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Title: DISCRETE MODELING OF FLOW SYSTEMS

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This study develops a general discrete flow model which is discrete both in time and space. A stirred tank network model (continuous time compartment model) is summarized and then compared with the discrete flow model. Both models make use of a fractional input matrix with elements representing the fraction of flow into the jth region which originates in the ith region. It is shown that the discrete flow model is more general and computationally much simpler than the stirred tank network model.

The fractional input matrix is used to find the sizes of the regions, to predict the residence time distribution (RTD) of the fluid in flow systems, and to compute the conversion for chemical reaction occurring in a flow system. Direct methods for finding the fractional input matrix from either steady state or transient data are developed, and methods and problems of fitting the model to data are presented. Two simple numerical examples are given to demonstrate the use of the model.

Lumping is important for modeling flow systems with very many regions, thus a lumping analysis for discrete flow systems is presented. The methods for obtaining the sizes of the regions and the fractional input matrix provide an important tool to analyze the lumping problems in flow systems.

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DISCRETE MODELING OF FLOW SYSTEMS

I. INTRODUCTION

Discrete modeling of flow systems using a fractional input matrix (or stochastic matrix) may become a useful tool in chemical engineering practice in the near future. This is mainly due to many practical uses of such a model. For example, it is possible to apply this technique to solve important problems which are encountered in such applications as water pollution treatment in the rivers and oceans, drug distribution in human body, flow of chemical through complex process equipments, solid particle movement in fluidized beds, and the mixing problems in the design of chemical reactors.

In studying a physical phenomenon in a flow process, chemical engineers often use sets of mathematical equations (both ordinary and partial differential equations) which approximate the process under investigation. But once the process becomes quite complex, particularly, when many unknown factors are involved in that process (like most of flow systems, for example), it is too difficult and often impractical to formulate the mathematical equations which describe the behavior of that system. The discrete flow model proposed in this study may be a useful approach in such a case.

No general work has been reported in the literatures on modeling continuous time, continuous space flow systems. But there has been some work on modeling special kinds of flow systems. Among them, most of the studies have been made on modeling continuous time, discrete space flow systems with a known set of interregion flows. In 1967, Gibilaro, et al. [8] used a discrete time Markov process to evaluate the response of a continuous time flow system consisting of six well-mixed vessels to input disturbances. They arbitrarily assigned the volumes of the vessels and the magnitude of the flows connecting the vessels. A network combing technique for modeling stirred vessel arrays was introduced in 1969 by Buffham, et al. [4]. An arbitrary flow network with identical linear dynamic mixing characteristics at the nodes, according to their work, may be replaced by an equivalent parallel-series arrangement. In this manner, the total response can be expressed as a sum of the individual series responses. That technique can be used only when values of the sizes of the vessels and the interconnected flows between the vessels are specified. In 1971, Schmalzer ahd Hoelscher [19] presented a stochastic model of a packed bed and discussed the consequences on mixing and mass transfer within that bed. In that model it was assumed that each packet of fluid has three velocity states and then related the movement of the packet of fluid in velocity states to a random walk problem. The transition probabilities in the velocity space with time as a discrete parameter were chosen arbitrarily. This was extended to the continuous parameter case later by

Srinivasan and Mehata [20]. In 1972, Chen, et al. [5] used a Markov chain model to model the axial mixing of a binary homogeneous solid particle mixture in a motionless mixer having no moving parts. One step transition probabilities were determined experimentally by them. The experimental results were in good agreement with those predicted from the model. But, according to their work, transition probabilities were difficult to obtain experimentally and the determination of those probabilities was time-consuming. This was extended to the case of mixing of a multicomponent solid particles later by Lai and Fan [13]. A mathematical model called compartmental analysis was presented in 1971 by Rubinow and Winzer [17]. It has been developed and used extensively in physiology to model flow within an organism [6, 15, 18]. According to that model, the information of the steady state fluxes between the compartments in a compartment system consisting of n interconnected well-mixed compartments can be inferred by observing the tracer concentration as a function of time in one or more compartments. There are only $(2n-1)$ algebraic equations which can be written down by relating the interconnected flux matrix to experimentally determined quantities and its invariants. In making inferences regarding n^2 unknown elements of the interconnected flux matrix, some elements of that matrix are assumed to be null. The computation in that model is tedious and the result is not unique.

For many flow systems (like rivers and oceans, for example) that are of interest in this study, there are very many regions inside the systems. In practice we do not know the interregion flows connecting the regions inside the systems. We do not know the sizes of the regions either. The only thing we may have is the transient concentrations of tracer at various points from multiple probe measurements. This thesis seeks to find out what use can be made of these sets of data measured by multiple probes in a flow system. Can they tell what is going on inside the system? Is it possible to develop a method to find the interregion flows from those measured data alone?

The approach in this study is to model the flow systems as discrete both in time and space and to develop general methodologies for determining the fractional input matrix (or transition matrix) based on multiple steady state or transient tracer measurements within the system. The use of that matrix to find the sizes of the regions, to predict the residence time distribution (RTD) of the fluid in the flow system, and to compute the reaction conversion if chemical reaction occurs will also be developed.

II. DISCRETE FLOW MODEL

Description of the Model

The model proposed in this study assumes that the behavior of a given flow system can be represented by an n regions which are connected by an arbitrary flow network. A schematic diagram of this flow model is shown in Figure 1. The volumes of the regions are not necessarily equal. We index the regions by i, running from 1 to n, denote the volume of the ith region by v_i and the volumetric flow rate from the ith region to the ith region itself by q_{ii} and the volumetric flow rate from the ith region to the jth by q_{ij}. The volumetric flow rate from the inlet station (or feed station) to the jth region is denoted by Q_j and the volumetric flow rate from the ith region to the outlet station is $q_{i,out}$.

In order to visualize a physical phenomenon which exactly corresponds to the mathematical model, we consider each region to contain a piston which moves from the top of the region down to the bottom in one transition and then discontinuously moves back to the top position ready for next transition. Material entering any region mixes completely on entering.

Consider the system at some time t after a tracer has been introduced. The state of the system is described by the tracer concentrations in each of the n regions. After a time Δt, during

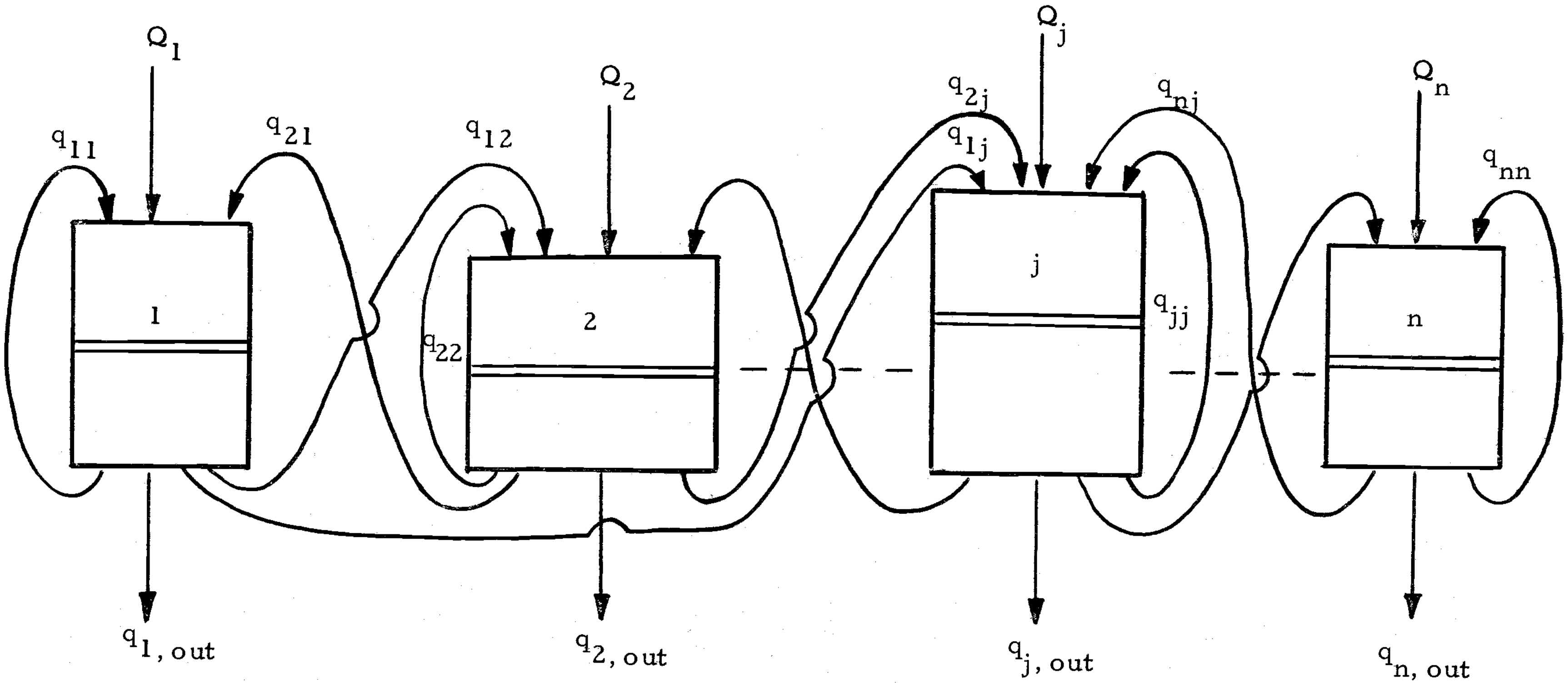

Figure 1. A schematic diagram of discrete flow model.

which the material flows out of the bottom of each cell and back into the top of other cells (or the same cell, or exits), we have a new set of concentrations or a new state. Each redistribution of this kind will be called a state transition.

State Transition Equation of the Model

Before we start the derivations, some assumptions about the actual system for this model are listed as follows:

1. The flow is incompressible.
2. The flow pattern is unchanging (not a function of time).
3. The scale of turbulence compared to the size of the regions is small and thus negligible. Hence measurements are reproducible.
4. No chemical reactions are involved in the flow process.

At time t, we inject a tracer into a flow system assumed to consist of n regions as shown in Figure 1. Let one step time interval be Δt. Then from the mass balance of the tracer around the jth region at time $t+\Delta t$, we find

$$v_j c_j(t+\Delta t) = \sum_{i=1}^{n} (q_{ij}\Delta t)c_i(t) + (Q_j \Delta t)f_j(t) , \qquad (1a)$$

for all $t \geq 0$ $j = 1, 2, \ldots, n$

where $c_j(t+\Delta t)$ is the tracer concentration in region j at time $t+\Delta t$, $c_i(t)$ is the tracer concentration in region i at time t, and $f_j(t)$ is the input tracer concentration from the feed station to region j at time t. Dividing by v_j on both sides of Equation (1a), we get

$$c_j(t+\Delta t) = \sum_{i=1}^{n} \left(\frac{q_{ij}\Delta t}{v_j}\right) c_i(t) + \left(\frac{Q_j \Delta t}{v_j}\right) f_j(t) , \qquad (1b)$$

for all $t \geq 0$ $j = 1, 2, \ldots, n$

Now define

$$p_{ij} = \frac{q_{ij}\Delta t}{v_j} , \qquad i, j = 1, 2, \ldots, n \qquad (2)$$

$$\pi_j = \frac{Q_j \Delta t}{v_j} , \qquad j = 1, 2, \ldots, n \qquad (3)$$

Equation (2) defines the fractional input coefficients (or transition probabilities) p_{ij} in this flow model from a physical viewpoint. They can be interpreted as the fraction of all material that will end up in the jth region that transfers from the ith region in one step. Similarly, the feed coefficients π_j (defined by Equation (3)) can be interpreted as the fraction of all material that will end up in the jth region that moves from the feed station in one step.

Substituting Equation (2) and Equation (3) into Equation (1b), we obtain

$$c_j(t+\Delta t) = \sum_{i=1}^{n} p_{ij} c_i(t) + \pi_j f_j(t) , \qquad (4)$$

for all $t \geq 0$ $j = 1, 2, \ldots, n$

In a general form, Equation (4) becomes

$$c_j(t+(m+1)\Delta t) = \sum_{i=1}^{n} p_{ij} c_i(t+m\Delta t) + \pi_j f_j(t+m\Delta t) , \qquad (5)$$

for all $t \geq 0$ $j = 1, 2, \ldots, n$ $m = 0, 1, 2, \ldots$

The above equation can be written in matrix notation as

$$C(t+(m+1)\Delta t) = C(t+m\Delta t)P + F(t+m\Delta t)\Pi , \qquad (6)$$

for all $t \geq 0$ $m = 0, 1, 2, \ldots$

In a shorthand, Equation (6) can also be written as

$$C(m+1) = C(m)P + F(m)\Pi, \quad m = 0, 1, 2, \ldots \qquad (7)$$

where $C(m)$ is the concentration row vector at time $m\Delta t$, i.e., $C(m) = [c_1(m)\ c_2(m) \ldots c_n(m)]$, $F(m)$ is input concentration row vector at time $m\Delta t$, i.e., $F(m) = [f_1(m)\ f_2(m) \ldots f_n(m)]$, P is the fractional input matrix (or transition matrix) of the flow system with elements p_{ij}, i.e.,

$$P = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ p_{21} & p_{22} & \cdots & p_{2n} \\ \vdots & \vdots & & \vdots \\ p_{n1} & p_{n2} & \cdots & p_{nn} \end{bmatrix},$$

and Π is the feed matrix with diagonal elements π_i, i.e.,

$$\Pi = \begin{bmatrix} \pi_1 & & & \\ & \pi_2 & & \\ & & \ddots & \\ & & & \pi_n \end{bmatrix}.$$

Equation (7) is the general formula of state transition equation for this flow model.

For an instantaneous or pulse tracer input at $t = 0^-$, the input tracer concentration row vector $F(m)$ becomes zero for $m \geq 0$. Then Equation (7) becomes

$$C(m+1) = C(m)P, \quad m = 0, 1, 2, \ldots \tag{8}$$

Since by recursion

$$C(1) = C(0)P$$
$$C(2) = C(1)P = C(0)P^2$$
$$C(3) = C(2)P = C(0)P^3$$

in general,

$$C(m) = C(0)P^{m}, \quad m = 0, 1, 2, \ldots \tag{9}$$

Equation (9) is the state transition equation for an instantaneous or pulse tracer input at $t = 0^-$.

Properties of the Fractional Input Matrix

1. The elements p_{ij} of matrix P are non-negative and not greater than one, i.e.,

$$0 \leq p_{ij} \leq 1$$

2. The summation over the column (i.e., $\sum_{(i)} p_{ij}$)

From Equation (2), we know

$$p_{ij} = \frac{q_{ij}\Delta t}{v_j}, \quad i, j = 1, 2, \ldots, n$$

Thus,

$$\sum_{i=1}^{n} p_{ij} = \sum_{i=1}^{n} \frac{q_{ij}\Delta t}{v_j} = \frac{\sum_{i=1}^{n} q_{ij}\Delta t}{v_j}, \quad j = 1, 2, \ldots, n \tag{10}$$

Case 1. If region j has an inlet from the inlet station, then

$$\sum_{i=1}^{n} q_{ij}\Delta t < v_j, \quad j = 1, 2, \ldots, n \tag{11}$$

Substituting Equation (11) into Equation (10), we get

$$\sum_{i=1}^{n} p_{ij} < 1, \qquad j = 1, 2, \ldots, n \tag{12}$$

Case 2. If region j has no inlet from the inlet station, then

$$\sum_{i=1}^{n} q_{ij} \Delta t = v_j , \qquad j = 1, 2, \ldots, n \tag{13}$$

Substituting Equation (13) into Equation (10), we get

$$\sum_{i=1}^{n} p_{ij} = 1, \qquad j = 1, 2, \ldots, n \tag{14}$$

From Equation (12) and Equation (14), we can summarize these as follows: if $\sum_{(i)} p_{ij} < 1$, then we can say that region j has an inlet from the inlet station; if $\sum_{(i)} p_{ij} = 1$, then we can say that region j has no inlet from the inlet station. Both conditions are true whether the volumes of the regions are all equal or not.

3. The summation over the row (i.e., $\sum_{(j)} p_{ij}$)

From Equation (2), we know

$$p_{ij} = \frac{q_{ij} \Delta t}{v_j} , \qquad i, j = 1, 2, \ldots, n$$

Thus,

$$\sum_{j=1}^{n} p_{ij} = \sum_{j=1}^{n} \frac{q_{ij}\Delta t}{v_j} \lesseqgtr 1, \quad i = 1, 2, \ldots, n \tag{15}$$

From Equation (15), we know that the sum of all the elements of each row could be any positive number (i.e., less than or equal to or greater than one) depending on individual flow rates and the volumes of the individual regions. The sum of the ith row will be equal to one if both of the following conditions are satisfied: (a) the volumes of the regions are all equal. (b) Region i has no outlet to the outlet station. We can summarize this as follows:

(1) If the sum of all the rows except the ones which have the outlet to the outlet station are equal to one, then we may assume that the volumes of the regions are all equal. In this case, region i has no outlet to the outlet station if the sum of the ith row is equal to one. Otherwise, region i has an outlet to the outlet station.

(2) If only some of the rows sum to one, then we may say that the volumes of the regions are not all equal. In this case, Equation (15) alone can not tell much whether region i has an outlet or not. From the flow diagram of the system, we can reasonably assume that some of the regions have

outlet to the outlet station and then check it later (check $\sum_{(i)} v_i$) to see if the assumption is correct or not.

Stability for the Flow Systems

For a real flow system, a pulse of tracer which was injected into system at $t = 0^-$ will eventually all wash out of the system. We would like to know what conditions must exist for the fractional input matrix P such that the concentration row vector C(m) will approach 0 as m approaches infinity.

