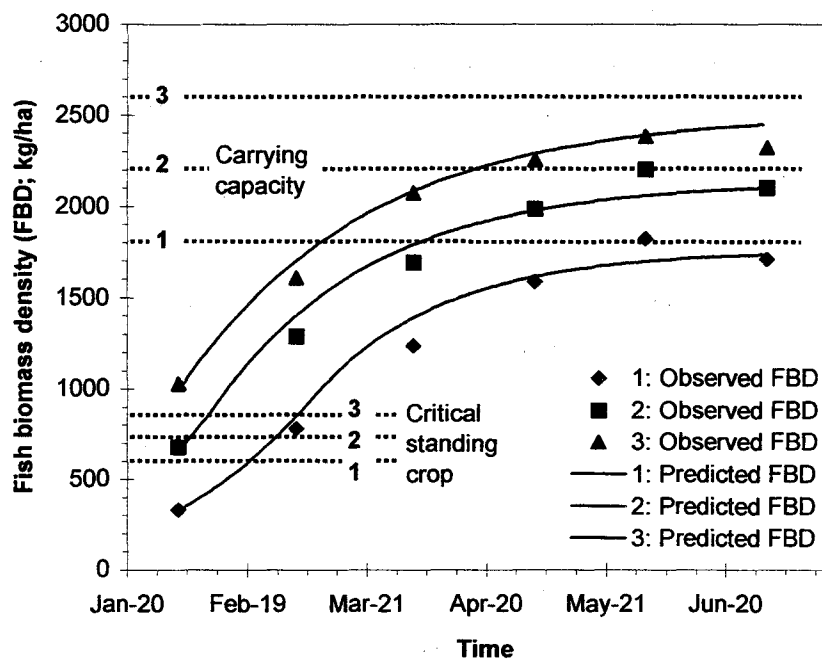


Figure 8.44. Predicted fish biomass densities by the DSGR-NFP model (Nile tilapia), for three fish stocking densities: (1) 1.0 fish/m², (2) 2.0 fish/m², and (3) 3.0 fish/m², showing the respective critical standing crop and carrying capacity fish densities used in the NFP model

8.4.4 Fish weight distribution modeling

Methods used to model fish weight distributions, and typical trends in these distributions in response to fish culture conditions, were described in Chapter 7. Simulation exercises for qualitative validation of weight distribution modeling are described here. Quantitative calibration and validation of the fish performance index (FPI) and feed competition index (FCI) parameters used in this model remain to be completed. Preliminary simulation trials showed that an FPI of about 1.1 to 1.3 and an FCI of about 1.5 provided reasonable results.

The predicted response of the coefficient of variation for fish weight (CV, %; $CV = 100 \text{ SD} / \text{mean}$, where SD = standard deviation) to FPI conformed to expected patterns (Figures 8.45 and 8.46). Conditions for this exercise included: Nile tilapia DSGR growth model, constant temperature, satiation feeding, growout from 1.0 to 400+ g, and initial CV 20%. Growth compensation (decrease in CV) and growth depensation (increase in CV) (Ricker, 1975) of varying degrees were predicted in accordance with varying degrees of genetic variability in growth potential. Empirical results reported by Ernst et al. (1989) for tilapia growout under satiation feeding (1-g to 470-g fish in 170 days), for which weight variability decreased from a CV of 44% to 25%, were matched by simulation using an FPI of 1.25. Using these same conditions at a range of feeding rates, where FPI was 1.1 and FCI was 1.5, a second exercise yielded the expected trend of an increase in weight variability in response to a decrease in food availability and increase in feeding competition (Figures 8.47 and 8.48). As food availability was successively reduced over a series of simulations, weight CV went from a declining trend (with time) to incrementally higher increasing trends and weight distributions expanded and skewed toward higher weights.

Whether weight distributions expand or contract, when individual fish lots are divided or combined, their fish weight distributions are also divided or combined. Divided distributions are truncated at the fish grade size, and combined distributions become multi-modal. In both cases, all resemblance to normal distributions is typically lost and distribution profiles may become markedly uneven (e.g., Figures 8.49, 8.50, and 8.51). The use of histograms (versus distribution functions) to represent these fish weight distributions is clearly required. Distribution recalculation for reducing the number of histogram bins for combined fish lots is illustrated by comparing Figures 8.50 (before compression) and 8.51 (after compression). Some resolution is lost in this recalculation, but the use of more than 30 distribution bins to model a single fish lot would not likely have significant impact on the accuracy of predicted results. Therefore, the additional calculation intensity required for uncompressed distributions would not be justified.

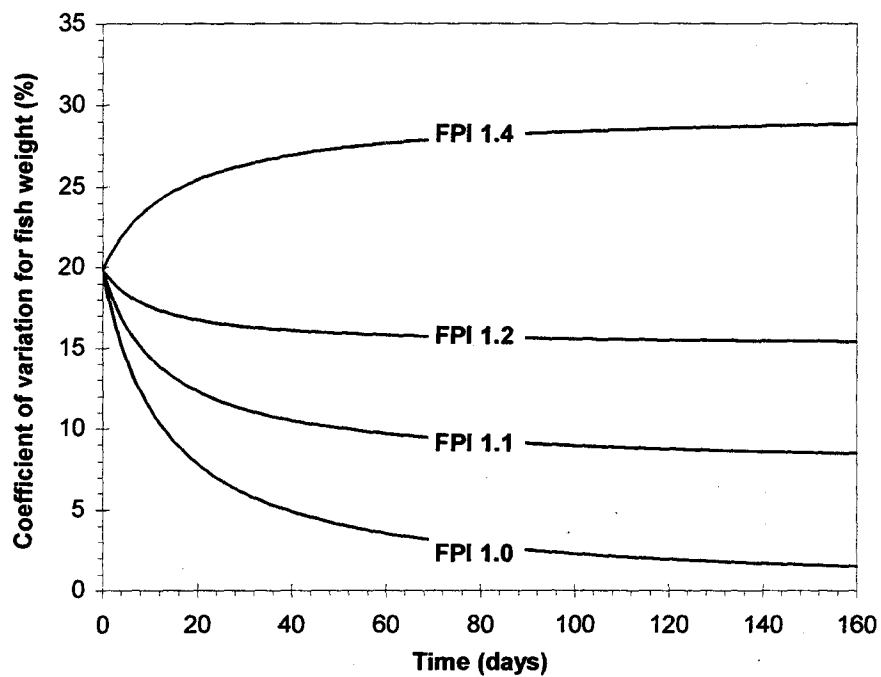


Figure 8.45. Predicted coefficient of variation for fish weight over the fish culture period, using a range of values for fish performance index (FPI)

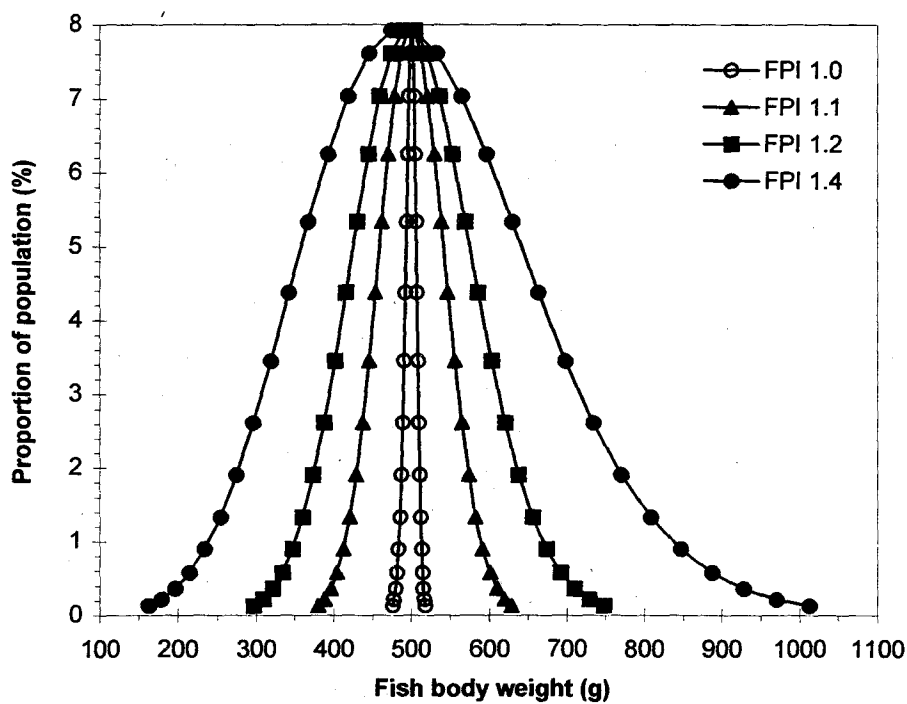


Figure 8.46. Predicted distributions for fish body weight at the end of the culture period, using a range of values for fish performance index (FPI)

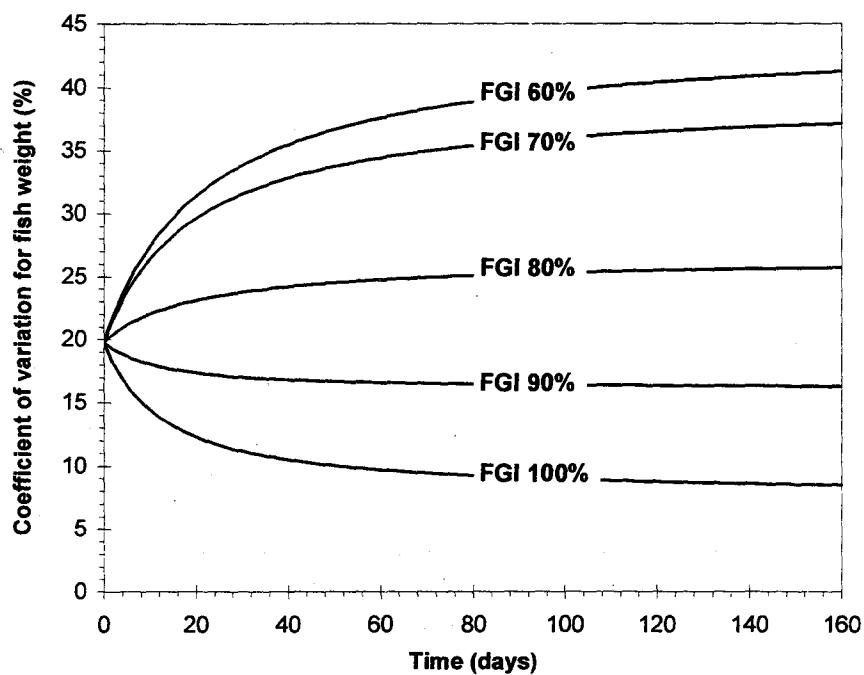


Figure 8.47. Predicted coefficient of variation for fish weight over the fish culture period, using a range of values for fish growth index (FGI; FPI = 1.1 and FCI = 1.5)