First, we introduce two important factors of the matrices so called eigenvector and eigenvalue and then show how to find them. Let x be an eigenvector of matrix P. Then, from the definition of x, there must exist an eigenvalue λ such that

$$Px = \lambda x$$

Or,

$$(P - \lambda I)x = 0 \qquad (16)$$

Equation (16) can be used to compute the eigenvector x which corresponds to the eigenvalue λ of matrix P. If $\det(P - \lambda I) \neq 0$, then Equation (16) has the trivial solution. We disregard this solution since x is an eigenvector of the matrix P and can not be a zero-vector by definition. Therefore, x will be an eigenvector of matrix P if and only if

$$\det(P-\lambda I) = 0 \tag{17}$$

The Equation (17) is called the characteristic equation of matrix P and the roots of that equation determine the eigenvalue λ of matrix P.

Next, from Equation (9), we know

$$C(m) = C(0)P^m, \quad m = 0, 1, 2, \ldots$$

Define

$$D = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_k \end{bmatrix} \qquad S_r = \begin{bmatrix} \lambda_r & 1 & 0 & \ldots & 0 & 0 \\ 0 & \lambda_r & 1 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & \lambda_r & 1 \\ 0 & 0 & 0 & \ldots & 0 & \lambda_r \end{bmatrix}$$

Here D is a diagonal matrix and S_r $(r = 1, 2, \ldots)$ is called a semi-diagonal matrix that has all its diagonal elements equal to λ_r, all of its superdiagonal elements equal to one, and all of its other elements equal to zero. Using the standard method [3, 22] to compute the matrix P, we obtain

$$P = MJM^{-1} \tag{18a}$$

where M is eigenvector matrix of matrix P, i.e., $M = [x_1, x_2, \ldots, x_n]$ and J is called a matrix in Jordan canonical form.[1/] A square matrix is in Jordan canonical form if it is a diagonal matrix or can be expressed in either one of the following two partitioned diagonal forms:

$$\begin{bmatrix} D & & & \\ & S_1 & & \\ & & \ddots & \\ & & & S_r \end{bmatrix}$$

or

$$\begin{bmatrix} S_1 & & \\ & \ddots & \\ & & S_r \end{bmatrix}$$

Then from Equation (18a), we know

$$P^2 = PP = (MJM^{-1})(MJM^{-1}) = (MJ)(M^{-1}M)(JM^{-1})$$

$$= (MJ)(I)(JM^{-1}) = MJ^2M^{-1} \ ,$$

$$P^3 = P^2P = (MJ^2M^{-1})(MJM^{-1}) = (MJ^2)(M^{-1}M)(JM^{-1})$$

$$= (MJ^2)(I)(JM^{-1}) = MJ^3M^{-1} \ ,$$

and, in general,

$$P^m = MJ^mM^{-1}, \qquad m = 0, 1, 2, \ldots \tag{18b}$$

[1/] A matrix in Jordan canonical form has nonzero elements only on the main diagonal and superdiagonal, and that the elements on the superdiagonal are restricted to be either zero or one.

Now, consider an arbitrary $n \times n$ matrix J in the Jordan canonical form

$$J = \begin{bmatrix} D & & & \\ & S_1 & & \\ & & \ddots & \\ & & & S_r \end{bmatrix} \tag{19a}$$

Using the method for multiplying together partitioned matrices, we find

$$J^m = \begin{bmatrix} D^m & & & \\ & S_1^m & & \\ & & \ddots & \\ & & & S_r^m \end{bmatrix}, \quad m = 0, 1, 2, \ldots \tag{19b}$$

Substituting Equation (18b) and Equation (19b) into Equation (9), we get

$$C(m) = C(0)M \begin{bmatrix} D^m & & & \\ & S_1^m & & \\ & & \ddots & \\ & & & S_r^m \end{bmatrix} M^{-1} \tag{20}$$

Since an arbitrary $k \times k$ diagonal matrix D is defined by

$$D = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_k \end{bmatrix}$$

Thus,

$$D^m = \begin{bmatrix} \lambda_1^m & & & \\ & \lambda_2^m & & \\ & & \ddots & \\ & & & \lambda_k^m \end{bmatrix} \qquad (21)$$

Since an arbitrary $\nu \times \nu$ semi-diagonal matrix S_r is defined as

$$S_r = \begin{bmatrix} \lambda_r & 1 & 0 & \cdots & 0 & 0 \\ 0 & \lambda_r & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \lambda_r & 1 \\ 0 & 0 & 0 & \cdots & 0 & \lambda_r \end{bmatrix}$$

It can be shown that [7]

$$S_r^m = \begin{bmatrix} \lambda_r^m & \frac{m\lambda_r^{m-1}}{1!} & \frac{m(m-1)\lambda_r^{m-2}}{2!} & \cdots & \frac{m(m-1)\ldots(m-\nu+2)\lambda_r^{m-\nu+1}}{(\nu-1)!} \\ 0 & \lambda_r^m & \frac{m\lambda_r^{m-1}}{1!} & \cdots & \frac{m(m-1)\ldots(m-\nu+3)\lambda_r^{m-\nu+2}}{(\nu-2)!} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{m\lambda_r^{m-1}}{1!} \\ 0 & 0 & 0 & \cdots & \lambda_r^m \end{bmatrix} \qquad (22)$$

From Equation (20), Equation (21), and Equation (22), we know that the system will be stable if the magnitude of all the eigenvalues of the fractional input matrix P computed by Equation (17) are less than one.

III. USE OF DISCRETE FLOW MODEL

Computation of the Volumes of the Regions in Flow Systems

From Equation (2), we know

$$p_{ij} = \frac{q_{ij}\Delta t}{v_j}, \qquad i,j = 1,2,\ldots,n$$

Thus,

$$p_{ij}v_j = q_{ij}\Delta t, \qquad i,j = 1,2,\ldots,n$$

Or,

$$\sum_{j=1}^{n} p_{ij}v_j = \sum_{j=1}^{n} q_{ij}\Delta t, \qquad i = 1,2,\ldots,n \qquad (23)$$

Case 1. If region i has no outlet to the outlet station, then

$$\sum_{j=1}^{n} q_{ij}\Delta t = v_i, \qquad i = 1,2,\ldots,n \qquad (24)$$

Substituting Equation (24) into Equation (23), we get

$$\sum_{j=1}^{n} p_{ij}v_j = v_i, \qquad i = 1,2,\ldots,n \qquad (25)$$

Case 2. If region i has an outlet to the outlet station, then

$$\sum_{j=1}^{n} q_{ij} \Delta t = v_i - (q_{i,out} \Delta t) , \qquad i = 1, 2, \ldots, n \tag{26}$$

Substituting Equation (26) into Equation (23), we get

$$\sum_{j=1}^{n} p_{ij} v_j = v_i - (q_{i,out} \Delta t) , \qquad i = 1, 2, \ldots, n \tag{27}$$

Now suppose that a flow system assumed to consist of n regions has some outlets to the outlet station, say from region k and region n for example, then Equation (25) and Equation (27) can be written together in matrix form as

$$P. \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_k \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_k - (q_{k,out}) \Delta t \\ \vdots \\ v_n - (q_{n,out}) \Delta t \end{bmatrix} \tag{28}$$

Or,

$$P. \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_k \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_k \\ \vdots \\ v_n \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \vdots \\ -(q_{k,out}) \Delta t \\ \vdots \\ -(q_{n,out}) \Delta t \end{bmatrix} \tag{29}$$

Thus,

$$(P-I)\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_k \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ -(q_{k,out})\Delta t \\ \vdots \\ -(q_{n,out})\Delta t \end{bmatrix} \quad (30)$$

If (P-I) is non-singular (none of the eigenvalues of matrix P is equal to one), then the matrix (P-I) is invertible.

Then, the above equation becomes

$$\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_k \\ \vdots \\ v_n \end{bmatrix} = (P-I)^{-1} \begin{bmatrix} 0 \\ 0 \\ \vdots \\ -(q_{k,out})\Delta t \\ \vdots \\ -(q_{n,out})\Delta t \end{bmatrix} \quad (31)$$

Equation (31) states that the volumes of the regions in flow systems can be computed easily by that equation if the fractional input matrix P is known.

Negative (or imaginary) volume, from a physical viewpoint, does not make sense at all. Thus, one simple question may be raised: Is there any guarantee to get only positive volumes of the regions by using Equation (31)? The answer of that question is shown as follows:

From Equation (31), we know

$$\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_k \\ \vdots \\ v_n \end{bmatrix} = (P-I)^{-1} \begin{bmatrix} 0 \\ 0 \\ \vdots \\ -(q_{k,out})\Delta t \\ \vdots \\ -(q_{n,out})\Delta t \end{bmatrix}$$

By a simple expansion of $(P-I)^{-1}$, we get

$$(P-I)^{-1} = -(I+P+P^2+P^3+P^4+\dots) \tag{32}$$

This series must converge because all the eigenvalues of the matrix P must be less than one.

Substituting Equation (32) into Equation (31), we find

$$\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_k \\ \vdots \\ v_n \end{bmatrix} = -(I+P+P^2+P^3+P^4+\dots) \begin{bmatrix} 0 \\ 0 \\ \vdots \\ -(q_{k,out})\Delta t \\ \vdots \\ -(q_{n,out})\Delta t \end{bmatrix} \tag{33a}$$

Or,

$$\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_k \\ \vdots \\ v_n \end{bmatrix} = (I+P+P^2+P^3+P^4+\ldots) \begin{bmatrix} 0 \\ 0 \\ \vdots \\ +(q_{k,out})\Delta t \\ \vdots \\ +(q_{n,out})\Delta t \end{bmatrix} \tag{33b}$$

Thus, if all the elements of the fractional input matrix P are positive, then, obviously, all the v_i are positive according to Equation (33b).

Prediction of the I (Internal Age Distribution) Curves and the F (Step Response) Curve in Flow Systems

The I curves of the regions and the F curve of a flow system can be calculated easily if the fractional input matrix P of that system is known. We assume that all the material enter the system from a single inlet station and all leave into a single outlet station.

Suppose that a flow system consists of n regions. Then the matrix P is $n \times n$ matrix. In order to compute the I curves and the F curve simultaneously, we have to include an accumulating outlet station, i.e., $i = n+1$. Then the augmented fractional input matrix $\overline{P}$ can be written as

$$\overline{P} = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1n} & p_{1,n+1} \\ p_{21} & p_{22} & \cdots & p_{2n} & p_{2,n+1} \\ \vdots & \vdots & & \vdots & \vdots \\ p_{n1} & p_{n2} & \cdots & p_{nn} & p_{n,n+1} \\ p_{n+1,1} & p_{n+1,2} & \cdots & p_{n+1,n} & p_{n+1,n+1} \end{bmatrix} \quad (34a)$$

Once the tracer elements enter the outlet station, they stay there permanently, hence

$$p_{n+1,i} = \begin{cases} 0 & i \neq n+1 \\ 1 & i = n+1 \end{cases}$$

Thus, Equation (34a) becomes

$$\overline{P} = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1n} & p_{1,n+1} \\ p_{21} & p_{22} & \cdots & p_{2n} & p_{2,n+1} \\ \vdots & \vdots & & \vdots & \vdots \\ p_{n1} & p_{n2} & \cdots & p_{nn} & p_{n,n+1} \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix} \quad (34b)$$

If no tracer is introduced for $t > 0$, we may write (analogous to Equation (9))

$$\overline{C}(m) = \overline{C}(0)\overline{P}^m , \qquad m = 0, 1, 2, \ldots \quad (35)$$

where $\overline{C}(0)$ is tracer concentration row vector including the outlet station at $t = 0$, i.e., $\overline{C}(0) = [c_1(0)\ c_2(0) \ldots c_n(0)\ c_{n+1}(0)]$, and

$\overline{C}(m)$ is tracer concentration row vector including the outlet station at $t = m\Delta t$, i.e., $\overline{C}(m) = [c_1(m)\ c_2(m) \ldots c_n(m)\ c_{n+1}(m)]$.

Suppose that we inject a unit of tracer into the inlet station at $t = 0^-$, then $c_1(m), c_2(m), \ldots,$ and $c_n(m)$, $m = 0, 1, 2, \ldots,$ computed by Equation (35) are the I curves corresponding to region 1, region 2, ..., and region n of the flow system. Also, $c_{n+1}(m)$, $m = 0, 1, 2, \ldots,$ computed by Equation (35) is the F curve (step response) of the system. If the flow system only has one outlet to the outlet station, say region n for example, then $c_n(m)$, $m = 0, 1, 2, \ldots,$ computed by Equation (35) is the RTD curve (impulse response) of the flow system.

Calculation of Reaction Conversion

Suppose that chemical reaction occurs in a flow system assumed to consist of n regions as shown in Figure 1. The reaction is

$$A \longrightarrow \text{Products} \tag{36a}$$

In a constant volume system, the reaction rate of component A is a known function as

$$r_A = -\frac{dc_A}{dt} = f(c_A) \tag{36b}$$

We assume that at the beginning of each time interval, each region exchanges material instantaneously with the others according to the matrix P. The new material mixes immediately and then the reaction proceeds according to Equation (36a) for a time interval of Δt. At the end of this interval, there is an immediate redistribution and mixing followed by reaction during the next time interval. The mechanism of this reaction-flow model is shown in Figure 2. During the first time interval, $c_i(t)$ reacts to form $c_i^r(t+\Delta t)$. Here $c_i(t)$ is the concentration of component A in region i at time t, and $c_i^r(t+\Delta t)$ is the concentration of component A in the fluid streams from region i at time $t+\Delta t$ (just before redistribution). $c_i^r(t+\Delta t)$ can be computed from Equation (36b) if $c_i(t)$ is known.

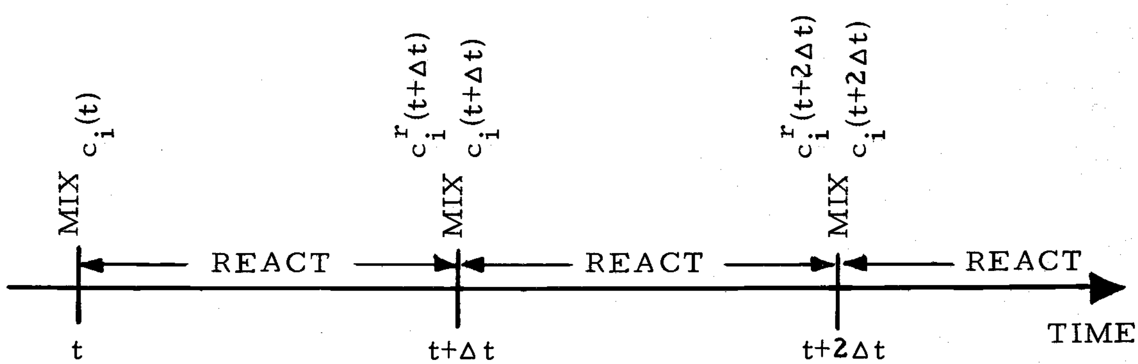

Figure 2. A schematic mechanism of the reaction-flow model.

Then from the state transition equation of discrete flow model (Equation (7)), we know

$$C(m+1) = C(m)P + F(m)\Pi , \qquad m = 0, 1, 2, \ldots$$

Replacing $C(m)$ by $C^r(m+1)$ and $F(m)$ by $F^r(m+1)$, then Equation (7) becomes

$$C(m+1) = C^r(m+1)P + F^r(m+1)\Pi , \qquad m = 0, 1, 2, \ldots \tag{37}$$

where $C^r(m+1)$ is concentration row vector in the fluid streams at time $(m+1)\Delta t$, i.e., $C^r(m+1) = [c_1^r(m+1)\ c_2^r(m+1) \ldots c_n^r(m+1)]$, and $F^r(m+1)$ is input concentration row vector in the input streams at time $(m+1)\Delta t$, i.e., $F^r(m+1) = [f_1^r(m+1)\ f_2^r(m+1) \ldots f_n^r(m+1)]$.

Thus, the concentration of component A in each region at time $(m+1)\Delta t$ can be calculated by using Equation (36b) and Equation (37) if the fractional input matrix P and the feed matrix of the flow model are known.

IV. COMPARISON OF DISCRETE FLOW MODEL AND STIRRED TANK NETWORK MODEL

The stirred tank network model shown in Figure 3 assumes that the behavior of a flow system can be represented by an n stirred tanks which are connected by an arbitrary flow network. The volumes of the tanks are not necessarily equal. The nomenclature used in this model as shown in Figure 3 is analogous to that of discrete flow model as shown in Figure 1. Since the time between state transitions in this model is a continuous random variable (not a constant), we can consider it to be a continuous time process.

Now suppose that at time $t = 0^-$ we inject a pulse of tracer into a flow system assumed to consist of n stirred tanks as shown in Figure 3. Then from the mass balance of the tracer in the jth tank at time t, we find

$$v_j \frac{dc_j(t)}{dt} = \Big(- \sum_{\substack{i=1 \\ i \neq j}}^{n} q_{ji} \Big) c_j(t) + \sum_{\substack{i=1 \\ i \neq j}}^{n} q_{ij} c_i(t) - q_{j,out} c_j(t), \qquad (38)$$

$$\text{for all } t \geq 0 \quad j = 1, 2, \ldots, n$$

where $c_j(t)$ is the tracer concentration in the tank j at time t, v_j is the volume of tank j, and q_{km} is volumetric flow rate from tank k to tank m.