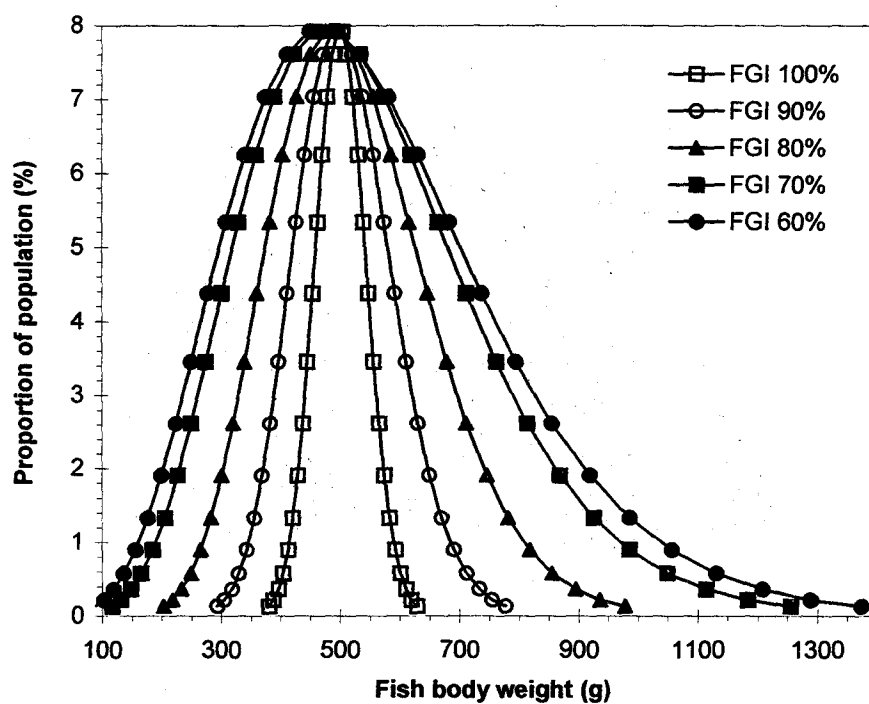


Figure 8.48. Predicted distributions for fish body weight at the end of the culture period, using a range of values for fish growth index (FGI; FPI = 1.1 and FCI = 1.5)

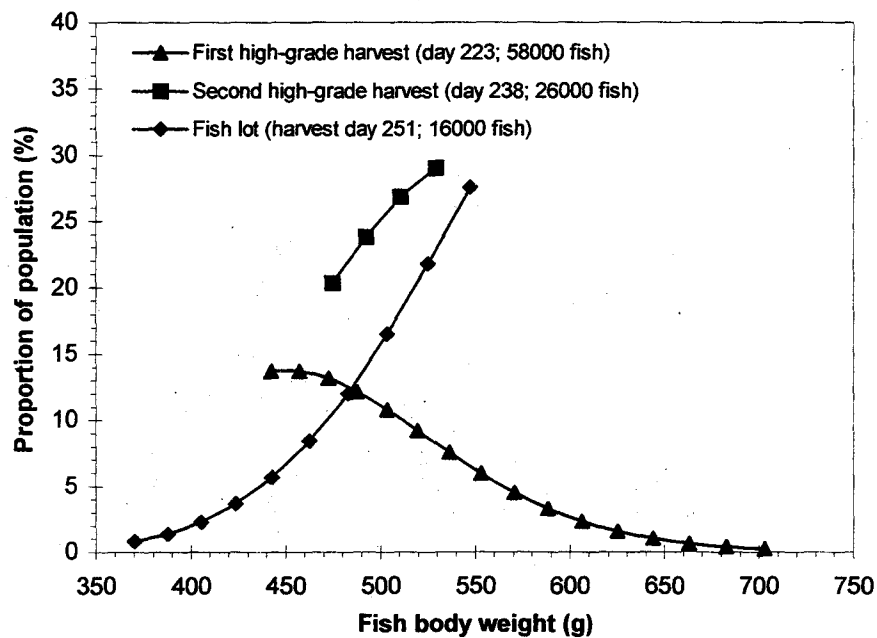


Figure 8.49. Predicted distributions for fish body weight for three harvest groups from the same fish lot, consisting of two high-grade harvests and a final complete harvest

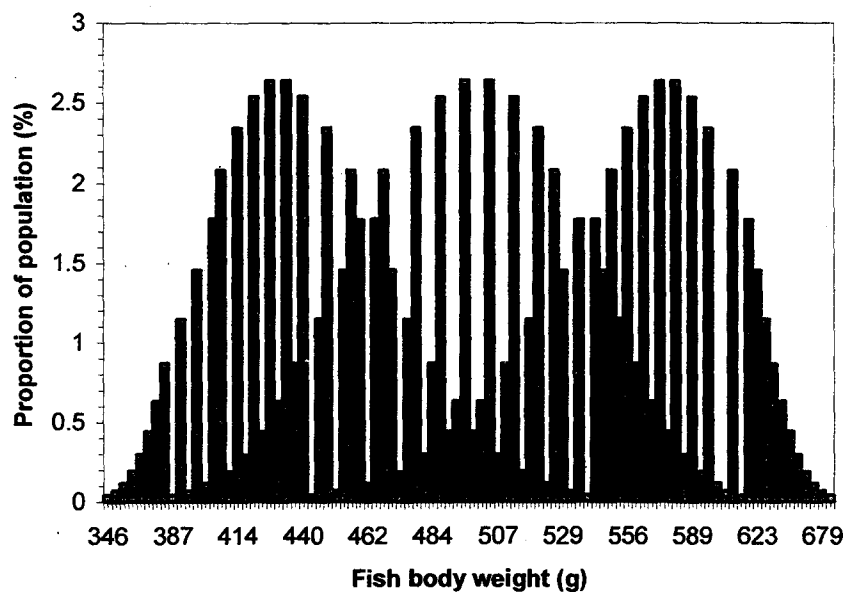


Figure 8.50. Predicted distribution for fish body weight at the end of the culture period, for a fish lot that had two fish lots combined into it over the course of the culture period and weight distributions were combined without combining the bins of the distributions (90 bins)

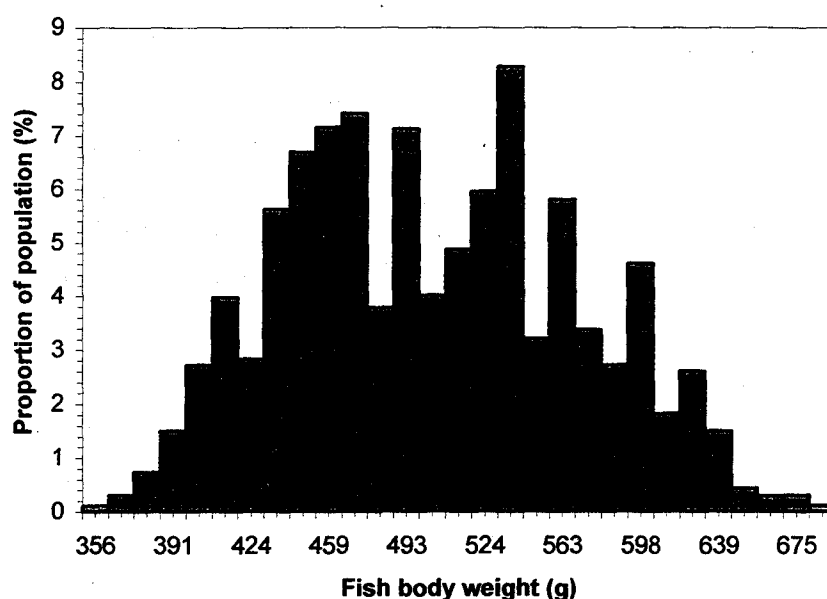


Figure 8.51. Predicted distribution for fish body weight at the end of the culture period, for a fish lot that had two fish lots combined into it over the course of the culture period and weight distributions were combined with bin recalculation (30 bins)

8.5 System-level validation

In the prior section, validation exercises were focused on isolated unit processes or closely associated groups of unit processes. Some additional validation considerations and exercises are described below, for which the simulation context includes additional processes of fish rearing units and their linkage into aquaculture facilities. This follows a short discussion of findings regarding the use of alternative simulation processing methods and the behavior of process control.

8.5.1 Simulation processing

In the application of AquaFarm to a full range of aquaculture system types (extensive to intensive), it was found that simplified, analytical-Eulerian integration, using 1-day and 1-hr time-steps for daily and diurnal simulations, provided results that normally matched those achieved by more rigorous, fourth-order Runge-Kutta integration (RK4; Elliot, 1984). As described in Chapter 3, the simplified integration method represents Eulerian numerical integration (Elliot, 1984), for which the accuracy of finite difference terms is enhanced by the use of analytical integration where

possible. These results indicate that for the simulation of aquaculture systems in general, using 1-day and 1-hr time-steps for daily and diurnal simulations, rates of change of state variables are typically low enough that the simplifying assumptions used to uncouple some simultaneous processes and first-order reactions are sufficiently supported.