Define

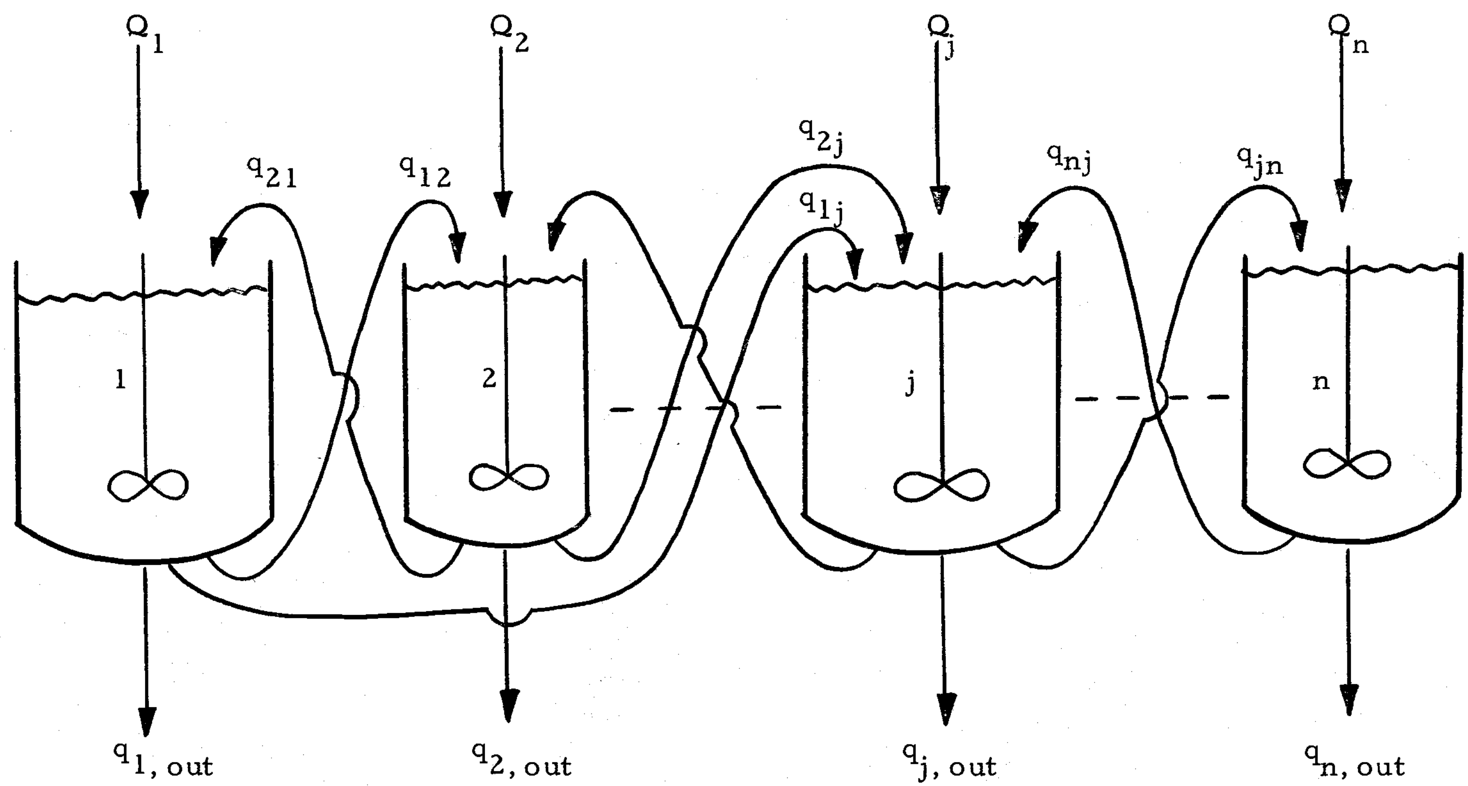

Figure 3. A schematic diagram of stirred tank network model.

$$q_{jj} = - \sum_{\substack{i=1 \\ i \neq j}}^{n} q_{ji} , \qquad j = 1, 2, \ldots, n \tag{39}$$

Substituting Equation (39) into Equation (38), we obtain

$$v_j \frac{dc_j(t)}{dt} = \sum_{i=1}^{n} q_{ij} c_i(t) - q_{j,out} c_j(t) , \tag{40}$$

for all $t \geq 0 \quad j = 1, 2, \ldots, n$

Dividing by v_j on both sides of Equation (40), we get

$$\frac{dc_j(t)}{dt} = \sum_{i=1}^{n} \left(\frac{q_{ij}}{v_j}\right) c_i(t) - \left(\frac{q_{j,out}}{v_j}\right) c_j(t) , \tag{41}$$

for all $t \geq 0 \quad j = 1, 2, \ldots, n$

Now, define

$$r_{ij} = \frac{q_{ij}}{v_j} , \qquad i, j = 1, 2, \ldots, n \tag{42}$$

$$a_j = \frac{q_{j,out}}{v_j} , \qquad j = 1, 2, \ldots, n \tag{43}$$

Equation (42) and Equation (43) define the transition rate coefficients r_{ij} and output coefficients a_j respectively.

Substituting Equation (42) and Equation (43) into Equation (41), we obtain

$$\frac{dc_j(t)}{dt} = \sum_{i=1}^{n} r_{ij} c_i(t) - a_j c_j(t) \, , \qquad (44)$$

$$\text{for all } t \geq 0 \quad j = 1, 2, \ldots, n$$

where r_{ij} is the transition rate coefficient from tank i to tank j, and a_j is the output coefficient from tank j. The above equation can be written in a matrix notation as

$$\frac{dC(t)}{dt} = C(t)R - C(t)A = C(t)(R-A), \quad \text{for all } t \geq 0 \qquad (45)$$

where $C(t)$ is tracer concentration row vector with elements $c_i(t)$ at time t, R is the transition rate matrix with elements r_{ij}, i.e.,

$$R = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ r_{21} & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & & \vdots \\ r_{n1} & r_{n2} & \cdots & r_{nn} \end{bmatrix} ,$$

and A is the output matrix with diagonal elements a_j, i.e.,

$$A = \begin{bmatrix} a_1 & & \\ & a_2 & \\ & & \ddots \\ & & & a_n \end{bmatrix} .$$

Taking the Laplace Transform of Equation (45) with respect to t, we get

$$s\bar{C}(s) - C(0) = \bar{C}(s)(R-A) \tag{46a}$$

where $\bar{C}(s)$ is the row vector of the Laplace Transforms of the tracer concentrations. Thus,

$$\bar{C}(s)(sI-(R-A)) = C(0) \tag{46b}$$

Or,

$$\bar{C}(s) = C(0)(sI-(R-A))^{-1} \tag{46c}$$

Inverting the Laplace Transform of Equation (46c), we obtain

$$C(t) = C(0)\exp((R-A)t), \quad \text{for all } t \geq 0 \tag{47}$$

Equation (47) is the state transition equation of the stirred tank network model for a pulse tracer input at $t = 0^-$. From the definition of r_{ij} (Equation (42)), we know

$$r_{ij} = \frac{q_{ij}}{v_j}, \qquad i,j = 1,2,\ldots,n$$

Thus,

$$r_{ij}v_j = q_{ij}, \qquad i,j = 1,2,\ldots,n$$

Then,

$$\sum_{j=1}^{n} r_{ij}v_j = \sum_{j=1}^{n} q_{ij}, \qquad i = 1,2,\ldots,n \tag{48}$$

From Equation (39), we know

$$\sum_{j=1}^{n} q_{ij} = 0 \, , \qquad i = 1, 2, \ldots, n \tag{49}$$

Substituting Equation (49) into Equation (48), we find

$$\sum_{j=1}^{n} r_{ij} v_j = 0 \, , \qquad i = 1, 2, \ldots, n \tag{50a}$$

Thus,

$$r_{ii} v_i + \sum_{\substack{j=1 \\ j \neq i}}^{n} r_{ij} v_j = 0 \, , \qquad i = 1, 2, \ldots, n \tag{50b}$$

Adding $-a_i v_i$ on both sides of Equation (50b), we obtain

$$(r_{ii} - a_i) v_i + \sum_{\substack{j=1 \\ j \neq i}}^{n} r_{ij} v_j = -a_i v_i \, , \qquad i = 1, 2, \ldots, n \tag{51}$$

Substituting Equation (43) into Equation (51), we get

$$(r_{ii} - a_i) v_i + \sum_{\substack{j=1 \\ j \neq i}}^{n} r_{ij} v_j = -q_{i,out} \, , \qquad i = 1, 2, \ldots, n \tag{52}$$

The above equation can be written in matrix form as

$$(R-A)\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}_{\text{stirred tank network}} = \begin{bmatrix} -q_{1,out} \\ -q_{2,out} \\ \vdots \\ -q_{n,out} \end{bmatrix} \tag{53}$$

If matrix (R-A) is non-singular, then the unique solution of Equation (53) is

$$\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}_{STN} = (R-A)^{-1} \begin{bmatrix} -q_{1,out} \\ -q_{2,out} \\ \vdots \\ -q_{n,out} \end{bmatrix} \tag{54}$$

Equation (54) states that if we can find matrix (R-A), then we can find the volumes of the tanks for this model. Once the volumes of the stirred tanks are found, then, from Equation (42) and Equation (43), we can find the volumetric flow rates connecting the tanks.

Next, let us look at the discrete flow model. As we know, the state transition equation of discrete flow model for a pulse tracer input at $t = 0^-$ is (see Equation (9))

$$C(m) = C(0)P^m, \qquad m = 0, 1, 2, \ldots$$

And,

$$\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}_{DFM} = (P-I)^{-1} \begin{bmatrix} -(q_{1,out})\Delta t \\ -(q_{2,out})\Delta t \\ \vdots \\ -(q_{n,out})\Delta t \end{bmatrix} \tag{31}$$

Suppose that we would like to find a matrix $(R-A)$ for stirred tank network model (continuous time process) that will have the same tracer concentrations as the discrete flow model (discrete time process) described by matrix P at $t = 0, \Delta t, 2\Delta t, \ldots,$ where one step time interval Δt is defined as the time for one transition of the discrete time process.

By comparison of Equation (47) and Equation (9) when $t = m\Delta t$, we know that

$$\exp((R-A)\Delta t) = P \tag{55}$$

Or,

$$R - A = \frac{\ell n\, P}{\Delta t} \tag{56}$$

From Equation (55) and Equation (56), we know that Matrix P for discrete flow model and matrix $(R-A)$ for stirred tank network model are nearly interchangeable in many cases. For every case of stirred tank network model we can find the corresponding case of discrete flow model according to Equation (55), while it is not true in the other direction according to Equation (56) since the convergence of

$\ell n\ P$ depends on the eigenvalues λ of matrix P. Hence, we may say that discrete flow model is a more general model than stirred tank network model.

Now, if we substitute Equation (56) into Equation (54) and then compare it with Equation (31), we find

$$\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}_{STN} = (\ell n\ P)^{-1}(P-I) \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}_{DFM} \tag{57}$$

Similarly,

$$\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}_{DFM} = \left(\frac{\exp((R-A)\Delta t)-I}{\Delta t}\right)^{-1}(R-A) \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}_{STN} \tag{58}$$

Equation (57) and Equation (58) give the relationship between the volumes of the regions for discrete flow model and the volumes of the stirred tanks for stirred tank network model

V. DETERMINATION OF FRACTIONAL INPUT COEFFICIENTS FROM EXPERIMENTAL DATA

The fractional input coefficients p_{ij} play an important role in the discrete flow model. Hence, the general methodologies for determining them based on multiple steady state or transient tracer measurements are developed.

From Steady State Tracer Measurements

Consider a flow system which is assumed to consist of n regions as shown in Figure 1. Then from the state transition equation of this flow model (see Equation (7)), we know

$$C(m+1) = C(m)P + F(m)\Pi \,, \qquad m = 0, 1, 2, \ldots$$

Now, suppose

$$C(0) = [0 \quad 0 \ldots 0] \,,$$

$$F(m) = [\frac{1}{\pi_1} \; 0 \ldots 0] \,, \qquad m = 0, 1, 2, \ldots$$

Then,

$$F(m)\Pi = [\frac{1}{\pi_1} \quad 0 \ldots 0] \begin{bmatrix} \pi_1 & & & \\ & \pi_2 & & \\ & & \ddots & \\ & & & \pi_n \end{bmatrix}$$

$$= [1 \quad 0 \ldots 0]$$

Substituting this into Equation (7), we find

$$C(1) = C(0)P + F(0)\Pi = [0 \;\; 0 \; \ldots \; 0] + [1 \;\; 0 \; \ldots \; 0]$$

$$= [1 \;\; 0 \; \ldots \; 0] \, ,$$

$$C(2) = C(1)P + F(1)\Pi$$

$$= [1 \;\; 0 \ldots 0]P + [1 \;\; 0 \ldots 0] \, ,$$

$$C(3) = C(2)P + F(2)\Pi$$

$$= [1 \;\; 0 \ldots 0]P^2 + [1 \;\; 0 \ldots 0]P + [1 \;\; 0 \ldots 0] \, ,$$

in general,

$$C(m+1) = [1 \;\; 0 \ldots 0]P^m + [1 \;\; 0 \ldots 0]P^{m-1} + \ldots$$

$$+ [1 \;\; 0 \ldots 0]P + [1 \;\; 0 \ldots 0]$$

$$= [1 \;\; 0 \ldots 0](P^m + P^{m-1} + \ldots + P + I) \tag{59}$$

We define the limit as $m \rightarrow \infty$ as

$$\lim_{m \rightarrow \infty} C(m+1) = [s_{11} \;\; s_{12} \cdots s_{1n}] \tag{60}$$

Here s_{ij} is the steady response at region j to a steady input at region i.

Substituting Equation (60) into Equation (59), we obtain

$$[s_{11} \;\; s_{12} \cdots s_{1n}] = [1 \;\; 0 \ldots 0] \lim_{m \rightarrow \infty} (P^m + P^{m-1} + \ldots + P + I) \tag{61}$$

Since

$$\lim_{m \to \infty} (P^m + P^{m-1} + \ldots + P + I) = (I-P)^{-1}$$

Thus, Equation (61) becomes

$$[s_{11} \ \ s_{12} \cdots s_{1n}] = [1 \ \ 0 \ldots 0](I-P)^{-1} \tag{62}$$

Similarly,

$$\begin{aligned} [s_{21} \ \ s_{22} \cdots s_{2n}] &= [0 \ \ 1 \ldots 0](I-P)^{-1} \\ &\vdots \\ [s_{n1} \ \ s_{n2} \cdots s_{nn}] &= [0 \ \ 0 \ldots 1](I-P)^{-1} \end{aligned} \tag{63}$$

Combining Equation (62) and Equation (63) together, we know

$$\begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1n} \\ s_{21} & s_{22} & \cdots & s_{2n} \\ \vdots & \vdots & & \vdots \\ s_{n1} & s_{n2} & \cdots & s_{nn} \end{bmatrix} = \begin{bmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \ldots & 1 \end{bmatrix} (I-P)^{-1} \tag{64}$$

Define

$$S = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1n} \\ s_{21} & s_{22} & \cdots & s_{2n} \\ \vdots & \vdots & & \vdots \\ s_{n1} & s_{n2} & \cdots & s_{nn} \end{bmatrix} \tag{65}$$

where S is the steady response matrix with elements s_{ij}. Then Equation (64) becomes

$$S = I(I-P)^{-1} = (I-P)^{-1} \tag{66}$$

Hence

$$P = I - S^{-1} \tag{67}$$

Equation (67) simply tells that in order to find the fractional input coefficients p_{ij} for steady tracer inputs, the only information we need to know is n^2 measurements of steady tracer responses from the experiment. Conversely, the fractional input coefficients p_{ij} can be used to obtain the steady state responses from Equation (66).

From Transient Tracer Measurements

Consider a flow system which is assumed to consist of n regions as shown in Figure 1. For an instantaneous or pulse tracer input at $t = 0^-$, then the state transition equation of this flow model becomes (see Equation (9))

$$C(m) = C(0)P^m, \qquad m = 0, 1, 2, \ldots$$

Thus,

$$\begin{aligned} C(1) &= C(0)P \\ C(2) &= C(0)P^2 = C(1)P \\ C(3) &= C(0)P^3 = C(2)P \\ &\vdots \\ C(n-1) &= C(0)P^{n-1} = C(n-2)P \\ C(n) &= C(0)P^n = C(n-1)P \end{aligned} \tag{68}$$

Equation (68) can be written as

$$\begin{bmatrix} C(1) \\ C(2) \\ C(3) \\ \vdots \\ C(n-1) \\ C(n) \end{bmatrix} = \begin{bmatrix} C(0) \\ C(1) \\ C(2) \\ \vdots \\ C(n-2) \\ C(n-1) \end{bmatrix} P \tag{69}$$

If the first square matrix in the right-hand side of Equation (69) is non-singular, then the unique solution of Equation (69) is

$$P = \begin{bmatrix} C(0) \\ C(1) \\ C(2) \\ \vdots \\ C(n-2) \\ C(n-1) \end{bmatrix}^{-1} \begin{bmatrix} C(1) \\ C(2) \\ C(3) \\ \vdots \\ C(n-1) \\ C(n) \end{bmatrix} \tag{70a}$$

Or,

$$P = \begin{bmatrix} c_1(0) & c_2(0) & \dots & c_n(0) \\ c_1(1) & c_2(1) & \dots & c_n(1) \\ c_1(2) & c_2(2) & \dots & c_n(2) \\ \vdots & \vdots & & \vdots \\ c_1(n-2) & c_2(n-2) & \dots & c_n(n-2) \\ c_1(n-1) & c_2(n-1) & \dots & c_n(n-1) \end{bmatrix}^{-1} \begin{bmatrix} c_1(1) & c_2(1) & \dots & c_n(1) \\ c_1(2) & c_2(2) & \dots & c_n(2) \\ c_1(3) & c_2(3) & \dots & c_n(3) \\ \vdots & \vdots & & \vdots \\ c_1(n-1) & c_2(n-1) & \dots & c_n(n-1) \\ c_1(n) & c_2(n) & \dots & c_n(n) \end{bmatrix} \tag{70b}$$

Equation (70b) (or Equation (70a)) simply tells that in order to find the fractional input coefficients p_{ij} for a pulse tracer input, the only information we need to know is n^2 transient tracer measurements from the experiment if the initial condition is known.