Simplified integrations were found to fail, as shown by negative and/or oscillating compound concentrations or water temperatures, for certain types of daily simulations using a 1-day time-step. Failures occurred within short-term periods (e.g., 1-5 days) during the first few days of a simulation or when high water flow rates were suddenly started or stopped in conjunction with fish stocking and harvest (or release). RK4 numerical integration for daily simulations using a 1-day time-step was also found to fail under such extreme conditions, although it is considerably more robust than the simplified approach. In general, discrete events have the potential to create disequilibria, cause high rates of change of state variables, and require reduced time-steps. To avoid the use of a reduced time-step for an entire simulation due to short-term constraints, methods were added to AquaFarm so that a time-step of one-tenth the size of the user specified time-step (e.g., 0.1 days) is used for the first five days of a daily simulation and for one day following any major fish additions or large changes in water flow rates. This functionality is transparent to the user and the frequency of collection of simulation-generated data is held constant.

Simplifying assumptions of analytical-Eulerian integration consist of the unlinking of some simultaneous processes and representation of some first-order processes as constants within a simulation time-step. Simultaneous linkage between facility units consists of water flow between facility units. However, at time-steps of 1-day for daily simulations and 1-hr for diurnal simulations, it was typically found that simulation results were not significantly impacted by consideration of advective linkage. Therefore, influent water quality for a given facility unit could be considered constant within a simulation step, using the current effluent water quality of upstream facility units(s) (facility units are simulated in the order of up to down stream).

A third method of integration, consisting of combined analytical and RK4 numerical integration (Chapter 3), was successful in using much larger time steps (e.g., ten fold) than allowed by RK4 integration alone, while achieving identical results. This offered a considerable reduction in required calculation intensity and prompted the removal of purely numerical RK4 integration from further use. This left two, alternative integration methods available in AquaFarm, consisting of either Eulerian or RK4 numerical integration aided by analytical integration where possible.

In summary, a significant degree of interaction of simultaneous processes both between and within facility units clearly exists, but not of such a magnitude that modeling of these processes cannot be somewhat simplified. The use of 1-day and 1-hr time-steps for daily and diurnal simulations, respectively, as required to simulate facility management and to provide the needed periodicity in simulation generated data, constrains the simulation time-step to a degree such that the mathematical constraints of integration are largely satisfied.

8.5.2 Control of active processes

As described in Chapter 3, process control methods include (1) constant rate, (2) on-off with a fixed on rate, (3) proportional (throttled) process control (variable on rates), and (4) proportional integral-derivative control (PID controllers). Any of these methods can be managed manually or automatically, where the use of manual control assumes that the human counterpart of the simulated facility manager carries out the necessary calculations. The only difference between static and flowing water conditions is that the latter has an advective load component. For compound addition and the application of active heat transfer, method validity was confirmed by achievement of specified set-point concentrations for a variety of water quality and static and flowing water conditions. Furthermore, simulation results yielded expected behaviors for the alternative process control methods. For example, PID controllers are used to minimize oscillation of the controlled variable around its set-point level (Heisler, 1984). This effect was demonstrated by diurnal simulation of water chilling under a diurnally varying heat load (ambient climate) (Figure 8.52). The relatively superior performance of PID control was found to be even more pronounced when loading rates were varied to a greater degree. The performance of simulated PID was found to be somewhat dependent on the simulation time-step, as illustrated by the lack of a flat line for PID control in Figure 8.52. Actual controllers use sampling rates on the order of seconds to milliseconds, in contrast to the 1.0-hr time-step used to generate Figure 8.52.

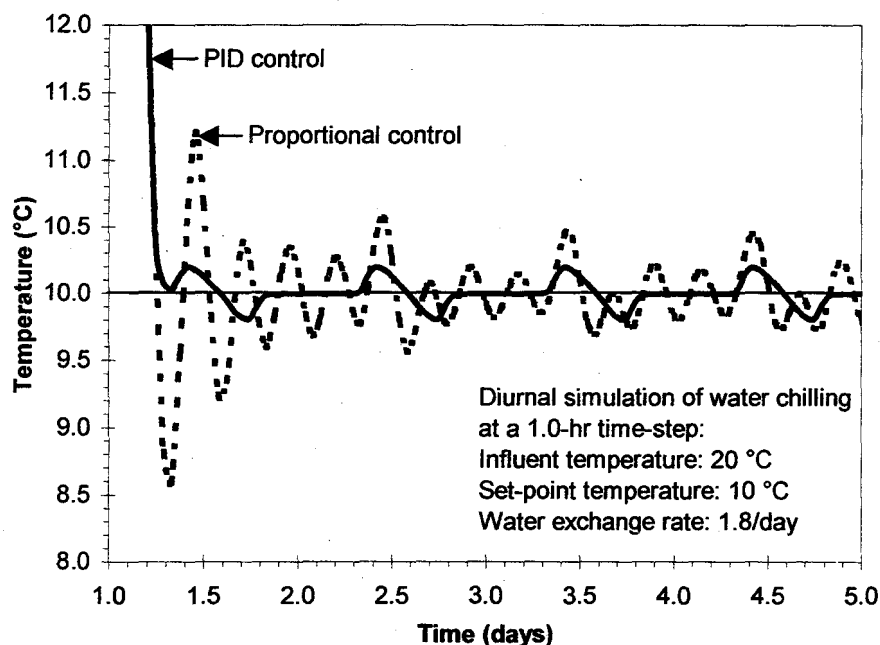


Figure 8.52. Diurnal simulation of water chilling under a diurnally varying heat load (ambient climate)

8.5.3 Selected case studies

Application of AquaFarm to various aquaculture systems and engineering analyses is demonstrated in the following examples. For each exercise, site-specific design specifications and management strategies were entered into AquaFarm, and standard parameter values were generally used for unit-process models. Simulations were then used to generate fish culture schedules, chronologies of state variables and processes, and required resources to achieve production objectives. Finally, predicted performance data were compared to empirical data from representative studies in the literature.

Reporting of the specifications and results of these simulation exercises is limited to overviews, with a focus on core issues of fish performance and dominant facility processes. The specifications and results presented illustrate the range of detail and analytical capacities available in AquaFarm. The design procedure presented in Chapter 2 is not demonstrated in these exercises, and the results of a single simulation are presented for each system type. Enterprise budgets are not presented, for which unit costs are highly specific to location and budget formats were described in Chapter 2. While not shown, however, any of these examples could use a series of simulations to

consider resource use, management intensity, and budgetary requirements over a range of fish production levels and alternative design and management strategies.

For all of these exercises, the accuracy of simulation results relative to empirical observations was dependent on the accuracy of site-specific specifications. When simulation results are said to be comparable to the referenced studies, it is meant that these results were within reported ranges and showed similar cause-and-effect behavior between independent and dependent variables. Conclusions for these exercises include the caveat that fully comprehensive reporting of methods and results were not available in the studies used, as is typically the case in technical papers, requiring the estimation of some design and management variables.

Given the scope and resolution of AquaFarm, required levels supporting data for calibration and validation procedures are considerable and present an ultimate constraint to this endeavor. Ideally, these datasets should include complete descriptions of environmental conditions, system components, management protocols, and resulting fish and facility performance variables. For intensive, water reuse and recirculating aquaculture systems, most available research has been conducted on individual unit processes or system components, and calibration and validation efforts must often proceed at this level. System level studies are mainly available as technical papers, which generally lack sufficient reporting of methods and results to support detailed calibration and validation exercises. In contrast, for extensive and semi-intensive, pond based aquaculture, publicly available databases are available and their usefulness in the development of pond simulation models and decision support systems has been demonstrated (e.g. Froese and Pauly, 1996; Piedrahita et al., 1997; Ernst et al., 1997; Ernst and Bolte, 1999; Bolte et al., 1999). In addition, many technical papers available for pond based aquaculture contain fairly comprehensive reporting of methods and results, given that their scope can normally be limited to individual ponds with no need to consider integrated water transport and treatment systems. However, results from pond studies can also be more difficult to interpret, given the stochastic nature of these systems, the difficulty of isolating individual unit processes (e.g. components of oxygen mass balances), and the difficulty of monitoring site-specific conditions and processes such as pond micro-climates, soil processes, sediment accumulation, nitrogen fixation and denitrification, and water seepage.

8.5.3.1 Tilapia production in ponds

AquaFarm was applied to the production of Nile tilapia (*Oreochromis niloticus*) in tropical (10 - 15° latitude) solar-algae ponds. Conditions of this exercise are provided in Table 8.8. Diurnal simulations were used and water stratification was considered. Agriculture limestone (calcium carbonate) and fertilizer were applied to maintain DIC (in terms of alkalinity), DIN, and DIP nutrient levels for primary productivity. Fertilized ponds received lime and fertilizer only. Fertilized-fed ponds received lime and fertilizer by the same management criteria as fertilized ponds, with additional application of pelletized feed as required to achieve target fish growth rates. Fertilizer consisted of combined chicken manure and ammonium nitrate, with the latter added to achieve a nitrogen-phosphorous ratio of 5.0, based on the nitrogen and phosphorous contents of the chicken manure (Kwei Lin et al., 1997).

Similar to the tilapia production exercise described earlier, simulations used natural fish productivity in conjunction with the DSGR growth model. For fertilized ponds, critical standing crop (CSC, 1600 kg/ha) with respect to natural food resources occurred at the peak fish biomass productivity (FBP) and inflection point of fish growth rate (Figure 8.53). For fertilized and fed ponds, CSC (1600 kg/ha) with respect to natural food resources was achieved, followed by a short decline in FBP until the onset of supplemental feeding. For all ponds, simulated fish growth rates, total production per hectare, fish density at the onset of feeding, and required feed application rates were comparable to reported results (Diana et al., 1996; Diana, 1997; Kwei Lin et al., 1997).