VI. A LUMPING ANALYSIS IN DISCRETE FLOW SYSTEMS

Lumping is important for modeling flow systems. Particularly, when a flow system has many regions, it is convenient and practical to lump all these smaller regions into larger regions and treat them as non-overlapping lumped regions. So far, no work has been done on lumping of flow systems, probably, because it requires a priori knowledge of the whole set of flow rates connecting the regions, and the volumes of the regions. Such information is rarely directly available for most of flow systems. Therefore, the methods shown in Chapter III and Chapter V for obtaining the sizes of the regions and the fractional input coefficients will provide an important tool to analyze the lumping problems in flow systems.

In 1969, Wei and Kuo [21] introduced a lumping theory for monomolecular reaction systems in a discrete mixture. This was extended to a continuous mixture later by Bailey [1]. Although lumping in the flow systems is more complicated and more difficult[2/] than that of in monomolecular reaction systems, many of the lumping concepts in their work are still useful for the flow systems.

[2/] Due to the following reasons:
1. One more variable set, i.e., the volumes of the regions, involved.
2. Flow systems usually possess inlet-outlet stations while the monomolecular reaction systems do not have those.

Lumping is a linear transformation from an n element vector, CV, into an k element vector, $\hat{C}\hat{V}$, of smaller dimension (i.e., $k < n$) by an $n \times k$ lumping matrix L,

$$\hat{C}\hat{V} = (CV)L \tag{71}$$

where V and $\hat{V}$ are the diagonal volume matrices of the original system and the lumped system respectively, i.e.,

$$V = \begin{bmatrix} v_1 & & & \\ & v_2 & & \\ & & \ddots & \\ & & & v_n \end{bmatrix},$$

$$\hat{V} = \begin{bmatrix} \hat{v}_1 & & & \\ & \hat{v}_2 & & \\ & & \ddots & \\ & & & \hat{v}_k \end{bmatrix},$$

and C and $\hat{C}$ are concentration row vectors of the original system and the lumped system respectively, and thus,

$$CV = [c_1 v_1 \;\; c_2 v_2 \; \ldots \; c_n v_n],$$

$$\hat{C}\hat{V} = [\hat{c}_1 \hat{v}_1 \;\; \hat{c}_2 \hat{v}_2 \; \ldots \; \hat{c}_k \hat{v}_k].$$

In order to retain the property of dividing all the regions into a few larger regions for the lumping, each row of lumping matrix L must be a unit vector u_i. If the system is lumped by such an L, then the lumping is called proper [21]. For instance, suppose that we want to lump region 1 and region 2 of a flow system consisting of four regions into a larger region called region $\hat{1}$, then the proper lumping matrix is

$$L = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Now suppose that there are n regions in a given flow system. Then from Equation (9), we know

$$C(m) = C(0)P^m, \qquad m = 0, 1, 2, \ldots$$

Similarly, from the mass balance of the lumped system consisting of k regions (k < n), we know

$$\hat{C}(m) = \hat{C}(0)\hat{P}^m, \qquad m = 0, 1, 2, \ldots \tag{72}$$

where $\hat{P}$ is the fractional input matrix of the lumped system, i.e.,

$$\hat{P} = \begin{bmatrix} \hat{p}_{11} & \hat{p}_{12} & \cdots & \hat{p}_{1k} \\ \hat{p}_{21} & \hat{p}_{22} & \cdots & \hat{p}_{2k} \\ \vdots & \vdots & & \vdots \\ \hat{p}_{k1} & \hat{p}_{k2} & \cdots & \hat{p}_{kk} \end{bmatrix}$$

Now, in order to estimate the magnitude of errors resulting from lumping in a given flow system, a criterion which has some resemblance to Wei and Kuo's work [21] is established. Usually, there are two ways to compute the concentration row vector $\hat{C}(m)$ of the lumped system. The right way is to compute $C(m)$ first (by Equation (9)) and then lump $C(m)$ into $\hat{C}(m)$ by using Equation (71), as

$$\hat{C}^{(r)}(m) = C(m)VL\hat{V}^{-1} = C(0)P^{m}VL\hat{V}^{-1} \tag{73}$$

where $\hat{C}^{(r)}(m)$ is the concentration row vector of the lumped system computed in the right way.

The wrong way is first to lump $C(0)$ into $\hat{C}(0)$ (by Equation (71)) and then compute $\hat{C}(m)$ by using Equation (72), as

$$\hat{C}^{(w)}(m) = \hat{C}(0)\hat{P}^{m} = C(0)VL\hat{V}^{-1}\hat{P}^{m} \tag{74}$$

where $\hat{C}^{(w)}(m)$ is the concentration row vector of the lumped system computed in the wrong way.

Thus, the error of lumping is

$$\hat{C}^{(r)}(m) - \hat{C}^{(w)}(m) = C(0)(P^m VL\hat{V}^{-1} - VL\hat{V}^{-1}\hat{P}^m) \tag{75}$$

Let

$$B = VL\hat{V}^{-1} \tag{76}$$

Substituting Equation (76) into Equation (75), we get

$$\hat{C}^{(r)}(m) - \hat{C}^{(w)}(m) = C(0)(P^m B - B\hat{P}^m) \tag{77}$$

<u>Case 1</u>. If the system is exactly lumpable, then

$$\hat{C}^{(r)}(m) - \hat{C}^{(w)}(m) = 0$$

Substituting this into Equation (77), we know

$$P^m B - B\hat{P}^m = 0 \tag{78a}$$

Or,

$$P^m B = B\hat{P}^m \tag{78b}$$

<u>Case 2</u>. If the system is not exactly lumpable (like most of flow systems), then

$$\hat{C}^{(r)}(m) - \hat{C}^{(w)}(m) \neq 0$$

Substituting this into Equation (77), we know

$$P^m B - B\hat{P}^m \neq 0 , \qquad m > 0 \tag{79}$$

Most of the flow systems are not exactly lumpable by a proper lumping matrix L, so here we examine only Case 2 in more detail. We define a new matrix called the <u>error matrix</u>, $E(m)$, which has the lumping error vector at $C(0) = u_i$ as its ith row vector. More precisely, the element $e_{ij}(m)$ of the error matrix $E(m)$ is defined as the lumping error at the region j of the lumped system to a unit tracer input at region i of the original system.

Then from Equation (77), we know

$$E(m) = P^m B - B\hat{P}^m, \qquad m > 0 \tag{80}$$

Using the standard method [3, 22] to diagonalize the matrices of P and $\hat{P}$ (if they are diagonalizable), we get

$$P^m = MD^m M^{-1} \tag{81}$$

$$\hat{P}^m = \hat{M}\hat{D}^m \hat{M}^{-1} \tag{82}$$

where M and $\hat{M}$ are eigenvector matrices of P and $\hat{P}$ respectively, D and $\hat{D}$ are diagonal eigenvalue matrices of P and $\hat{P}$ respectively.

Substituting Equation (81) and Equation (82) into Equation (80), we obtain

$$E(m) = MD^m M^{-1} B - B\hat{M}\hat{D}^m \hat{M}^{-1} \tag{83}$$

After rearrangement, Equation (83) becomes

$$E(m) = (MD^m M^{-1} B(\hat{M}\hat{M}^{-1}) - (MM^{-1})B\hat{M}\hat{D}^m\hat{M}^{-1})$$

$$= M(D^m(M^{-1}B\hat{M}) - (M^{-1}B\hat{M})\hat{D}^m)\hat{M}^{-1} \quad (84)$$

By expansion of Equation (84), the elements $e_{ij}(m)$ of the error matrix $E(m)$ will appear in a form as shown in the following:

$$e_{ij}(m) = \sum_{r=1}^{k} \sum_{\ell=1}^{n} a_{r\ell}^{(ij)} (\lambda_\ell^m - \hat{\lambda}_r^m) , \quad (85)$$

$$i = 1, 2, \ldots, n; \quad j = 1, 2, \ldots, k$$

where λ_ℓ is the eigenvalue of matrix P, $\hat{\lambda}_r$ is the eigenvalue of matrix $\hat{P}$, $a_{r\ell}^{(ij)}$ is the coefficient of an expansion for $e_{ij}(m)$, and $e_{ij}(m)$ is the element of the error matrix $E(m)$ at the ith row and jth column.

Now, if $C(0) = u_i$, then the ith row of the error matrix $E(m)$, i. e., $[e_{i1}(m)\ e_{i2}(m) \ldots e_{ik}(m)]$, is the lumping error vector. Here $e_{ij}(m)$ is the lumping error at region j of the lumped system to a unit tracer input at region i of the original system. We now compute

$$\max_{j=1,2,\ldots,k} |e_{ij}(m)| .\text{[3/]}$$

[3/] Let $de_{ij}(m)/dm = 0$.

If $\max_{j=1,2,\ldots,k} |e_{ij}(m)| \ll 1$, then we can conclude that the lumping error is small and the lumping is good. If $\max_{j=1,2,\ldots,k} |e_{ij}(m)|$ is larger than we can tolerate, then we may say that the lumping is poor.

The procedures for demonstrating a lumping analysis in discrete flow systems can be described as follows:

1. Compute the fractional input matrices P and $\hat{P}$ of original system and the lumped system respectively by using Equation (70b) (or Equation (70a)).
2. Compute the volumes of the regions of the original and the lumped system respectively by using Equation (31).
3. Compute the error matrix $E(m)$ by using Equation (84). The elements of $E(m)$ appear in a form as Equation (85).
4. If $C(0) = u_i$, then compute $\max_{j=1,2,\ldots,k} |e_{ij}(m)|$.
5. If $\max_{j=1,2,\ldots,k} |e_{ij}(m)| \ll 1$, then we can say that the lumping is good. If $\max_{j=1,2,\ldots,k} |e_{ij}(m)|$ is larger than we can tolerate, then we may say that the lumping is poor.

VII. FITTING THE FLOW MODEL TO REAL DATA

Assumptions

Before we start fitting the model to data, some assumptions about the system are listed as follows:

1. There are enough data points with good accuracy.
2. The inflows into and outflows from the system are known.
3. The system is stationary.

Selection of the Size of One Step Time Interval

From the definition of p_{ij} of Equation (2), we know that the fractional input coefficients p_{ij} of flow systems are function of time interval Δt. Thus, before we can compute the fractional input matrix P of a flow system by using Equation (70b) (or Equation (70a)), the size of Δt must be chosen.

As we know, the smaller the size of Δt we choose, the closer will be the concentration distributions in discrete time flow systems to those of continuous time flow systems. But the computation time increases proportionally with decreasing the size of Δt.

In modeling the flow systems, there are certain range of the size of Δt can be chosen. But once the size of Δt chosen is too small, some of the fractional input coefficients will turn out to be negative. It probably can be explained thus: When the size of Δt

chosen is too short, some of the fluid elements in the regions do not have enough time to mix uniformly. A negative coefficient corresponds to reversing the direction of time. In reverse time, material would have to leave a mixed region, unmix, and then go to other regions with different concentrations. Thus, negative input coefficients suggest a reversal of the mixing processes and likely correspond to a time interval Δt too short to allow uniform mixing to occur. Hence, the restrictions for choosing the size of Δt are described as follows:

(i) All the fractional input coefficients p_{ij} computed from a choosing size of Δt must be in the range of zero to one.

(ii) The sum of the volumes of the regions computed from a choosing size of Δt must be closed enough to the given total volume of the flow system, i.e., $\sum_{(i)} v_i \simeq v_{total}$.

From the above analysis, we may conclude that if we wish to have a best fit to a flow system under investigation, then an optimum size of Δt has to be chosen for modeling that system. In practice, it has been found by the author that only a few trials are needed to find the optimum size of Δt.

Selection of Numbers of Probes

Before we start to model a flow system, it is important to know what number of probes is needed to model that system. Such information is rarely available in advance for most flow systems. Thus, a trial and error method must be used. First, assume that a small number of probes, say k probes for example, is sufficient to model the flow system which is under investigation. If the values of some elements of the fractional input matrix P computed by Equation (70b) are not in the range of zero to one or the values of the sum in some columns of that matrix are greater than one (see Equation (12) and Equation (14)) no matter what size of Δt is chosen, then we may say that an k probes is not sufficient to model that system and we have to use more probes to model the flow system. If the first square matrix in the right-hand side of Equation (70b) (or Equation (70a)) turns out to be a singular or nearly singular no matter what size of Δt is chosen, then we may say that some of k probes are redundant or nearly redundant and we must remove those redundant probes (according to their cofactors in the overall matrix)[4/] and use fewer probes to model that system.

The n $(n \lesseqgtr k)$ probe model is a good fit to the flow system under investigation if the residence time distribution (RTD) curve

---

[4/] Remove probe j first if the cofactor of the element $c_j(n-1)$ in the concentration matrix (i. e., the first square matrix in the right-hand side of Equation (70b)) is largest and so on.

and the sum of the volumes computed from that model both are closed to the real RTD curve (if it is known) and the total volume of the flow system.

Numerical Examples

In order to demonstrate how to model flow systems by using the methods shown in Chapters III, IV, and V, two simple examples are given. The first example shows how to model a continuous time, discrete space flow system. The second example shows how to model a continuous time, pseudo-continuous space flow system.

For each example, assume that a finite number of transient tracer concentrations (each measured by a single probe) are known.[5/]

Example 1. Modeling a Continuous Time, Discrete Space Flow System

Suppose that we put probe 1, probe 2, and probe 3 simultaneously into a given flow system consisting of three well-mixed regions as shown in Figure E1. The transient concentrations of tracer in this flow system that would be measured by the three probes are tabulated in Table E1.[6/] What are the volumes of these

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[5/] In these examples, simulated data are given (see Appendix B for data source).

[6/] See Appendix B.

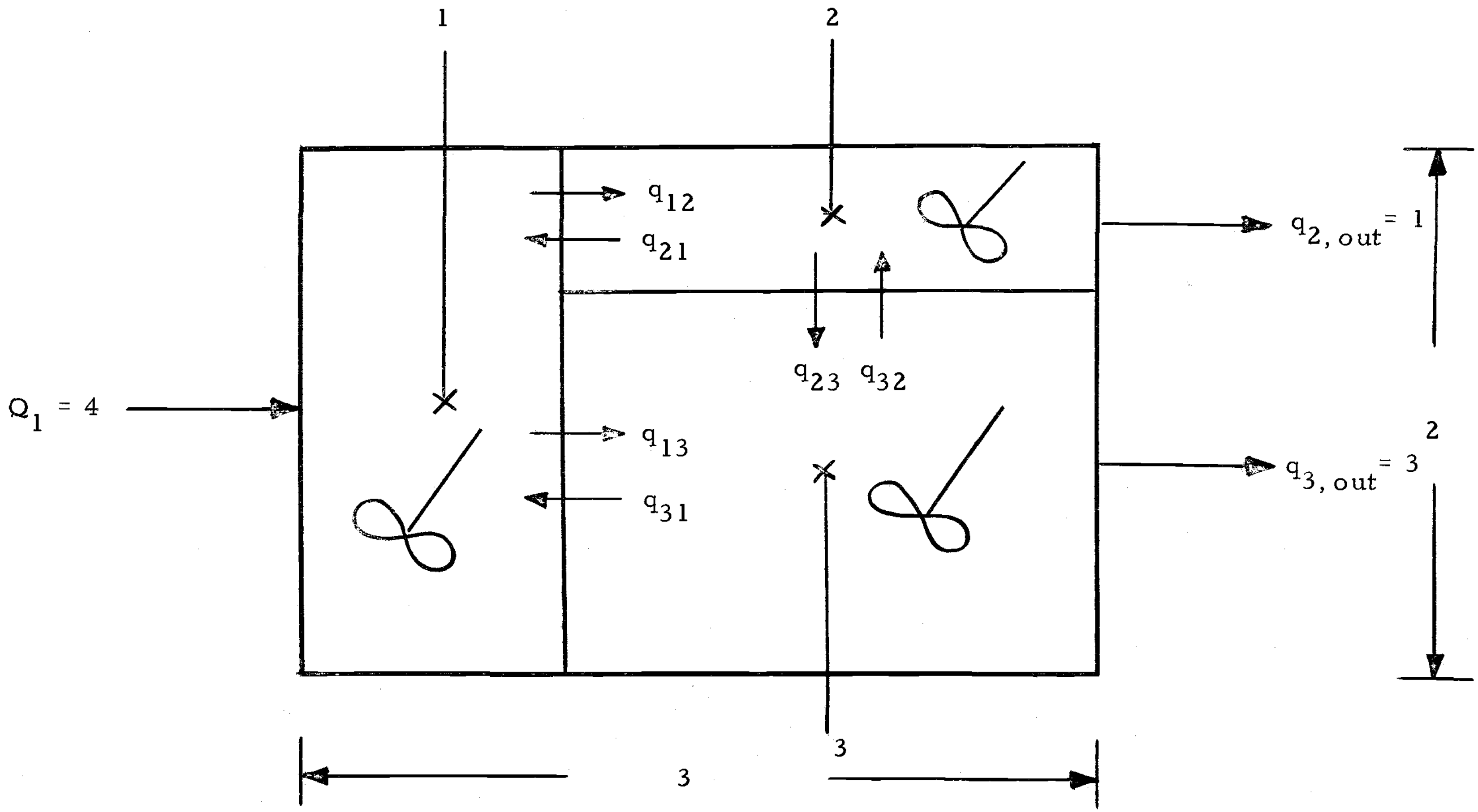

Figure E1. Diagram of the flow system in Example 1.

three regions? What are the interregion flow rates?