Predicted water quality regimes and fertilizer and feed requirements were comparable to reported values for tilapia production under similar site and management conditions. As expected, total lime application rates were in the low range of reported rates (Boyd, 1990; Boyd and Bowman, 1997), for which pond source water had low alkalinity but soils were assumed to already be neutralized with respect to exchange acidity (base unsaturation). The nitrogen and phosphorous application rates used were within reported ranges for tilapia production in fertilized ponds, which range from 2.0 to 4.0 kg N/ha/d at N:P ratios that range from 1:1 to 8:1 (Kwei Lin et al., 1997).

Fish production and application of fertilizer and feed were adequately estimated using a daily time-step with no consideration of water stratification. However, as generally found for solar-algae ponds, diurnal simulations and consideration of stratification were required to estimate extremes in water quality regimes. Diurnal profiles of temperature and dissolved oxygen (Figure 8.54; mid summer), were comparable to reported profiles for stratified tropical ponds (Losordo and Piedrahita,

1991; Piedrahita et al., 1993; Culberson and Piedrahita, 1994). Diurnal, stratified profiles of temperature and dissolved oxygen are shown in Figure 8.55, for the top layer, bottom layer, and water column mean. Daily water-column turnover occurred from approximately midnight to 0900. The maximum divergence in water quality between the top and bottom layers was controlled by the specified regime for the water mixing index (WMI, 1/day).

As found in this exercise and as generally the case for pond production systems, the prediction of pond nutrient budgets is hampered by the existence of poorly defined nutrient sinks. For example, reported nitrogen budgets typically include applied materials (stocked fish, fertilizers, and feeds), removed materials (harvested fish and removed solids), influent and effluent water, and initial and ending conditions for water and sediment nitrogen contents. Nitrogen losses through water seepage, nitrate denitrification and loss of nitrogen gas, and ammonia volatilization are not measured and are used to account for the missing nitrogen fraction in these budgets. Nitrogen gains through nitrogen fixation by blue-green algae are also not measured and are therefore included in this lumped fraction. Complicating this situation further, sediments and soils can be a major nitrogen sink but their consideration in reported studies is variable. The fraction of the total nitrogen loss attributed to these unmeasured sinks apparently ranges in the vicinity of 50% (Boyd, 1985; Briggs and Funge-Smith, 1994), clearly a major, if not dominate, budget component. Therefore, for simulations to predict representative nitrogen concentrations (ammonia and nitrate) in the water column and/or required fertilization rates, it is necessary to predict these poorly defined losses of nitrogen with some degree of accuracy. In the tilapia pond simulation exercise described here, nitrogen loss by nitrate denitrification, soil uptake, and ammonia volatilization were used, for which denitrification and soil uptake rates required some adjustment in order to achieve reported results. Similar concerns existed for phosphorous, for which soil uptake rates were also adjusted so that reported results were achieved. This calibration tuning detracts from the validation intent of this exercise, but the additional work needed in this area must be regionally, site, or even pond specific and is beyond the scope of this dissertation.

Table 8.8. Tilapia production in fertilized and fed ponds

Specifications	
Facility	<ul style="list-style-type: none"> • Location: 10 – 15° N latitude, low elevation • Weather: annual parameters for air temperature, cloud cover, precipitation, and water mixing index (stratification) • Source water quality: 20 mg/L alkalinity and equilibrium gas concentrations
Culture systems	<ul style="list-style-type: none"> • Levee type, clay lined ponds, 1.0-ha in area, and 1.0-m average depth • Water makeup to replace losses and maintain depth • Pond unit processes: water budget, passive heat transfer, seasonal water stratification, passive gas transfer, solids settling, primary productivity, bacterial processes (organic oxidation, nitrification, and denitrification), soil and seepage processes, and fish processes • Fertilizer composition: chicken manure with ammonium nitrate added to achieve an N:P ratio of 5.0, with a combined composition of 22.4% N, 4.48% P, and 70% dry wt. organic solids • Feed composition: 35% protein and 1.5% phosphorous • Fertilized ponds: agricultural limestone and mixed inorganic/organic fertilizer applied to maintain DIC (alkalinity ≥ 40 mg CaCO_3/L), DIN (≥ 1.0 mg N/L), and DIP (≥ 0.1 mg P/L), beginning 6 weeks prior to fish stocking • Fertilized-fed ponds: additional application of prepared feed as required to achieve target fish growth rates
Fish production objectives	<ul style="list-style-type: none"> • Culture period: March 1 to Oct. 1 (215 days) • Fish number: 10000 to 9000 fish/ha at 10% mortality • Fish weight: 1.0-g at stocking to weight available on Oct. 1 for fertilized ponds, and 1.0-g to 512-g target weight for fertilized-fed ponds
Results	
Fish production	<ul style="list-style-type: none"> • Fertilized pond applications: total lime applied 1870 kg/ha and fertilizer applied at a mean rate of 12.3 kg/ha/d (2.8 kg N/ha/d and 0.55 kg P/ha/d) over the pond pre-conditioning and fish rearing period • Fertilized-fed pond applications: total lime applied 1900 kg/ha, fertilizer requirements reduced about 10% compared to non-fed ponds, and supplemental feed applied at an increasing rate to a maximum of 65 kg/ha/d over the last 70 days of the culture period • Fertilized pond production: 332-g fish at 3000 kg fish/ha on Oct. 1 • Fertilized-fed pond production: 512-g fish at 4600 kg fish/ha on Oct. 1, 80% fish feeding index (% maximum ration) to achieve target weight, and 170% food conversion efficiency (based on applied feed only, mortality included) • Fertilized pond water quality (for fish culture period, including diurnal and stratification extremes): temperature 22 – 34 °C, pH 7.0 – 9.5, DO 2.8 – 14.5 mg O_2/L, DC 0.01 – 7.8 mg CO_2/L, NO_3 0.60 – 0.74 mg N/L, TAN 0.25 – 0.53 mg N/L, NH_3 0.01 – 0.25 mg N/L, phytoplankton 8.5 – 10.8 mg C/L, NPP -0.5 – 6.0 g $\text{C}/\text{m}^3/\text{d}$ (whole column) • Fertilized-fed pond water quality (for fish culture period, including diurnal and stratification extremes): similar to fertilized pond, except DO 1.6 – 14.5 mg O_2/L, pH 6.9 – 9.5, DC 0.01 – 10.3 mg CO_2/L

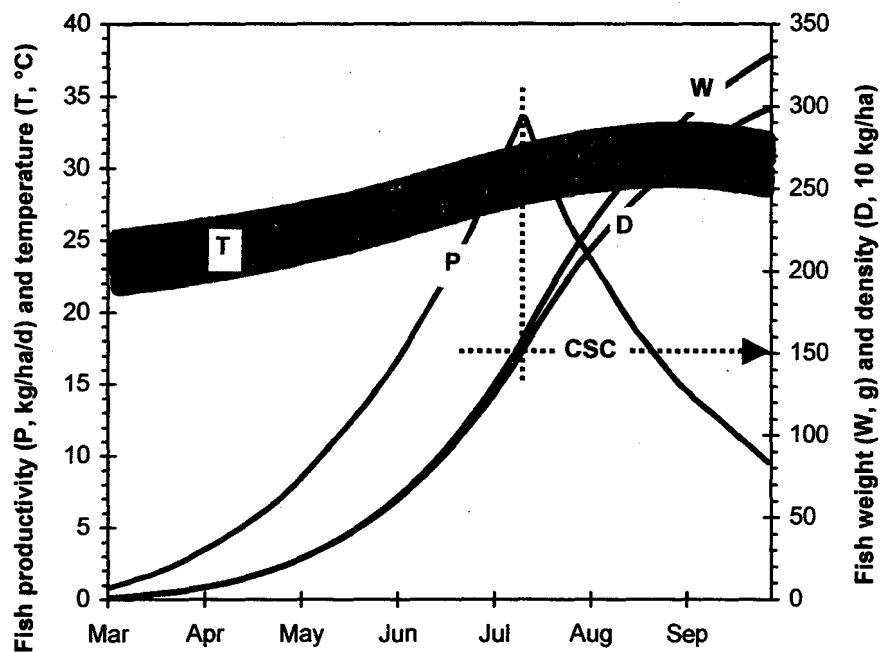


Figure 8.53. Simulated data (1-hour time step) for tilapia production in fertilized ponds over a 7-month culture period, for which the temperature band represents the diurnal temperature regime

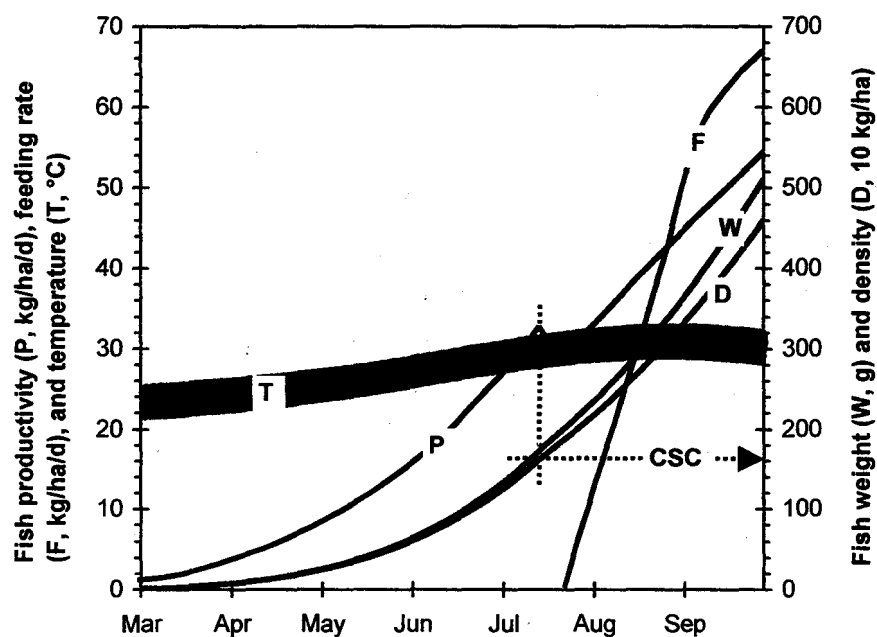


Figure 8.54. Simulated data (1-hour time step) for tilapia production in fertilized and fed ponds over a 7-month culture period, for which the temperature band represents the diurnal temperature regime