Table E1. Transient concentrations of tracer in the flow system of Example 1.

t	c_1	c_2	c_3
0	1.0000	0	0
0.1	0.7639	0.1625	0.0952
0.2	0.5906	0.2446	0.1633
0.3	0.4627	0.2811	0.2088
0.4	0.3676	0.2919	0.2366
0.5	0.2963	0.2885	0.2511
0.6	0.2424	0.2775	0.2558
0.7	0.2011	0.2627	0.2537
0.8	0.1693	0.2463	0.2469
0.9	0.1443	0.2294	0.2370
1.0	0.1246	0.2129	0.2252
1.1	0.1086	0.1970	0.2124
1.2	0.0956	0.1820	0.1992
1.3	0.0849	0.1679	0.1859
1.4	0.0758	0.1548	0.1730
1.5	0.0681	0.1426	0.1606
1.6	0.0615	0.1314	0.1488
1.7	0.0557	0.1209	0.1376
1.8	0.0506	0.1113	0.1271
1.9	0.0461	0.1024	0.1173
2.0	0.0421	0.0942	0.1081

Solution. 1. Modeling the well-mixed regions as discrete in time (use discrete flow model directly).

Case (i). Let $\Delta t = 0.3$. Then from Table E1, we know

$$C(0) = [c_1(0) \quad c_2(0) \quad c_3(0)] = [1.0000 \quad 0 \quad 0 \quad]$$

$$C(1) = [c_1(1) \quad c_2(1) \quad c_3(1)] = [0.4627 \quad 0.2811 \quad 0.2088]$$

$$C(2) = [c_1(2) \quad c_2(2) \quad c_3(2)] = [0.2424 \quad 0.2775 \quad 0.2558]$$

$$C(3) = [c_1(3) \quad c_2(3) \quad c_3(3)] = [0.1443 \quad 0.2294 \quad 0.2370]$$

Substituting these into Equation (70b), we find

$$P = \begin{bmatrix} 1.0000 & 0 & 0 \\ 0.4627 & 0.2811 & 0.2088 \\ 0.2424 & 0.2775 & 0.2558 \end{bmatrix}^{-1} \begin{bmatrix} 0.4627 & 0.2811 & 0.2088 \\ 0.2424 & 0.2775 & 0.2558 \\ 0.1443 & 0.2294 & 0.2370 \end{bmatrix}$$

$$= \begin{bmatrix} 0.4627 & 0.2811 & 0.2088 \\ 0.0380 & 0.2895 & 0.1291 \\ 0.0845 & 0.3164 & 0.5886 \end{bmatrix} \qquad \text{(E1)}$$

Substituting Equation (E1) into Equation (31), we obtain

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_{DFM} = (P-I)^{-1} \begin{bmatrix} -(q_{1,out})\Delta t \\ -(q_{2,out})\Delta t \\ -(q_{3,out})\Delta t \end{bmatrix}$$

$$= \begin{bmatrix} -0.5373 & 0.2811 & 0.2088 \\ 0.0380 & -0.7105 & 0.1291 \\ 0.0845 & 0.3164 & -0.4114 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ -(1)(0.3) \\ -(3)(0.3) \end{bmatrix}$$

$$= \begin{bmatrix} 1.9600 \\ 1.1598 \\ 3.4822 \end{bmatrix} \qquad \text{(E2)}$$

Substituting Equation (E1) and Equation (E2) into Equation (2), we get the interregion flow matrix

$$Q_d = \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{bmatrix} = \begin{bmatrix} 3.0230 & 1.0867 & 2.4236 \\ 0.2483 & 1.1192 & 1.4985 \\ 0.5521 & 1.2232 & 6.8321 \end{bmatrix} \quad \text{(E3)}$$

The off-diagonal elements of matrix Q_d in Equation (E3) are interregion flow rates based on $\Delta t = 0.3$.

Case (ii). Let $\Delta t = 0.1$. Then from Table E1, we know

$$C(0) = [c_1(0) \quad c_2(0) \quad c_3(0)] = [1.0000 \quad 0 \quad 0]$$

$$C(1) = [c_1(1) \quad c_2(1) \quad c_3(1)] = [0.7639 \quad 0.1625 \quad 0.0952]$$

$$C(2) = [c_1(2) \quad c_2(2) \quad c_3(2)] = [0.5906 \quad 0.2446 \quad 0.1633]$$

$$C(3) = [c_1(3) \quad c_2(3) \quad c_3(3)] = [0.4627 \quad 0.2811 \quad 0.2088]$$

Substituting these into Equation (70b), we find

$$P = \begin{bmatrix} 1.0000 & 0 & 0 \\ 0.7639 & 0.1625 & 0.0952 \\ 0.5906 & 0.2446 & 0.1633 \end{bmatrix}^{-1} \begin{bmatrix} 0.7639 & 0.1625 & 0.0952 \\ 0.5906 & 0.2446 & 0.1633 \\ 0.4627 & 0.2811 & 0.2088 \end{bmatrix}$$

$$= \begin{bmatrix} 0.7639 & 0.1625 & 0.0952 \\ 0.0165 & 0.6301 & 0.0819 \\ 0.0459 & 0.1899 & 0.8117 \end{bmatrix} \quad \text{(E4)}$$

Substituting Equation (E4) into Equation (31), we obtain

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_{DFM} = \begin{bmatrix} -0.2361 & 0.1625 & 0.0952 \\ 0.0165 & -0.3699 & 0.0819 \\ 0.0459 & 0.1899 & -0.1883 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ -(1)(0.1) \\ -(3)(0.1) \end{bmatrix}$$

$$= \begin{bmatrix} 1.9938 \\ 1.0553 \\ 3.1435 \end{bmatrix} \qquad \text{(E5)}$$

Substituting Equation (E4) and Equation (E5) into Equation (2), we get the interregion flow matrix

$$Q_d = \begin{bmatrix} 15.2308 & 1.7148 & 2.9926 \\ 0.3290 & 6.6493 & 2.5745 \\ 0.9152 & 2.0040 & 25.5155 \end{bmatrix} \qquad \text{(E6)}$$

The off-diagonal elements of matrix Q_d in Equation (E6) are interregion flow rates based on $\Delta t = 0.1$.

<u>Summary</u>. <u>Case (i)</u>. $\Delta t = 0.3$

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_{DFM} = \begin{bmatrix} 1.9600 \\ 1.1598 \\ 3.4822 \end{bmatrix} \qquad \text{(E2)}$$

$$Q_d = \begin{bmatrix} 3.0230 & 1.0867 & 2.4236 \\ 0.2483 & 1.1192 & 1.4985 \\ 0.5521 & 1.2232 & 6.8321 \end{bmatrix} \qquad \text{(E3)}$$

Case (ii). $\Delta t = 0.1$

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_{DFM} = \begin{bmatrix} 1.9938 \\ 1.0553 \\ 3.1435 \end{bmatrix} \qquad \text{(E5)}$$

$$Q_d = \begin{bmatrix} 15.2308 & 1.7148 & 2.9926 \\ 0.3290 & 6.6493 & 2.5745 \\ 0.9152 & 2.0040 & 25.5155 \end{bmatrix} \qquad \text{(E6)}$$

The true values of v_i $(i = 1, 2, 3)$ and q_{ij} $(i, j = 1, 2, 3)$ are (see Appendix B for data source)

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_{true} = \begin{bmatrix} 2.0000 \\ 1.0000 \\ 3.0000 \end{bmatrix} \qquad \text{(E7)}$$

$$Q_{true} = \begin{bmatrix} -(q_{12}+q_{13}+q_{1,out}) & q_{12} & q_{13} \\ q_{21} & -(q_{21}+q_{23}+q_{2,out}) & q_{23} \\ q_{31} & q_{32} & -(q_{31}+q_{32}+q_{3,out}) \end{bmatrix} =$$

$$= \begin{bmatrix} -5.5000 & 2.2000 & 3.3000 \\ 0.5000 & -4.8000 & 3.3000 \\ 1.0000 & 2.6000 & -6.6000 \end{bmatrix} \qquad \text{(E8)}$$

The off-diagonal elements of matrix Q_{true} in Equation (E8) are true interregional flow rates.

By comparison of calculated volumes (Equation (E2) and Equation (E5)) and true volumes (Equation (E7)), we see that the smaller the size of Δt we choose the closer are the volumes calculated from discrete flow model to the true volumes. This is also true for the calculated interregion flow rates as seen by comparing Equation (E3) and Equation (E6) to the true values (Equation (E8)).

2. Modeling the well-mixed regions as continuous in time (use discrete flow model as an intermediate).

Case (i). Let $\Delta t = 0.3$. From Equation (E1), we know

$$P = \begin{bmatrix} 0.4627 & 0.2811 & 0.2088 \\ 0.0380 & 0.2895 & 0.1291 \\ 0.0845 & 0.3164 & 0.5886 \end{bmatrix}$$

Let

$$f(P) = \ell n\, P$$

Using the polynomial method on matrices given in [3], we know

$$f(P) = \ell n\, P = r(P) = \alpha_2 P^2 + \alpha_1 P + \alpha_0 I \qquad \text{(E9)}$$

where $r(P)$ is the remainder and is of degree $n-1$ and α_i are constants.

Also,

$$f(\lambda_i) = \ell n\, \lambda_i = r(\lambda_i) = \alpha_2 \lambda_i^2 + \alpha_1 \lambda_i + \alpha_0 \qquad \text{(E10)}$$

where λ_i is the eigenvalue of matrix P.

Then from the characteristic equation of matrix P (Equation (17)), i.e., $\det(P - \lambda I) = 0$, we find

$$\lambda_1 = 0.7777$$
$$\lambda_2 = 0.3799$$
$$\lambda_3 = 0.1832$$

Substituting these into Equation (E10) to determine α_i, we obtain

$$\alpha_2 = -3.2075$$
$$\alpha_1 = 5.5140$$
$$\alpha_0 = -2.5997$$

Substituting the values of α_i into Equation (E9), we get

$$\ell n\, P = \begin{bmatrix} -0.8250 & 0.6599 & 0.3308 \\ 0.0828 & -1.4375 & 0.3228 \\ 0.1424 & 0.7773 & -0.6530 \end{bmatrix} \qquad \text{(E11)}$$

Substituting Equation (E11) into Equation (56), we find

$$R - A = \frac{\ell n\, P}{\Delta t} = \frac{\ell n\, P}{0.3}$$

$$= \begin{bmatrix} -2.7530 & 2.1997 & 1.1027 \\ 0.2760 & -4.7917 & 1.0760 \\ 0.4747 & 2.5910 & -2.1767 \end{bmatrix} \qquad \text{(E12)}$$

Substituting Equation (E12) into Equation (54), we obtain

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_{cont} = (R - A)^{-1} \begin{bmatrix} -q_{1,out} \\ -q_{2,out} \\ -q_{3,out} \end{bmatrix}$$

$$= \begin{bmatrix} -2.7530 & 2.1997 & 1.1027 \\ 0.2760 & -4.7917 & 1.0760 \\ 0.4747 & 2.5910 & -2.1767 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ -1 \\ -3 \end{bmatrix}$$

$$= \begin{bmatrix} 2.0002 \\ 0.9981 \\ 3.0026 \end{bmatrix} \qquad \text{(E13)}$$

Substituting Equation (E12) and Equation (E13) into Equation (42) and Equation (43), we get the interregion flow matrix

$$Q_{cont} = \begin{bmatrix} -(q_{12}+q_{13}+q_{1,out}) & q_{12} & q_{13} \\ q_{21} & -(q_{21}+q_{23}+q_{2,out}) & q_{23} \\ q_{31} & q_{32} & -(q_{31}+q_{32}+q_{3,out}) \end{bmatrix}$$

$$= \begin{bmatrix} -5.5065 & 2.1955 & 3.3110 \\ 0.5520 & -4.7826 & 3.2308 \\ 0.9495 & 2.5861 & -6.5357 \end{bmatrix} \tag{E14}$$

The off-diagonal elements of matrix Q_{cont} in Equation (E14) are interregion flow rates.

<u>Case (ii).</u> Let $\Delta t = 0.1$. From Equation (E4), we know

$$P = \begin{bmatrix} 0.7639 & 0.1625 & 0.0952 \\ 0.0165 & 0.6301 & 0.0819 \\ 0.0459 & 0.1899 & 0.8117 \end{bmatrix}$$

Then from the characteristic equation of matrix P (Equation (17)), i.e., $\det(P-\lambda I) = 0$, we find

$$\lambda_1 = 0.9199$$

$$\lambda_2 = 0.7196$$

$$\lambda_3 = 0.5662$$

Substituting these into Equation (E10) to determine α_i, we obtain

$$\alpha_2 = -0.9520$$

$$\alpha_1 = 2.7880$$

$$\alpha_0 = -1.8418$$

Substituting the values of α_i into Equation (E9), we get

$$\ell n\ P = \begin{bmatrix} -0.2743 & 0.2202 & 0.1099 \\ 0.0205 & -0.4804 & 0.1144 \\ 0.0561 & 0.2617 & -0.2250 \end{bmatrix} \qquad \text{(E15)}$$

Substituting Equation (E15) into Equation (56), we find

$$R - A = \frac{\ell n\ P}{0.1} = \begin{bmatrix} -2.7430 & 2.2020 & 1.0990 \\ 0.2050 & -4.8040 & 1.1440 \\ 0.5610 & 2.6170 & -2.2500 \end{bmatrix} \qquad \text{(E16)}$$

Substituting Equation (E16) into Equation (54), we obtain

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_{cont} = \begin{bmatrix} -2.7430 & 2.2020 & 1.0990 \\ 0.2050 & -4.8040 & 1.1440 \\ 0.5610 & 2.6170 & -2.2500 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ -1 \\ -3 \end{bmatrix}$$

$$= \begin{bmatrix} 2.0203 \\ 1.0122 \\ 3.0143 \end{bmatrix} \qquad \text{(E17)}$$

Substituting Equation (E16) and Equation (E17) into Equation (42) and Equation (43), we get the interregion flow matrix

$$Q_{cont} = \begin{bmatrix} -5.5417 & 2.2289 & 3.3127 \\ 0.4142 & -4.8626 & 3.4484 \\ 1.1334 & 2.6489 & -6.7822 \end{bmatrix} \qquad \text{(E18)}$$

The off-diagonal elements of matrix Q_{cont} in Equation (E18) are interregion flow rates.

Summary. Case (i). $\Delta t = 0.3$

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_{cont} = \begin{bmatrix} 2.0002 \\ 0.9981 \\ 3.0026 \end{bmatrix} \qquad \text{(E13)}$$

$$Q_{cont} = \begin{bmatrix} -5.5065 & 2.1955 & 3.3110 \\ 0.5520 & -4.7826 & 3.2308 \\ 0.9495 & 2.5861 & -6.5357 \end{bmatrix} \qquad \text{(E14)}$$

Case (ii). $\Delta t = 0.1$

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_{cont} = \begin{bmatrix} 2.0203 \\ 1.0122 \\ 3.0143 \end{bmatrix} \qquad \text{(E17)}$$

$$Q_{cont} = \begin{bmatrix} -5.5417 & 2.2289 & 3.3127 \\ 0.4142 & -4.8626 & 3.4484 \\ 1.1334 & 2.6489 & -6.7822 \end{bmatrix} \quad \text{(E18)}$$

By comparison of calculated volumes (Equation (E13) or Equation (E17)) and the true volumes (Equation (E7)), we find that the agreement is good. By comparison of calculated interregion flow rates (Equation (E14) or Equation (E18)) and the true flow rates (Equation (E8)), we find that the agreement is also good. In fact the method is exact, and the only errors are due to computer roundoff and inaccuracies in calculating the eigenvalues. The larger size of Δt gives slightly more accurate values.

Example 2. Modeling a Continuous Time, Pseudo-Continuous Space Flow System

Consider a pseudo-continuous flow system shown in Figure E2a. Suppose that the total volume of this flow system is given. The total inlet flow rate to the system and the total outlet flow rate from the system are also given. In addition, the residence time distribution (RTD) of the fluid elements in the flow system is known as shown in Figure E2b.[7/] How does one model this flow system with a finite number of probes?

[7/] See Appendix B.