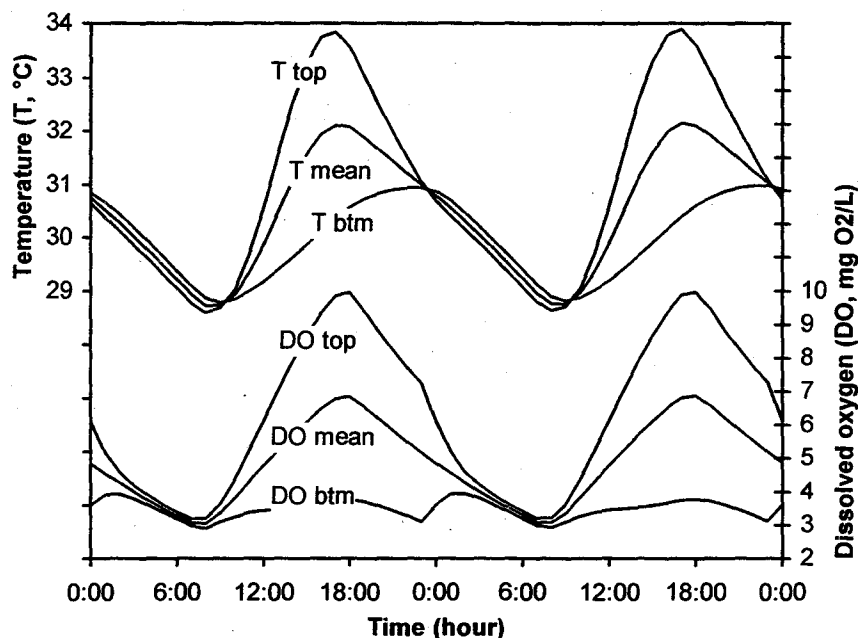


Figure 8.55. Simulated data (1-hour time step) for tilapia production in fertilized ponds, for a few mid-summer days within the 7-month culture period

8.5.3.2 Catfish production in ponds

AquaFarm was applied to the production of channel catfish (*Ictalurus punctatus*) in temperate (30° N latitude) solar-algae ponds. Conditions of this exercise are provided in Table 8.9. Diurnal simulations were used and water stratification was considered. Single fish stocking and harvest events were used to simplify this example, rather than the periodic high-grade harvesting and partial re-stocking methods typically employed for catfish production. Target fish numbers and weights were specified such that feed application rate increased to a maximum of 110 kg/ha/d, in order to emulate conditions used in Cole and Boyd (1986) and Tucker and van der Ploeg (1993). Aeration was used as required to maintain bottom-layer dissolved oxygen above a minimum level (30% saturation), for which aerator specifications were matched to Cole and Boyd (1986). The production period, from June 1 year 1 to October 31 year 2 (519 days) included a fish over-wintering period.

Feed application rates increased over the rearing period in association with increasing fish biomass density as well as varying with water temperature. Fish feeding and growth rates were within typical ranges (Tucker, 1985). Predicted water quality regimes and aeration requirements were comparable to reported values for catfish production (Cole and Boyd, 1986; Brune and Drapcho, 1991; Tucker and van der Ploeg, 1993; Schwartz and Boyd, 1994). Reported aeration

requirements were achieved (Cole and Boyd, 1986), including diurnal aeration timing, the maximum power requirement, and cumulative power use. Accurate prediction of active aeration required accurate specifications for the aerator size, standard aerator efficiency, and minimum allowed dissolved oxygen levels. In Figure 8.56 and 8.57, bands for water quality variables represent diurnal, stratified regimes. Means of the top and bottom layers of the water column are shown, daily water-column turnover is occurring, and bottom bands may overlay top bands to a large degree. In Figure 8.58, representing simulated oxygen budget data, diurnal water-column stratification and turnover are occurring. Oxygen budget components include top and bottom layer net primary productivity (NPP) and bacterial respiration (BR), passive and active gas transfer (PGT and AGT), and fish oxygen consumption. The accurate prediction of aeration requirements for this exercise indicates that the predicted oxygen budget was accurate.

Table 8.9. Channel catfish production in fed ponds

Specifications	
Facility	<ul style="list-style-type: none"> Location: 32° N latitude and 100 m elevation Weather: annual parameters for air temperature, cloud cover, precipitation, and water mixing index (stratification) Source water quality: 100 mg CaCO₃/L alkalinity and equilibrium gas concentrations
Culture systems	<ul style="list-style-type: none"> Levee type, clay lined ponds, 5.0-ha in area, and 1.0-m average depth Water makeup to replace losses and maintain depth Pond unit processes: water budget, passive heat transfer, seasonal water stratification, passive and active gas transfer, solids settling, primary productivity, bacterial processes (organic oxidation, nitrification, and denitrification), soil and seepage processes, and fish processes Aeration: on at ≤ 30% and off at ≥ 40% DO saturation based on water quality of bottom water layer, maximum aeration rate 6.25 kW/ha, and aerator SAE 1.2 kg O₂/kWhr
Fish production objectives	<ul style="list-style-type: none"> Culture period: June 1, year 1 to Oct. 31, year 2 (518 days) Fish number: 12000 to 10500 fish/ha at 12.5% mortality Fish weight: 1.0-g at stocking to 880-g target weight
Results	
Fish production	<ul style="list-style-type: none"> 80% fish feeding index (% maximum ration) 50% food conversion efficiency 9250 kg/ha maximum fish biomass density 110 kg/ha/d maximum feed application rate Aeration power use: total of 4260 kWhr/ha, for 672 total hours of operation, ranging from 2 to 7 hours per day over a period of 4 months Water quality (see Figures 8.56 and 8.57): DIN averaged 72% TAN and 28% NO₃, alkalinity 80 – 100 mg/L, and diurnal NPP -0.4 – 5.0 g C/m³/d (whole column)

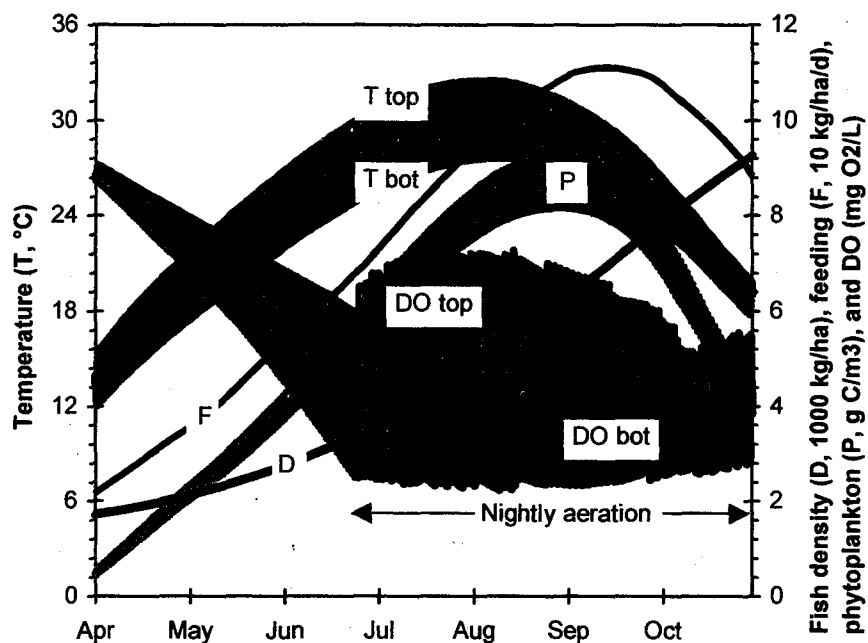


Figure 8.56. Simulated data (1-hour time step) for catfish production in fed ponds, showing the last 7 months of the 17 month culture period

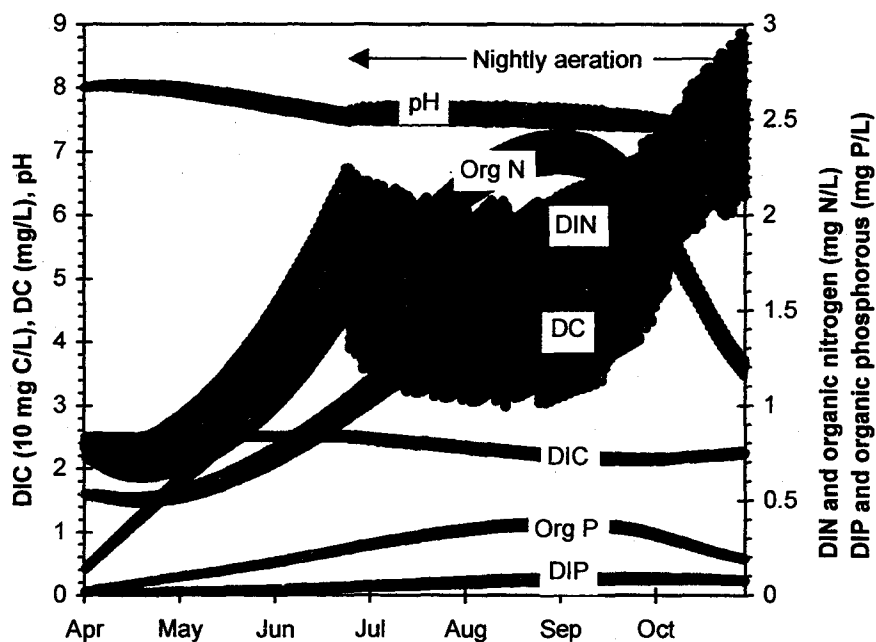


Figure 8.57. Simulated data (1-hour time step) for catfish production in fed ponds, showing the last 7 months of the 17 month culture period