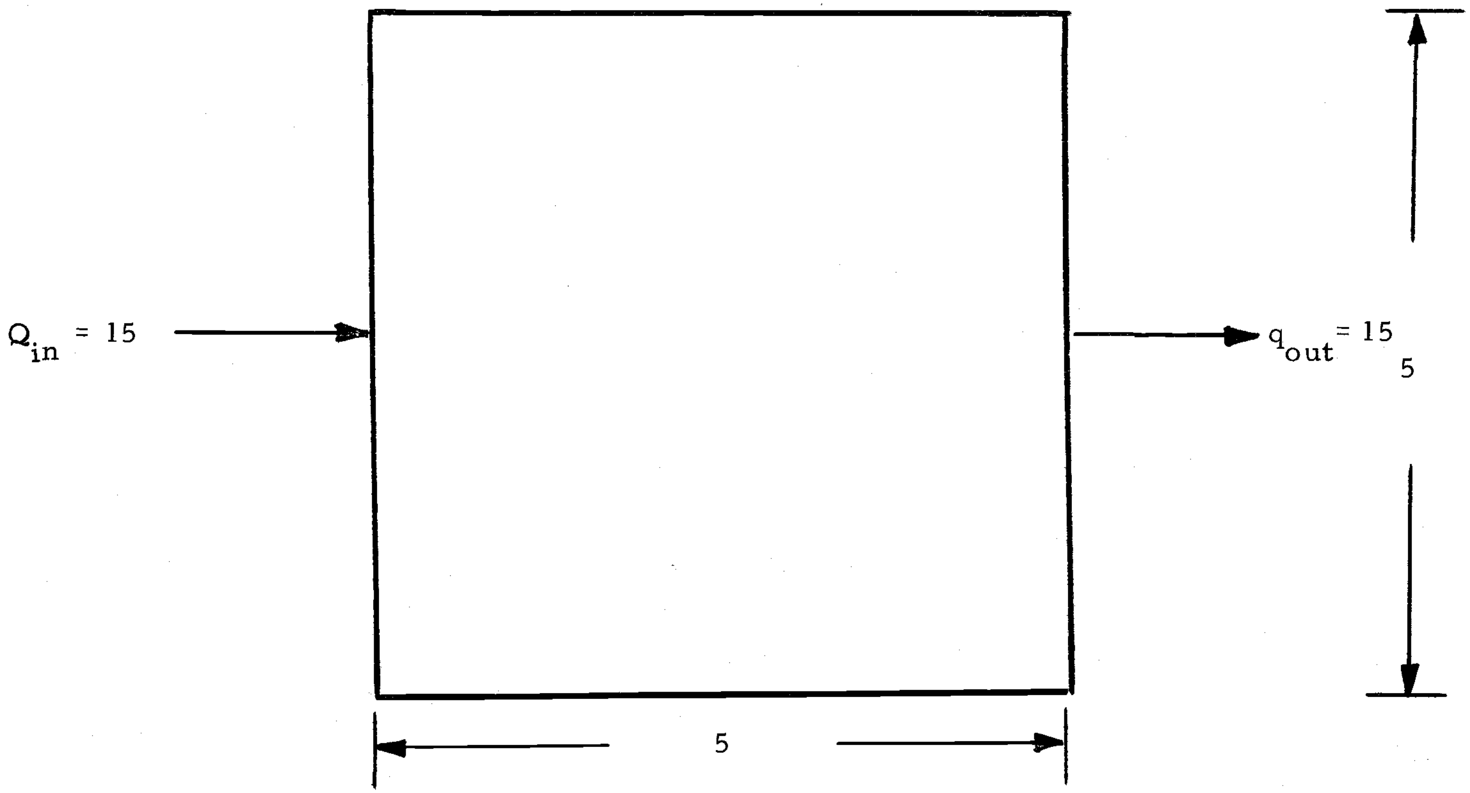

Figure E2a. Diagram of the flow system in Example 2.

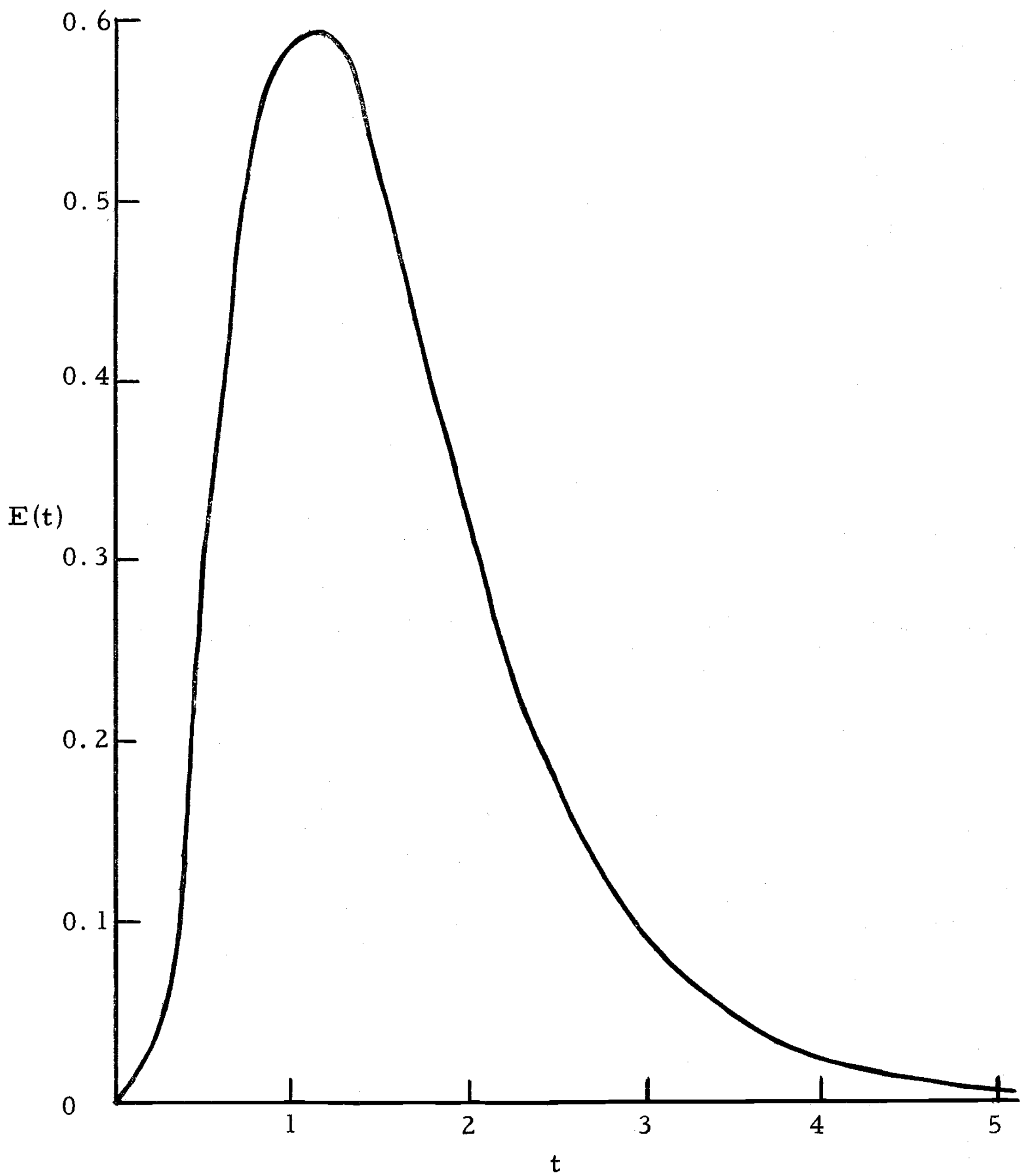

Figure E2b. The RTD curve of the flow system in Example 2.

Solution. Method 1. We would like to put three probes simultaneously into the flow system as shown in Figure E2c. The transient tracer concentrations measured by these three probes are tabulated in Table E2a.

Table E2a. Transient concentrations of tracer in the flow system of Example 2 measured by three probes.

t	c_1	c_2	c_3
0	0.2000	0	0
0.1	0.1316	0.0072	0
0.2	0.0913	0.0267	0.0003
0.3	0.0659	0.0423	0.0030
0.4	0.0490	0.0513	0.0086
0.5	0.0372	0.0546	0.0159
0.6	0.0288	0.0542	0.0234
0.7	0.0225	0.0514	0.0300
0.8	0.0178	0.0473	0.0350
0.9	0.0142	0.0427	0.0383
1.0	0.0115	0.0381	0.0400
1.1	0.0093	0.0337	0.0403
1.2	0.0076	0.0296	0.0395
1.3	0.0062	0.0258	0.0379
1.4	0.0051	0.0225	0.0357
1.5	0.0042	0.0195	0.0332
1.6	0.0035	0.0170	0.0306
1.7	0.0029	0.0147	0.0279
1.8	0.0024	0.0127	0.0253
1.9	0.0020	0.0110	0.0228
2.0	0.0017	0.0096	0.0204

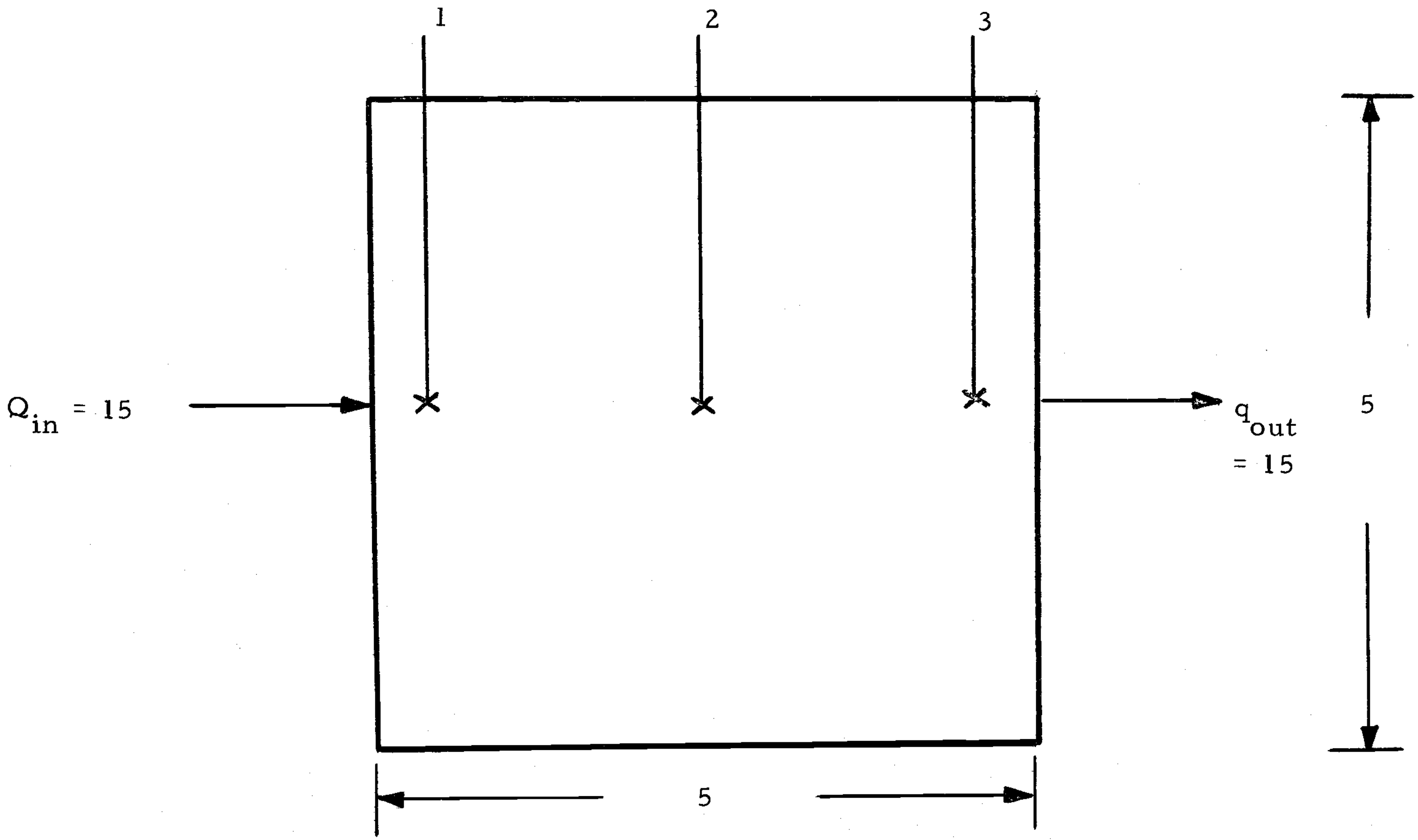

Figure E2c. The schematic diagram of the three probes inside the flow system in Example 2.

First, let $\Delta t = 0.4$. Then from Table E2a, we know

$$C(0) = C(t = 0.5) = [0.0372 \quad 0.0546 \quad 0.0159]$$

$$C(1) = C(t = 0.9) = [0.0142 \quad 0.0427 \quad 0.0383]$$

$$C(2) = C(t = 1.3) = [0.0062 \quad 0.0258 \quad 0.0379]$$

$$C(3) = C(t = 1.7) = [0.0029 \quad 0.0147 \quad 0.0279]$$

Substituting these into Equation (70b), we find

$$P = \begin{bmatrix} 0.0372 & 0.0546 & 0.0159 \\ 0.0142 & 0.0427 & 0.0383 \\ 0.0062 & 0.0258 & 0.0379 \end{bmatrix}^{-1} \begin{bmatrix} 0.0142 & 0.0427 & 0.0383 \\ 0.0062 & 0.0258 & 0.0379 \\ 0.0029 & 0.0147 & 0.0279 \end{bmatrix}$$

$$= \begin{bmatrix} 0.3192 & 0.5630 & 0.0761 \\ 0.0443 & 0.3896 & 0.5474 \\ 0 & 0.0306 & 0.3511 \end{bmatrix} \qquad \text{(E19)}$$

All the fractional input coefficients p_{ij} found in Equation (E19) are non-negative and less than one. Therefore, the choice of Δt is acceptable.

Since

$$\sum_{(i)} p_{i1} = 0.3192 + 0.0443 + 0 = 0.3635 < 1$$

$$\sum_{(i)} p_{i2} = 0.5630 + 0.3896 + 0.0306 = 0.9832 \simeq 1$$

$$\sum_{(i)} p_{i3} = 0.0761 + 0.5474 + 0.3511 = 0.9746 \simeq 1 ,$$

we can say that region 1 has an inlet from the inlet station, while region 2 and region 3 both have no inlet from the inlet station.

Now,

$$\sum_{(j)} p_{1j} = 0.3192 + 0.5630 + 0.0761 = 0.9583 \simeq 1$$

$$\sum_{(j)} p_{2j} = 0.0443 + 0.3896 + 0.5474 = 0.9813 \simeq 1$$

$$\sum_{(j)} p_{3j} = 0 + 0.0306 + 0.3511 = 0.3817 < 1 ,$$

we may say that the volumes of the regions are all nearly equal and region 1 and region 2 both have no outlet to the outlet station, while region 3 has an outlet to the outlet station.

Substituting Equation (E19) into Equation (31), we get

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_{DFM} = \begin{bmatrix} -0.6808 & 0.5630 & 0.0761 \\ 0.0443 & -0.6104 & 0.5474 \\ 0 & 0.0306 & -0.6489 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 0 \\ -(15)(0.4) \end{bmatrix}$$

$$= \begin{bmatrix} 8.7939 \\ 9.3246 \\ 9.6861 \end{bmatrix} \qquad \text{(E20)}$$

Since v_{total} is 25 (see Figure E2a), therefore the % error in the volume is

$$\frac{\left| \sum_{(i)} v_i - v_{total} \right|}{v_{total}} \times 100 = \frac{|27.8046 - 25|}{25} \times 100$$

$$= 11.21\ (\%)$$

Next, let region 4 be an accumulating outlet station. Substituting Equation (E19) into Equation (34b), we find

$$\overline{P} = \begin{bmatrix} 0.3192 & 0.5630 & 0.0761 & 0 \\ 0.0443 & 0.3896 & 0.5474 & 0 \\ 0 & 0.0306 & 0.3511 & 0.6183 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

and

$$\overline{C}(0) = \overline{C}(t = 0.5) = [0.0372 \quad 0.0546 \quad 0.0159 \quad 0.0000]$$

We use Equation (35) to compute $\overline{C}(m)$ for $m = 0, 1, 2, \ldots$. Here $c_1(m)$, $c_2(m)$, and $c_3(m)$, $m = 0, 1, 2, \ldots$, are the I curves corresponding to region 1, region 2, and region 3 respectively. Here $c_4(m)$, $m = 0, 1, 2, \ldots$, is the step response curve of the flow system. The normalized $c_3(m)$ curve is the RTD curve. Also, the adjusted $c_4(m)$ curve is the F curve. The RTD curve of this flow system computed from 3 probe model is shown in Figure E2d.

Summary. From Equation (E20), we know that the sum of the volumes computed from three probe model is only 11.21% off compared to the given total volume of the system. The RTD curve computed from this model (see Figure E2d) is very close to the real RTD curve of the flow system (see Figure E2b). Hence, we may say that three probe model is a good fit to the flow system under investigation.

Method 2. We would like to put four probes simultaneously into the flow system as shown in Figure E2e. The transient tracer concentrations measured by these four probes are tabulated in Table E2b.[8/]

[8/] See Appendix B.

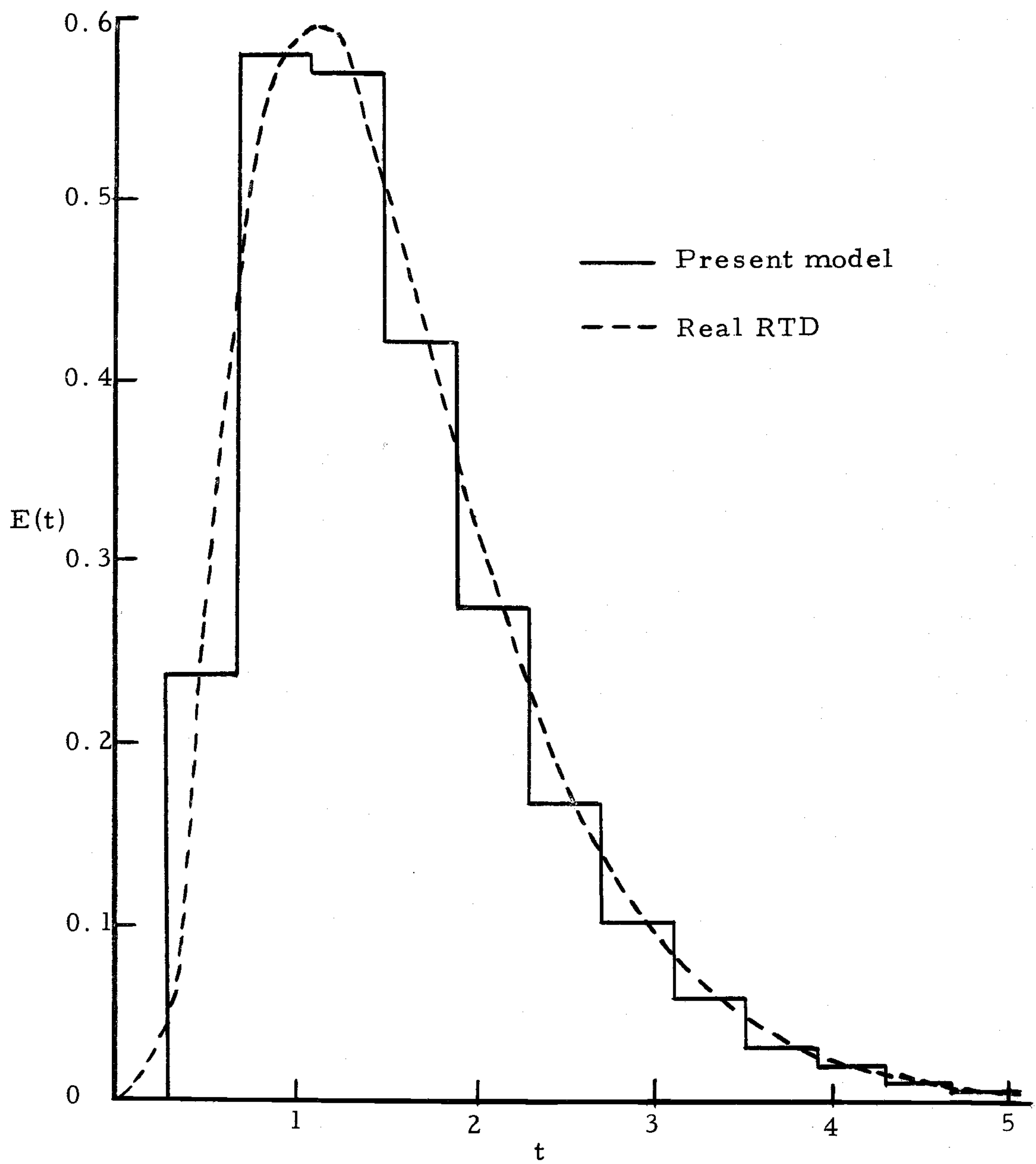

Figure E2d. The RTD curve of the flow system computed from three probe model in Example 2.