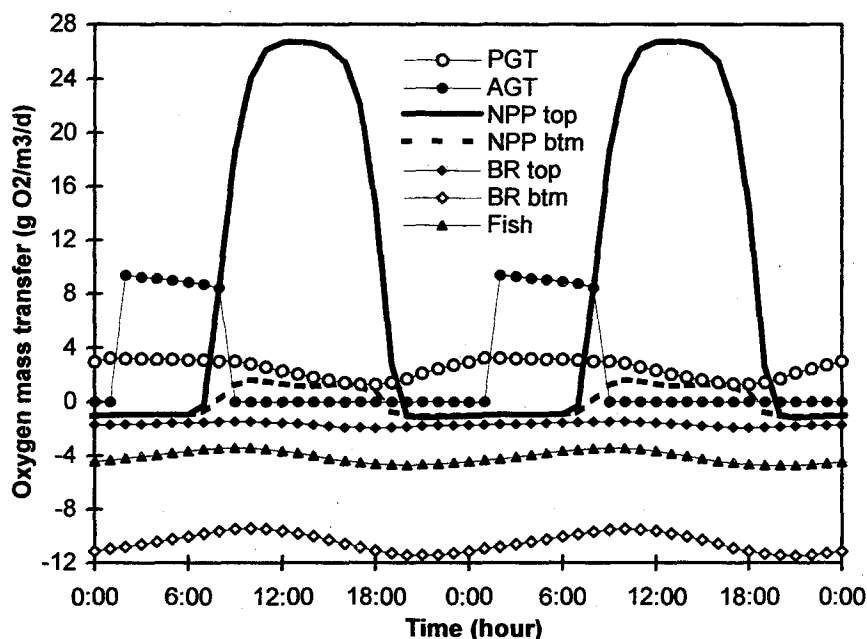


Figure 8.58. Simulated oxygen budget data (1-one hour time step) for catfish production in fed ponds, for a few days in late August in the last 7 months of the culture period and in the vicinity of peak feeding and NPP rates

8.5.3.3 Shrimp production in ponds

AquaFarm was applied to a range of production intensities (50,000 – 500,000 shrimp/ha) for marine shrimp (*Penaeus monodon* and *P. indicus*) in tropical (0 - 20° N latitude), brackish water (25 ppt), ponds (1.0-ha), with application of fertilizers and prepared feeds, demand aeration, and variable levels of water exchange as needed to maintain water quality. Production periods of 100 to 150 days were simulated (mean 120 days), where culture period lengths in conjunction with stocking densities were used to attain a range of feed application intensities. The DSGR growth model was applicable, given that common harvest sizes of 16 – 20 g for *P. indicus* (White/Indian shrimp) and 28 – 35 g for *P. monodon* (Black tiger/Grass shrimp) are well below maximum maturation shrimp sizes ($\geq 80 - 100+$ g; Kutty, 1995). Supporting this conclusion, growth data in the supporting literature showed exponential and linear growth stanzas for shrimp body weights up to at least 40 g, when growth was not limited by water quality or feed availability. For estimating natural food resources and timing the initiation of prepared feed application, empirically based critical standing crop (e.g., 100 – 300 kg/ha) and carrying capacity shrimp densities were used without consideration of water column NPP, given the benthic location and variety of food resources utilized by omnivorous shrimp. Application rates for prepared feeds were based on

reported food conversion efficiencies (e.g., 50% for complete feeds and 30% for lower quality feeds), considering contributions of natural foods. The DSGR growth model was used in conjunction with the natural fish productivity model. Overall, the processes and models used in this exercise were similar to those used earlier for tilapia production in ponds.

Results of this exercise (not shown) compared well to observed data for marine shrimp production studies (Wyban, 1992; Fast and Lester, 1992; Briggs and Funge-Smith, 1994; Kutty, 1995), including shrimp growth, feed requirements, aeration requirements, and water quality regimes. Pond water exchange rates of zero to 30 % per day were simulated, including impacts on pond water quality and stratification, tradeoffs in relation to aeration requirements, and compound and BOD loading rates on receiving waters. Pond nitrogen and phosphorous budgets were comparable to those reported by Briggs and Funge-Smith (1994), but as with other solar-algae pond exercises, soil uptake, seepage loss, and denitrification components had to be adjusted somewhat in order to achieve reported results.

Regarding shrimp biomass density constraints with respect to dissolved oxygen, it has been suggested that while air-water gas exchange limits production of finfish such as tilapia and catfish, advective transport of oxygen through the water column to the benthic region limits production of bottom-dwelling shrimp (Garcia and Brune, 1989; Brune and Drapcho, 1991). These authors propose that shrimp reside in a “diffusive boundary layer”, located in the bottom few centimeters of the water column. Simulation results indicated that consideration of this boundary layer was required to achieve reported aeration rates for shrimp ponds. This boundary layer is not considered in the two-layer thermal stratification model, it acts in addition to thermal stratification, and it is present in aerated/mixed ponds where thermal stratification is broken down. Therefore, it was accounted for by the minimum dissolved oxygen criterion used for aeration management. By increasing this criterion, the concentration gradient necessary to transfer oxygen into the benthic boundary layer was provided and aeration power requirements were increased to reported rates.

8.5.3.4 Salmon production in tanks and cages

AquaFarm was applied to Atlantic salmon (*Salmo salar*) production, including egg incubation, production of 45.0-g smolts in single-pass, flow-through tanks, and production of 4.0-kg marketable fish in seawater cages. Specifications and results of this exercise are provided in Table 8.10 and Figures 8.59 and 8.60. Egg, smolt, and growout production stages were linked by their temporal

Table 8.10. Atlantic salmon production in tanks and cages

Specifications				
Facility	<ul style="list-style-type: none">• Location: 57° N latitude and sea level• Weather: annual parameters for air temperature and cloud cover• Source water quality: annual water temperature regimes, 50 mg/L alkalinity for freshwater, 100 mg/L alkalinity and 35 ppt salinity for seawater, and equilibrium gas concentrations			
Culture systems	<ul style="list-style-type: none">• Egg incubators: parallel configuration, water flow rates at 2.0 L/min per 10,000 eggs and 5.0 L/min per 10,000 alevin (hatched fry)• Smolt tanks: 10 m³ cylindrical tanks, parallel configuration, maximum fish density 30 kg/m³, and water retention time 30 minutes• Growout cages: 1500 m³, cylindrical, seawater cages, maximum fish density 22 kg/m³, and assumed water retention time 1.0 hour			
Fish production objectives	Stage	Dates	Number	Weights
	Egg to first-feeding fry	Jan. 21, year 1 to May 1, year 1 (100days)	15000 to 12000	Egg to 0.2 g
	Fry to smolt	May 1, year 1 to May 1, year 2 (365 days)	12000 to 6600	0.2 to 45.0 g
	Smolt to harvest	May 1, year 2 to Oct. 1, year 3 (520 days)	10000 to 8500	45.0 to 4000 g
	<ul style="list-style-type: none">• Egg: 20% mortality• Smolt: 5% cull removal at 0.75 g fish, 5% cull removal at 2.0 g fish, 75% high-grade for potential yearling smolts at 10.0 g fish, 10% mortality, and 48% protein feed• Growout: no handling other than harvest, 15% mortality, and 45% protein feed			
Results				
Smolt production	<ul style="list-style-type: none">• Each smolt tank was stocked from the output of one egg incubator• Total fish loss due to mortality and low-grade removal required an initial 12,000 fish per tank to achieve a final target smolt density of 30 kg/m³• 70% fish feeding index (% maximum ration) and 67% food conversion efficiency (includes cull and mortality losses)• Maximum fish respiration rate: 170 mg O₂/kg fish/hr• Water quality: DO ≥ 77% sat., DC ≤ 355% sat., TAN ≤ 0.30 mg N/L, NH₃ ≤ 0.003 mg N/L, pH 7.7 – 8.2, and particulate solids ≤ 2.9 mg dw/L			
Cage growout	<ul style="list-style-type: none">• Each cage was stocked with the output of 1.5 smolt tanks• Total fish loss due to mortality required an initial 10,000 smolts per cage to achieve a final target fish density of 22 kg/m³• 90% fish feeding index (% maximum ration) and 52% food conversion efficiency (includes mortality losses)• Water quality: DO ≥ 65% sat., DC ≤ 178% sat., TAN ≤ 0.37 mg N/L, NH₃ ≤ 0.005, pH 8.0-8.2, and particulate solids ≤ 3.5 mg dw/L• Total compound loading on supporting water body per 1000-kg fish produced: 680 kg dry wt. solids, 750 kg BOD, 80 kg DIN, and 20 kg DIP			

sequence and population numbers, for which dates and population numbers were given for the input of fertilized eggs and output of harvested fish. Based on the intermediate target date for first-feeding fry, egg incubation was controlled by adjusting water temperatures to an increasing 8 – 10 °C regime using water blending. Smolt and harvest target fish weights were achieved through control of feed application rates.

This example demonstrates some of the detail that can be used in fish lot management, but results of multiple fish lots are not shown. Results were comparable to production data given in Laird and Needham (1988). Accurate estimations for expected source water quality and temperature regimes and assumed water exchange rates of cages were critical inputs for this exercise, in which unit processes of smolt tanks and salmon cages were dominated by fish metabolism and water advection. This example demonstrates the use of biomass densities and water exchange rates as management criteria. Alternatively, required water flow rates and allowed biomass loading rates could have been based on water quality variables such as dissolved oxygen, cumulative oxygen consumption, carbon dioxide, and/or unionized ammonia.

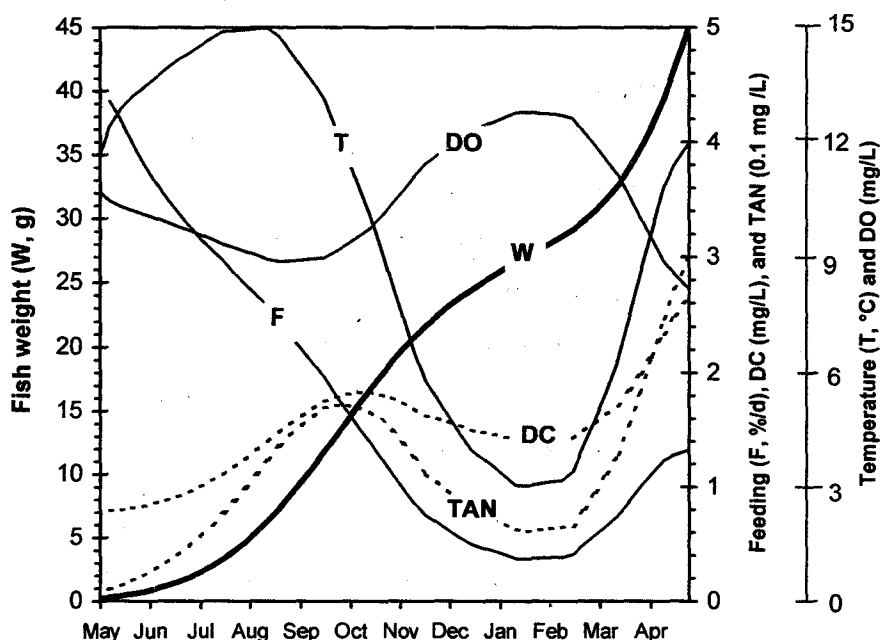


Figure 8.59. Simulated data (1-day time step) for Atlantic salmon smolt production in flow-through tanks over a 12-month culture period, for which values represent daily means

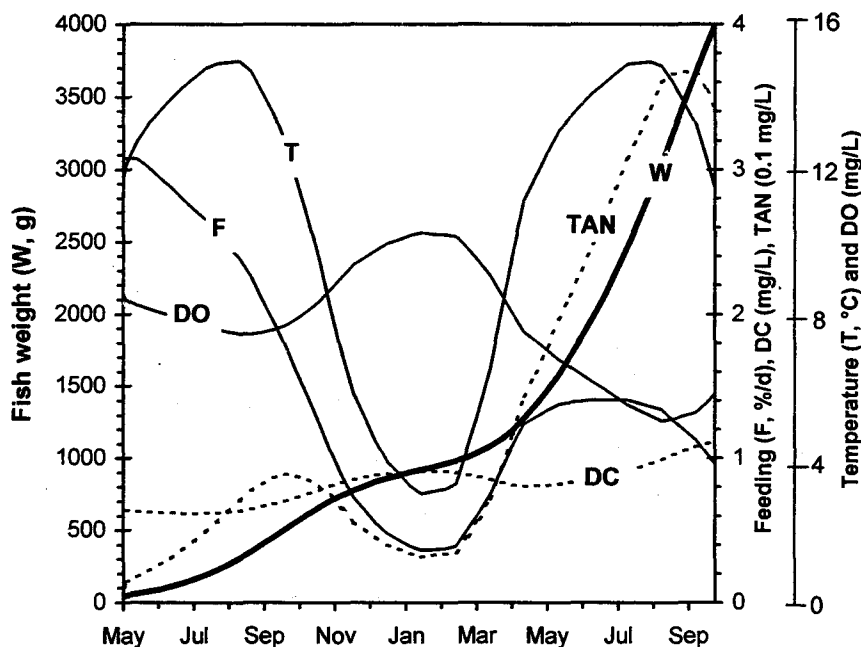


Figure 8.60. Simulated data (1-day time step) for Atlantic salmon growout in marine cages over a 17-month culture period, for which values represent daily means

8.5.3.5 Salmon production using serial water reuse

AquaFarm was applied to hatchery production of spring chinook salmon (*Oncorhynchus tshawytscha*) utilizing serial raceways, pure oxygen absorbers between raceways, and water reuse. Conditions of this exercise are provided in Table 8.11. The purpose of this exercise was to validate the simulation of diurnal fish metabolic rates resulting from feed application during daylight hours and diurnal temperature oscillations. Similar modeling can be applied to any fish species and type of aquaculture system, when it is desired to account for impacts of diurnal fish metabolism on water quality. No specific calibrations were performed for this exercise, other than for the diurnal water temperature regimes of the hatchery supply water (large stream), and the standard parameter set of AquaFarm was used.

Results were comparable to production data given in Ewing et al. (1994) and additional, unpublished, continuous monitoring data (author, 1995) from spring chinook hatcheries in the same region. Fish rearing-unit processes were dominated by fish metabolism and water advection, a relatively simple modeling exercise. In Figure 8.61, the data points shown for feeding represent the time of feeding and feeding rates. For observed data, clear associations between feeding times and

peaks in oxygen consumption rates are evident. For simulated data, these peak responses were smoothed, but the overall agreement of predicted and observed data was good. In Figure 8.62, oxygen was added between raceways so that influent DO levels of raceways were equal but fish metabolites accumulated as expected. Accurate prediction of diurnal temperatures for the hatchery supply water was an important aspect of this exercise. Fish rearing-unit temperatures closely followed source water temperatures and were a major determinant of fish metabolic rates.

This exercise demonstrates the use of diurnal simulations to analyze daily peak loading-rates of fish metabolism and cumulative impacts of fish metabolism on water quality under serial water reuse. Such analyses can be used to assess the impacts of alternative management strategies on water quality, including fish biomass loading, pure-oxygen addition by constant or demand-based process control, and temporal distribution of feeding events over daylight hours. Management tolerance for short term, sub-optimal water quality is an important variable in this regard. Daily peak-mean ratios of fish biomass support requirements (Colt and Orwicz, 1991b) can be derived for use in simulations using daily time-steps.

Table 8.11. Spring chinook production in raceways

Specifications	
Facility	<ul style="list-style-type: none"> • Location: 45° N latitude and 370 m elevation • Weather: annual parameters for air temperature and cloud cover • Source water quality: annual temperature regimes, 20 mg/L alkalinity, and equilibrium gas concentrations
Culture systems	<ul style="list-style-type: none"> • Serial rearing-unit configuration with water reuse • Pure oxygen absorbers placed between raceways, with automated oxygen addition rates based on a 100% saturation set-point • Three 105 m³ raceways per series, operated at a raceway water retention time of one hour and 6 kg/m³ fish density at the given fish size
Fish production objectives	<ul style="list-style-type: none"> • Fry to pre-smolt growout: culture period for purposes of this exercise limited to June 1 – 10, with 222000, 2.5 g fish per raceway on June 1 and using 50% protein feed
Results	
Fish production	<ul style="list-style-type: none"> • Mean values for 10 day analysis period: 2.9-g fish weight, 6.1 kg/m³ fish density, 3.7% bw/day feeding rate, and 85% food conversion efficiency • Fish respiration rate: 200 – 480 mg O₂/kg fish/hr, showing diurnal, sinusoidal profiles in rates and resulting impacts on water quality

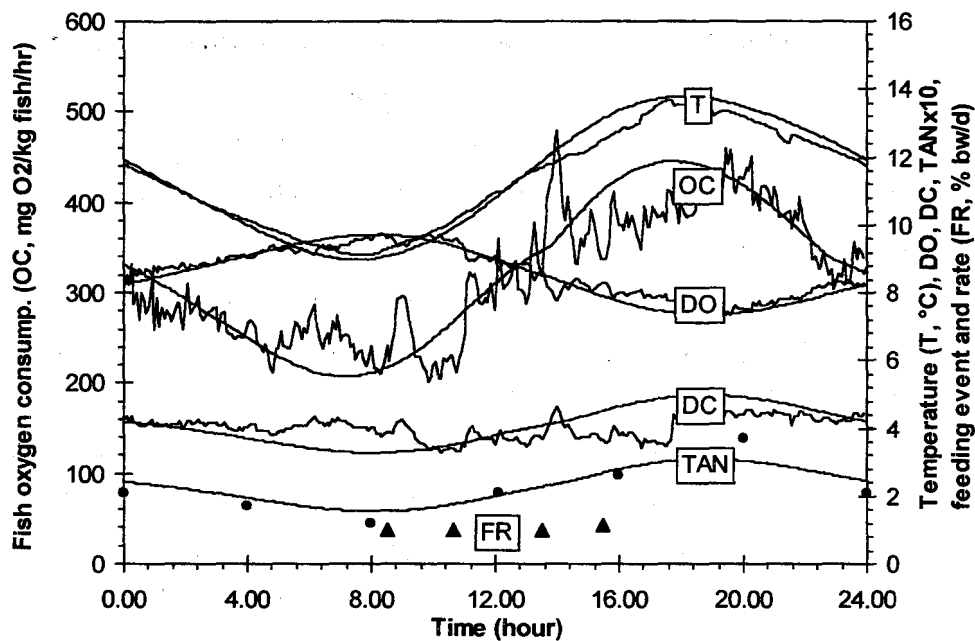


Figure 8.61. Simulated data (smooth lines; 1-hour time step) and empirical data (jagged lines; continuous monitoring) for Pacific salmon hatchery production in raceways, showing a single day (June 1) within the culture period