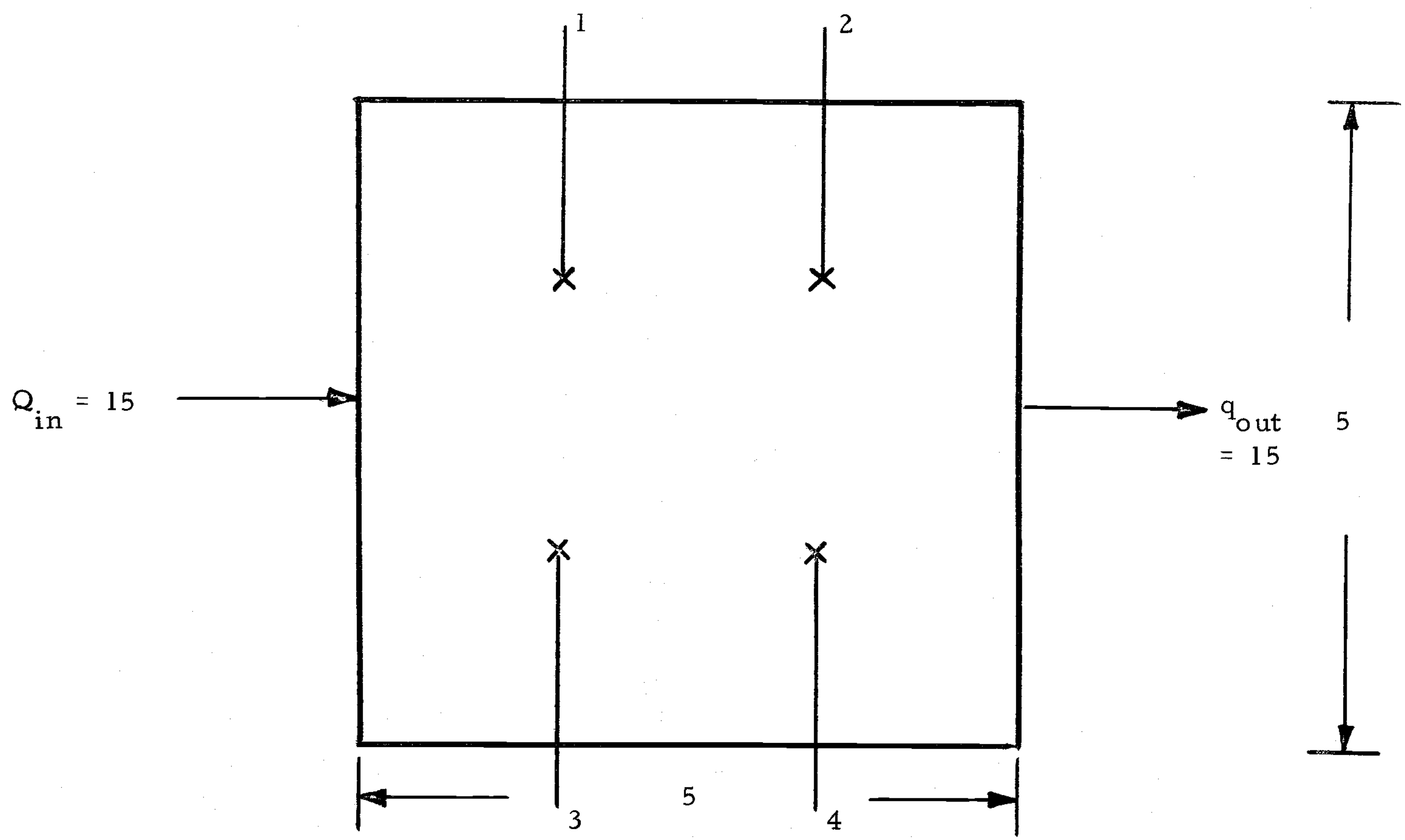

Figure E2e. The schematic diagram of the four probes inside the flow system in Example 2.

Table E2b. Transient concentrations of tracer in the flow system of Example 2 measured by four probes.

t	c_1	c_2	c_3	c_4
0	0	0	0	0
0.1	0.0574	0	0.0575	0
0.2	0.0777	0.0043	0.0690	0.0047
0.3	0.0799	0.0136	0.0654	0.0132
0.4	0.0741	0.0244	0.0575	0.0215
0.5	0.0655	0.0339	0.0492	0.0280
0.6	0.0564	0.0411	0.0417	0.0323
0.7	0.0479	0.0456	0.0351	0.0345
0.8	0.0404	0.0477	0.0296	0.0352
0.9	0.0339	0.0480	0.0250	0.0348
1.0	0.0285	0.0468	0.0212	0.0336
1.1	0.0239	0.0447	0.0180	0.0319
1.2	0.0201	0.0420	0.0153	0.0299
1.3	0.0169	0.0389	0.0131	0.0277
1.4	0.0142	0.0357	0.0112	0.0254
1.5	0.0120	0.0324	0.0096	0.0232
1.6	0.0101	0.0293	0.0082	0.0211
1.7	0.0086	0.0263	0.0071	0.0191
1.8	0.0073	0.0235	0.0061	0.0172
1.9	0.0062	0.0209	0.0053	0.0154
2.0	0.0053	0.0186	0.0046	0.0137
2.1	0.0045	0.0164	0.0039	0.0123
2.2	0.0039	0.0145	0.0034	0.0109
2.3	0.0033	0.0128	0.0030	0.0097
2.4	0.0028	0.0113	0.0026	0.0086
2.5	0.0024	0.0099	0.0022	0.0076

First, let $\Delta t = 0.4$. Then from Table E2b, we know

$$C(0) = C(t = 0.5) = [0.0655 \quad 0.0339 \quad 0.0492 \quad 0.0280]$$

$$C(1) = C(t = 0.9) = [0.0339 \quad 0.0480 \quad 0.0250 \quad 0.0348]$$

$$C(2) = C(t = 1.3) = [0.0169 \quad 0.0389 \quad 0.0131 \quad 0.0277]$$

$$C(3) = C(t = 1.7) = [0.0086 \quad 0.0263 \quad 0.0071 \quad 0.0191]$$

$$C(4) = C(t = 2.1) = [0.0045 \quad 0.0164 \quad 0.0039 \quad 0.0123]$$

Before substituting these into Equation (70b) (or Equation (70a)) to find the fractional input matrix P, we check the determinant of the first square matrix in the right-hand side of Equation (70b).

Let the concentration matrix

$$T = \begin{bmatrix} C(0) \\ C(1) \\ C(2) \\ C(3) \end{bmatrix} = \begin{bmatrix} 0.0655 & 0.0339 & 0.0492 & 0.0280 \\ 0.0339 & 0.0480 & 0.0250 & 0.0348 \\ 0.0169 & 0.0389 & 0.0131 & 0.0277 \\ 0.0086 & 0.0263 & 0.0071 & 0.0191 \end{bmatrix}$$

Then we find

$$\det(T) = 7.586 \times 10^{-10}, \quad \text{for} \quad \Delta t = 0.4 \tag{E21}$$

Similarly, we find

$$\begin{aligned} \det(T) &= 4.855 \times 10^{-10}, \quad \text{for} \quad \Delta t = 0.3 \\ \det(T) &= 4.672 \times 10^{-10}, \quad \text{for} \quad \Delta t = 0.5 \end{aligned} \tag{E22}$$

From Equation (E21) and Equation (E22), we know that the first square matrix in the right-hand side of Equation (70b) is nearly singular no matter what size of Δt is chosen. Hence, we may say that some of four probes are nearly redundant. By looking at the transient concentration distributions, we know that probe 1 and probe 3 are nearly redundant and also probe 2 and probe 4 are nearly redundant. Therefore, we must remove two probes according to their cofactors in the concentration matrix and use two probes only to model this flow system.

First, consider the case of $\Delta t = 0.4$. Comparing the cofactors of the elements $c_1(3)$ and $c_3(3)$ in the matrix T, we find

$$\text{cofactor of } c_1(3) = -0.415 \times 10^{-6}$$

$$\text{cofactor of } c_3(3) = 0.734 \times 10^{-6}$$

Since the cofactor of $c_3(3)$ is larger than the cofactor of $c_1(3)$, thus we remove probe 3.

After removing probe 3, we find a new concentration matrix T', we find

$$\text{cofactor of } c_2(2) = 13.302 \times 10^{-4}$$

$$\text{cofactor of } c_4(2) = 19.948 \times 10^{-4}$$

Since the cofactor of $c_4(2)$ is larger than the cofactor of $c_2(2)$, thus we remove probe 4.

The same results are obtained for the cases of $\Delta t = 0.3$ and $\Delta t = 0.5$.

Hence, after removing both probe 3 and probe 4, we would like to use probe 1 and probe 2 only to model the flow system shown in Figure E2a.

First, let $\Delta t = 0.4$. Then from Table E2b, we know

$$C(0) = C(t = 0.5) = [0.0655 \quad 0.0339]$$

$$C(1) = C(t = 0.9) = [0.0339 \quad 0.0480]$$

$$C(2) = C(t = 1.3) = [0.0169 \quad 0.0389]$$

Substituting these into Equation (70b), we find

$$P = \begin{bmatrix} 0.0655 & 0.0339 \\ 0.0339 & 0.0480 \end{bmatrix}^{-1} \begin{bmatrix} 0.0339 & 0.0480 \\ 0.0169 & 0.0389 \end{bmatrix}$$

$$= \begin{bmatrix} 0.5285 & 0.4939 \\ 0 & 0.4616 \end{bmatrix} \quad \text{(E23)}$$

All the fractional input coefficients p_{ij} found in Equation (E23) are non-negative and less than one. Therefore, it is acceptable. Since

$$\sum_{(i)} p_{i1} = 0.5285 + 0 \qquad = 0.5285 < 1$$

$$\sum_{(i)} p_{i2} = 0.4939 + 0.4616 = 0.9555 \simeq 1 ,$$

we can say that region 1 has an inlet from the inlet station, while region 2 has no inlet from the inlet station.

Since

$$\sum_{(j)} p_{1j} = 0.5285 + 0.4939 = 1.0224 \simeq 1$$

$$\sum_{(j)} p_{2j} = 0 \qquad + 0.4616 = 0.4616 < 1 ,$$

we may say that the volumes of the regions are nearly equal and region 1 has no outlet to the outlet station, while region 2 has an outlet.

Substituting Equation (E23) into Equation (31), we get

$$\begin{bmatrix} v_1 \\ v_2 \end{bmatrix}_{DFM} = \begin{bmatrix} -0.4715 & 0.4939 \\ 0 & -0.5384 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ -(15)(0.4) \end{bmatrix}$$

$$= \begin{bmatrix} 11.6736 \\ 11.1441 \end{bmatrix} \qquad \text{(E24)}$$

Since v_{total} is 25 (see Figure E2a), therefore the % error in the volume is

$$\frac{|22.8177 - 25|}{25} \times 100 = 8.73\ (\%)$$

Next, let region 3 be an accumulating outlet station.

Substituting Equation (E23) into Equation (34b), we find

$$\overline{P} = \begin{bmatrix} 0.5285 & 0.4939 & 0 \\ 0 & 0.4616 & 0.5384 \\ 0 & 0 & 1 \end{bmatrix}$$

and

$$\overline{C}(0) = \overline{C}(t = 0.5) = [0.0655 \quad 0.0339 \quad 0.0000]$$

We use Equation (35) to compute $\overline{C}(m)$ for $m = 0, 1, 2, \ldots$. Here $c_1(m)$, and $c_2(m)$, $m = 0, 1, 2, \ldots,$ are the I curves corresponding to region 1, and region 2 respectively. Here $c_3(m)$, $m = 0, 1, 2, \ldots,$ is the step response curve of the flow system. The normalized $c_2(m)$ curve is the RTD curve. Also, the adjusted $c_3(m)$ curve is the F curve. The RTD curve of this flow system computed from two probe model is shown in Figure E2f.

Summary. From Equation (E24), we know that the sum of the volumes computed from two probe model is only 8.73% off compared to the given total volume of the flow system. The RTD curve computed from this model (see Figure E2f) is fairly close to the real RTD curve of the flow system (see Figure E2b). Hence, we may say that two probe model is a fair fit to the flow system under investigation.

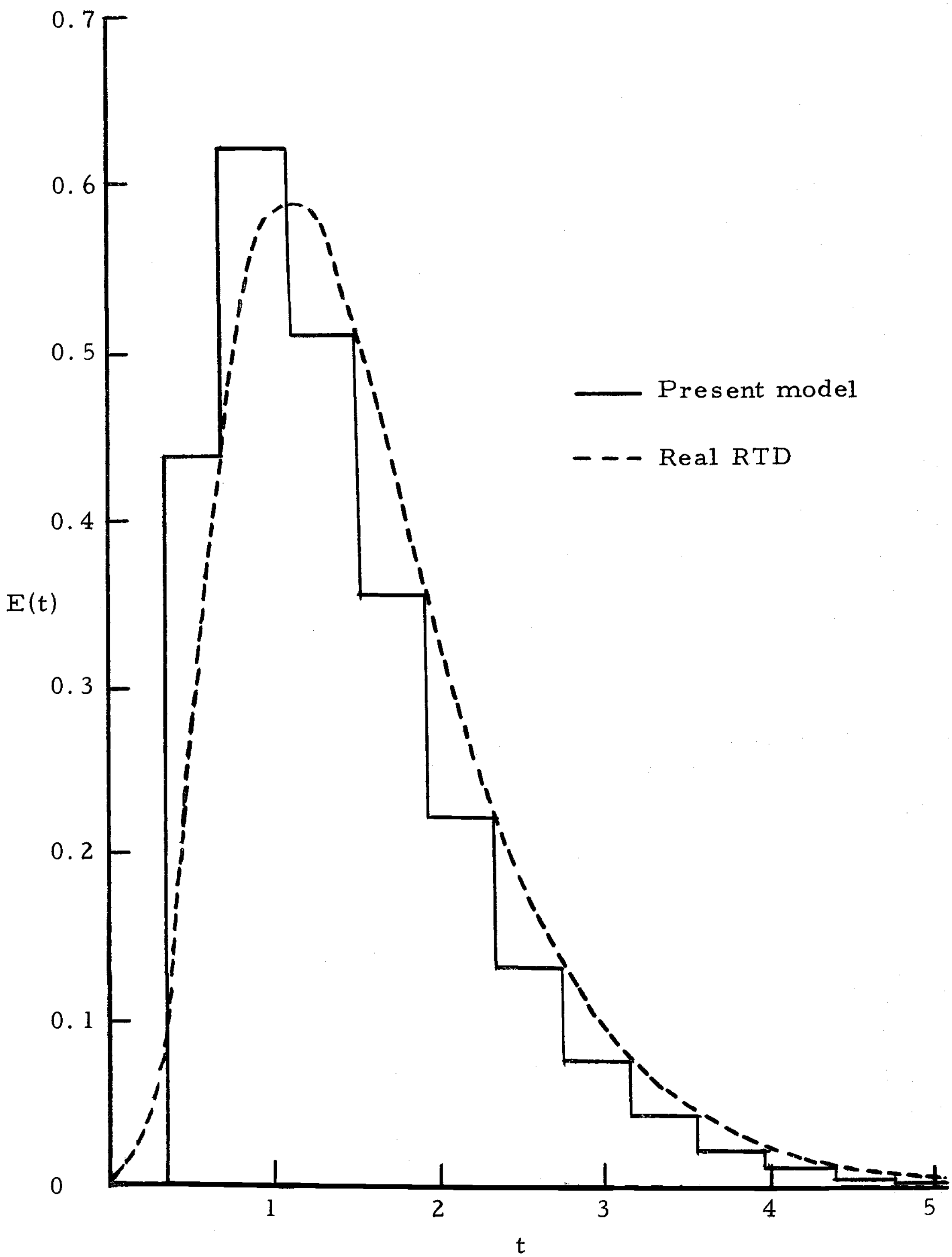

Figure E2f. The RTD curve of the flow system computed from two probe model in Example 2.