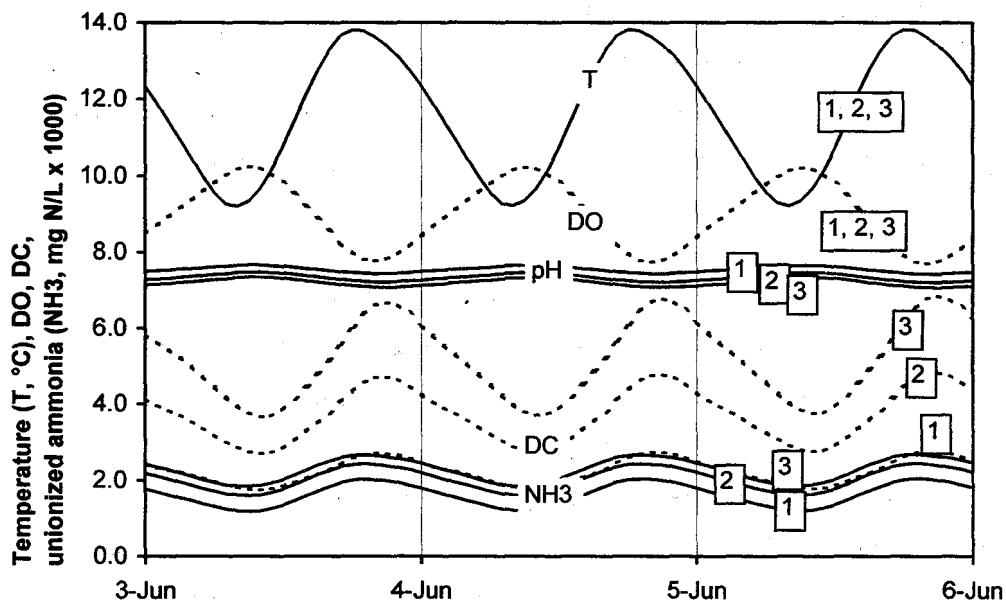


Figure 8.62. Simulated data (1-hour time step) for Pacific salmon hatchery production in three, serial raceways (numbered 1, 2, and 3, up to down stream), showing a few days at the beginning of June within the culture period

8.5.3.6 Fish production using water recirculation

AquaFarm was applied to the intensive production of rainbow trout (Heinen et al., 1996), hybrid striped bass (Tuncer et al., 1990; Singh et al., 1997), and tilapia (Twarowska et al., 1997; Rosati et al., 1997) in water recirculation systems. To match the conditions of these studies, systems were operated as semi-closed (2.0 system exchanges per day) or minimal-exchange (0.075 system exchanges per day). As described in the listed references, major systems components included (1) fish rearing units, including rectangular cross-flow and single and dual drain circular and polygonal tanks, (2) sump tanks and pumps, (3) water heaters, (4) aerators and oxygenators, (4) carbon dioxide strippers, (6) particle separators, parallel-tube settling basins, expandable granular media filters (bead filters), and microscreen filters for solids removal, (7) trickling, fluidized bed, and expandable granular media biofilters for nitrification, (8) alkalinity control by addition of various carbonate compounds, (9) water disinfection units, and (10) settling basins for discharged water/solids. Examples of facility maps for such systems were given in Chapter 2 (see AquaFarm user interface). In addition to the active processes associated with water treatment and transport, passive processes required to model these systems included heat transfer under controlled climates, gas transfer, solid settling, bacterial oxidation of organic solids, and nitrification.

AquaFarm was also applied to tilapia and catfish production in “green water” (phytoplankton present) recirculation systems (Drapcho and Brune, 1989; Cole et al., 1997; Lutz, 1997; Avnimelech, 1998). These systems varied widely in design but essentially consisted of intensively fed fish rearing units, coupled with one or more facility units for growth and/or harvesting of algae, oxidation of particulate solids, settling and physical removal of particulate solids, gas exchange, and water transport.

For each of these systems, a facility was constructed according to the supporting study, using estimated specifications when facility design and management were not sufficiently reported. Results of these exercises (not shown) were generally comparable to reported results, including fish production, solid waste production and composition, consumption of resources (e.g. energy, water, feed, oxygen, and alkalinity compounds), and water quality regimes. However, comparisons between simulated and reported results were limited by a lack of sufficient reporting detail in the studies used. Rigorous validation requires complete system specifications, management schedules, and water quality data at multiple points in the system. In contrast to simulation exercises with extensive systems, simulation results were largely a function of facility specifications (e.g. oxygenators, biofilters, and solid filters) and were less dependent on parameters of passive unit

processes. These actively managed unit processes are modeled in terms of their given efficiencies. For example, oxygen absorption efficiencies for oxygenators, nitrification efficiencies for biofilters, and solid removal efficiencies for solid filters are specified directly, rather than calculating these efficiencies from a host of additional specifications.

9. Conclusion

The informed decision-making required for aquaculture design and management planning presents a number of challenges. Major challenges include the application of widely ranging expertise areas encompassed by aquacultural engineering, the utilization of relevant data and information resources from empirical research, and the processing of numerically intensive, design and planning procedures. To address these challenges, the objective of this dissertation has been to construct an interactive, farm level, simulation and decision support system for aquaculture design and management planning (AquaFarm). AquaFarm provides expertise in aquacultural engineering, utilizes the findings of aquaculture research, and supports the major burden of data management and calculation processing. By providing this functionality within a flexible, interactive framework, AquaFarm offers decision support to end-users in aquaculture research, education, design, and production, for all types of crustacean and finfish aquaculture systems.

Existing simulation models and decision support systems for aquaculture that approach the analytical scope and resolution of AquaFarm were not found in the literature, especially regarding the degree of analytical rigor applied and the flexibility in system types and management strategies supported. While the existing literature was utilized to a large degree, original contributions of this dissertation include: (1) computer program architecture and user interface, (2) adaptation of existing unit-process models, (3) development of new unit-process models, (4) formulation of aquaculture management methods into rule-based structures, (5) synthesis of existing and new methods into an integrated analytical framework, (6) simulation processing procedures, and (7) formulation of the procedures of aquacultural engineering into design and planning templates.

The bulk of the work accomplished here concerned (1) the partitioning of aquaculture production systems into functional components and associated models, including unit processes, management procedures, and resource accounting and (2) the flexible reintegration of these components into system-level simulation models and design procedures that are adaptable to various aquaculture system types, production objectives, and user needs. The successful development of generic, analytical templates that could be applied to a wide range of specific problems demonstrated the accomplishment of these tasks. Considerable effort was required to accomplish these tasks due to (1) the wide scope of systems considered, (2) the rigorous levels of analytical resolution pursued, (3) the computer programming required to represent this functionality, and (4) the graphical user interface required to access this functionality.

The documentation provided in this dissertation is fully duplicated in the computer program code comprising AquaFarm. This body of software consists of a total of about 16 megabytes of C++ program and interface code. The AquaFarm executable package is about 5.0 megabytes (executable file, dynamic link libraries, and project data files). A listing of this program code is not provided here, due to space limitations, required familiarity with C++ program code, and lack of purpose to most readers. It should be noted that this dissertation provides complete documentation of AquaFarm from an aquacultural engineering and management perspective, but a considerable amount of the program algorithms used to support the user interface and to process simulations are not documented here, again due to space limitations and lack of purpose to most readers.

Specific conclusions regarding the methods, application, and predictive accuracy of AquaFarm as an aquaculture simulator were provided throughout this dissertation. Overall, applications to practical problems demonstrated a capacity to simulate a wide range of aquaculture systems within an acceptable degree of accuracy. However, it was not necessarily demonstrated that this functionality represented a useful decision support system for users with limited technical expertise. The paramount concern is that the degree of responsibility required from a user for the input data and decisions of a given design project may exceed that user's capacity. While AquaFarm supports the engineering analyses that would otherwise be used, with full access to parameters and the benefit of computerization, non-technical users may lack the capacity to recognize when incorrect conditions exist or to accomplish the necessary adjustments.

In order to further minimize user responsibility for unit-process parameters, an argument for additional calibration-validation work can be made. However, the simplifying assumptions and aggregated processes used to develop AquaFarm make it unlikely that a single, best parameter set exists for all culture conditions of a given aquaculture species. Furthermore, user responsibility for site-specific parameters and variables, such as specifications of the proposed or existing facility, cannot be avoided. Given these ultimate constraints to parameterization and considering the good calibration and validation results that have been achieved, the use of additional exercises to further refine the standard parameter set of AquaFarm is considered to lack a clear rationale. Similarly, the use of additional sensitivity studies to rank the impact of input parameters and variables on simulation results is not felt to offer significant benefits relative to the work required. In general, all of the input parameters and variables considered by AquaFarm can significantly impact results under certain conditions and a sufficient understanding has been developed regarding where the user's attention to accurate, site-specific input data should be directed.

Given these conclusions, ongoing development work for AquaFarm is concerned with responsive, empirically based mechanisms to alleviate user responsibilities, which can be used in the course of a design project. This represents a flexible, case specific, run-time approach to calibration that can be used to enhance the standard parameter set where needed and assist the specification of system design and management variables. The second major area of ongoing work concerns the development of a representative user base and incorporation of user feedback regarding the user interface and functionality provided by AquaFarm. Specific tasks include:

- 1) Methods are being developed to utilize user-supplied datasets (e.g., historical fish production and water quality data) for the derivation of site-specific parameters. This approach will be particularly useful to users with existing facilities or knowledge of representative facilities. Efforts are currently focused on the calibration of fish growth and feeding models from user-supplied datasets. Some additional areas of interest include thermal stratification and primary productivity in solar algae ponds and system capacity constraints encountered in intensive aquaculture.
- 2) Users that lack an empirical basis for their specific projects would be better served by the availability of a representative facility in their area of interest. To address this need, a number of pre-designed aquaculture facilities are being developed for a range of systems types, cultures species, and management intensities. These systems can be used as a starting point for new projects or as tutorials for new users. This effort mainly concerns facility and management specifications, and these systems will be available at the user interface for loading from file.
- 3) Range checking for all input data and message generation regarding specifications that exceed typical ranges are being further developed to facilitate user data entry. In addition, interface navigation aids are being developed to guide users through procedures of project specification, simulation, evaluation, and adjustment.
- 4) In conjunction with these tasks, a representative base of users from aquaculture research, engineering, education, and production is being developed. Feedback from these users will be used to improve the capacity of AquaFarm to address user needs, present reasonable levels of user responsibility, and provide a navigable interface. AquaFarm will not be widely released until completion of this user application and testing stage.

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