VIII. CONCLUSIONS

A general discrete flow model which is discrete both in time and space is developed and is used to model flow systems. A stirred tank network model (continuous time compartment model) is summarized and the relationship between these two models is developed. Both models make use of fractional input matrices with elements representing the fraction of flow into the jth region which originates in the ith region. The fractional input matrices for the discrete and continuous models are shown to be related to each other. The discrete flow model is more general and computationally much simpler than the stirred tank network model, and gives data which agrees precisely with continuous model at regularly spaced discrete values of time.

The fractional input matrix can be used to find the sizes of the regions, to predict the residence time distribution (RTD) of the fluid in the flow system, and to compute the reaction conversion if chemical reaction occurs. Direct methods are given for finding the fractional input matrix from either steady state or transient tracer data.

Two simple numerical examples are given to demonstrate how well the discrete flow model works. Use of the data fitting techniques allows data generated by a high order stirred tank model to be fitted quite well with a lower order discrete time model.

Lumping is important for modeling flow systems with very many regions, thus a lumping analysis for discrete flow systems is presented. The methods for obtaining the sizes of the regions and the fractional input matrix provide an important tool to analyze the lumping problems in flow systems.

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APPENDICES

APPENDIX A

Nomenclature

Letter	Definition
a_i	output coefficient from tank i
$a_{r\ell}^{(ij)}$	coefficient in Equation (85)
A	output matrix
B	defined by Equation (76)
$c_i(m)$	concentration in the ith region at time $m\Delta t$
$c_i(t)$	concentration in the ith tank at time t
C(m)	concentration row vector at time $m\Delta t$
C(t)	concentration row vector at time t
$\bar{C}(m)$	defined by Equation (35)
$\bar{C}(s)$	row vector of Laplace Transform of concentration
$c_i^r(m)$	concentration of component A in the fluid streams from region i at time $m\Delta t$
$C^r(m)$	concentration row vector in the flow streams at time $m\Delta t$
$C^{(r)}(m)$	defined by Equation (73)
$C^{(w)}(m)$	defined by Equation (74)
D	diagonal matrix
$e_{ij}(m)$	lumping error at region j of the lumped system to a unit tracer input at region i of the original system

Letter	Definition
$E(m)$	error matrix
$E(t)$	residence time distribution of fluid
f	function
$f_i(m)$	input concentration from the inlet station to region i at time $m\Delta t$
$F(m)$	input concentration row vector at time $m\Delta t$
$f_i^r(m)$	input concentration in the input streams to region i at time $m\Delta t$
$F^r(m)$	input concentration row vector in the input streams at time $m\Delta t$
I	identity matrix
J	a matrix in Jordan canonical form
L	lumping matrix
M	eigenvector matrix
n	number of regions
p_{ij}	fractional input coefficient from region i to region j
P	fractional input matrix
$\bar{P}$	defined by Equation (34a) and Equation (34b)
q_{ij}	volumetric flow rate from region i to region j
$q_{i, out}$	volumetric flow rate from region i to the outlet station
Q_{cont}	interregion flow matrix for continuous time flow systems

Letter	Definition
Q_d	interregion flow matrix for discrete time flow systems
Q_j	volumetric flow rate from the inlet station to the jth region
r	the remainder
r_{ij}	transition rate coefficient from tank i to tank j
R	transition rate matrix
s	Laplace variable
s_{ij}	steady response at region j to a steady input at region i
S	steady response matrix
S_r	semi-diagonal matrix
t	time
T	concentration matrix
u_i	unit vector with 1 as its ith element
v_i	volume of region i
v_{total}	total volume of the flow system
V	diagonal volume matrix
x	eigenvector

Greek Letters

α_i	constant in Equation (E9) and Equation (E10)
λ	eigenvalue
Δt	one step time interval

Letter	Definition
π_i	feed coefficient from the inlet station to region i
Π	feed matrix

Overhead

$\wedge$	any property related to lumped system

APPENDIX B

Data Source for Numerical Examples

Data Source for Example 1

Suppose that at time $t = 0^-$ we inject a pulse of tracer into a flow system consisting of three well-mixed regions as shown in Figure E1. Then from the material balance, we know

$$v_1 \frac{dc_1}{dt} = -(q_{12}+q_{13})c_1 + q_{21}c_2 + q_{31}c_3$$

$$v_2 \frac{dc_2}{dt} = q_{12}c_1 - (q_{21}+q_{23}+q_{2,out})c_2 + q_{32}c_3 \qquad \text{(A1)}$$

$$v_3 \frac{dc_3}{dt} = q_{13}c_1 + q_{23}c_2 - (q_{31}+q_{32}+q_{3,out})c_3$$

Let

$$q_{12} = 2.2 \quad q_{21} = 0.5 \quad q_{31} = 1.0$$

$$q_{13} = 3.3 \quad q_{23} = 3.3 \quad q_{32} = 2.6$$

and

$$v_1 = 2.0$$

$$v_2 = 1.0$$

$$v_3 = 3.0$$

with the initial conditions:

$$c_1(0) = 1, \quad c_2(0) = c_3(0) = 0$$

A digital computer was used to solve Equation (A1). The results were tabulated in Table E1.

Data Source for Example 2

Consider a flow system consisting of 25 regions as shown in Figure A1. In order to obtain discrete data for this system, the values of the initial condition and the fractional input matrix were assigned arbitrarily. The elements of the fractional input matrix were tabulated in Table A1. Then the transient concentrations were generated using Equation (9). The results are tabulated in Table A2. The residence time distribution (RTD) of the fluid elements in the flow system are computed by taking the flow weighted average of the transient concentrations of region 5, region 10, region 15, region 20, and region 25. The RTD curve of this system was shown in Figure E2b.

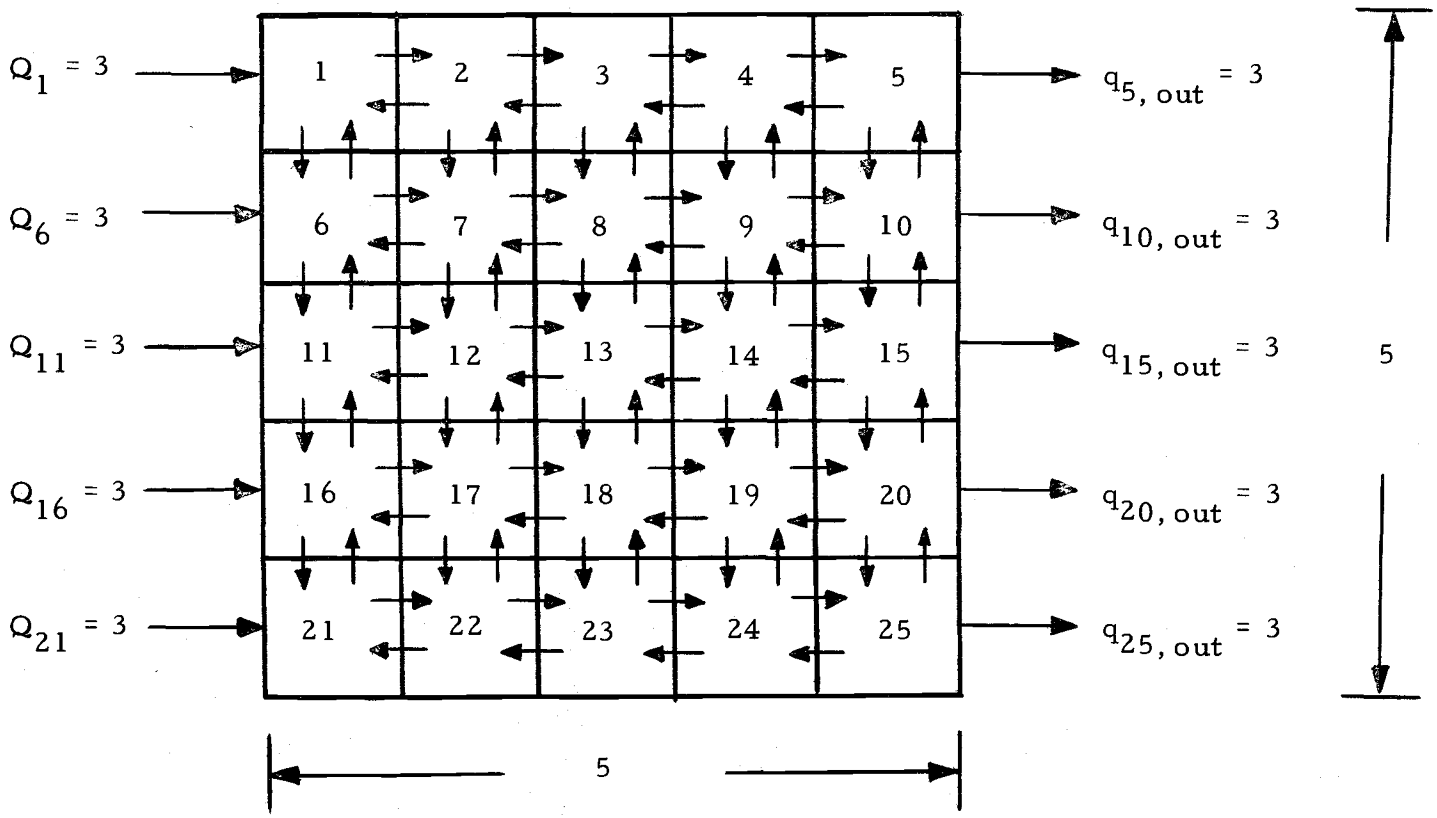

Figure A1. Diagram of the flow system with 25 regions.

Table A1. Fractional input matrix of the flow system with 25 regions.

.775	.200	.000	.000	.000	.025	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.050	.745	.180	.000	.000	.000	.025	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.000	.040	.750	.190	.000	.000	.000	.020	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.000	.000	.050	.705	.210	.000	.000	.000	.035	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.000	.000	.000	.075	.750	.000	.000	.000	.000	.025	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.025	.000	.000	.000	.000	.745	.175	.000	.000	.000	.055	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.000	.015	.000	.000	.000	.030	.725	.195	.000	.000	.000	.035	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.000	.000	.020	.000	.000	.000	.040	.710	.200	.000	.000	.000	.030	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.000	.000	.000	.030	.000	.000	.000	.050	.685	.225	.000	.000	.000	.010	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.000	.000	.000	.000	.040	.000	.000	.000	.065	.715	.000	.000	.000	.000	.030	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
.000	.000	.000	.000	.000	.050	.000	.000	.000	.000	.725	.200	.000	.000	.000	.025	.000	.000	.000	.000	.000	.000	.000	.000	.000
.000	.000	.000	.000	.000	.000	.035	.000	.000	.000	.045	.725	.180	.000	.000	.000	.015	.000	.000	.000	.000	.000	.000	.000	.000
.000	.000	.000	.000	.000	.000	.000	.025	.000	.000	.000	.025	.735	.205	.000	.000	.000	.010	.000	.000	.000	.000	.000	.000	.000
.000	.000	.000	.000	.000	.000	.000	.000	.015	.000	.000	.000	.045	.690	.230	.000	.000	.000	.020	.000	.000	.000	.000	.000	.000
.000	.000	.000	.000	.000	.000	.000	.000	.000	.035	.000	.000	.000	.055	.710	.000	.000	.000	.000	.050	.000	.000	.000	.000	.000
.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.025	.000	.000	.000	.000	.730	.190	.000	.000	.000	.055	.000	.000	.000	.000
.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.015	.000	.000	.000	.045	.700	.215	.000	.000	.000	.025	.000	.000	.000
.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.010	.000	.000	.000	.065	.695	.195	.000	.000	.000	.035	.000	.000
.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.040	.000	.000	.000	.055	.670	.210	.000	.000	.000	.025	.000
.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.030	.000	.000	.000	.070	.705	.000	.000	.000	.000	.045
.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.050	.000	.000	.000	.000	.725	.225	.000	.000	.000
.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.030	.000	.000	.000	.070	.695	.205	.000	.000
.000	.000	.000	.000	.000	.000	..000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.025	.000	.000	.000	.055	.730	.190	.000
.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.045	.000	.000	.000	.030	.705	.220
.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.035	.000	.000	.000	.080	.735

Table A2. Transient concentrations of tracer in the flow system with 25 regions.

t	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	c_9	c_{10}	c_{11}	c_{12}	c_{13}	c_{14}	c_{15}	c_{16}	c_{17}	c_{18}	c_{19}	c_{20}	c_{21}	c_{22}	c_{23}	c_{24}	c_{25}
0	.3000	0	0	0	0	.2000	0	0	0	0	.2000	0	0	0	0	.2000	0	0	0	0	.1000	0	0	0	0
0.1	.1912	.0927	.0108	0	0	.1391	.0574	.0068	0	0	.1316	.0630	.0072	0	0	.1238	.0575	.0082	0	0	.0707	.0354	.0046	0	0
0.2	.1295	.1142	.0387	.0062	.0004	.0984	.0777	.0265	.0043	.0003	.0913	.0801	.0267	.0046	.0003	.0816	.0690	.0275	.0047	.0003	.0523	.0452	.0173	.0027	.0002
0.3	.0919	.1096	.0596	.0183	.0038	.0712	.0799	.0432	.0136	.0029	.0659	.0787	.0423	.0139	.0030	.0566	.0654	.0403	.0132	.0028	.0400	.0451	.0275	.0084	.0018
0.4	.0675	.0967	.0705	.0312	.0106	.0526	.0741	.0535	.0244	.0084	.0490	.0706	.0513	.0241	.0086	.0409	.0575	.0460	.0215	.0076	.0312	.0414	.0334	.0148	.0052
0.5	.0509	.0823	.0738	.0419	.0194	.0396	.0655	.0579	.0339	.0161	.0372	.0608	.0546	.0328	.0159	.0306	.0492	.0468	.0280	.0135	.0248	.0367	.0357	.0204	.0098
0.6	.0392	.0690	.0721	.0493	.0284	.0304	.0564	.0581	.0411	.0242	.0288	.0512	.0542	.0388	.0234	.0235	.0417	.0449	.0323	.0195	.0200	.0319	.0355	.0245	.0148
0.7	.0306	.0574	.0677	.0536	.0365	.0236	.0479	.0556	.0456	.0317	.0225	.0428	.0514	.0423	.0300	.0184	.0351	.0416	.0345	.0247	.0163	.0275	.0337	.0271	.0193
0.8	.0242	.0477	.0619	.0553	.0428	.0186	.0404	.0516	.0477	.0376	.0178	.0355	.0473	.0436	.0350	.0147	.0296	.0378	.0352	.0286	.0134	.0237	.0312	.0285	.0230
0.9	.0193	.0396	.0557	.0551	.0472	.0148	.0339	.0470	.0480	.0418	.0142	.0295	.0427	.0432	.0383	.0118	.0250	.0339	.0348	.0313	.0111	.0203	.0284	.0287	.0256
1.0	.0156	.0329	.0495	.0534	.0496	.0119	.0285	.0421	.0468	.0442	.0115	.0245	.0381	.0417	.0400	.0096	.0212	.0301	.0336	.0328	.0092	.0174	.0255	.0282	.0273
1.1	.0126	.0274	.0438	.0508	.0504	.0096	.0239	.0374	.0447	.0450	.0093	.0203	.0337	.0393	.0403	.0079	.0180	.0267	.0319	.0332	.0077	.0149	.0227	.0272	.0280
1.2	.0103	.0229	.0385	.0476	.0498	.0078	.0201	.0330	.0420	.0445	.0076	.0169	.0296	.0366	.0395	.0066	.0153	.0235	.0299	.0328	.0065	.0128	.0201	.0258	.0279
1.3	.0085	.0192	.0337	.0441	.0482	.0064	.0169	.0290	.0389	.0431	.0062	.0141	.0258	.0335	.0379	.0055	.0131	.0207	.0277	.0318	.0055	.0109	.0177	.0241	.0273
1.4	.0070	.0161	.0295	.0404	.0459	.0052	.0142	.0254	.0357	.0410	.0051	.0118	.0225	.0305	.0357	.0046	.0112	.0182	.0254	.0303	.0046	.0094	.0156	.0224	.0262
1.5	.0058	.0136	.0257	.0368	.0431	.0043	.0120	.0222	.0324	.0384	.0042	.0099	.0195	.0275	.0332	.0039	.0096	.0160	.0232	.0284	.0039	.0081	.0137	.0206	.0248
1.6	.0048	.0115	.0224	.0333	.0401	.0036	.0101	.0193	.0293	.0355	.0035	.0083	.0170	.0247	.0306	.0033	.0082	.0140	.0211	.0265	.0034	.0070	.0120	.0188	.0232
1.7	.0040	.0097	.0196	.0300	.0369	.0030	.0086	.0168	.0263	.0326	.0029	.0070	.0147	.0220	.0279	.0028	.0071	.0123	.0191	.0244	.0029	.0060	.0105	.0171	.0215
1.8	.0034	.0083	.0170	.0269	.0336	.0025	.0073	.0146	.0235	.0297	.0024	.0059	.0127	.0196	.0253	.0024	.0061	.0108	.0172	.0223	.0025	.0052	.0092	.0154	.0198
1.9	.0028	.0070	.0148	.0240	.0305	.0021	.0062	.0127	.0209	.0268	.0020	.0050	.0110	.0173	.0228	.0020	.0053	.0095	.0154	.0203	.0021	.0045	.0081	.0139	.0181
2.0	.0024	.0060	.0129	.0214	.0275	.0018	.0053	.0111	.0186	.0241	.0017	.0042	.0096	.0153	.0204	.0017	.0046	.0083	.0137	.0183	.0018	.0039	.0071	.0125	.0165
2.1	.0020	.0051	.0113	.0190	.0247	.0015	.0045	.0096	.0164	.0216	.0014	.0036	.0083	.0135	.0182	.0015	.0039	.0073	.0123	.0165	.0016	.0033	.0062	.0112	.0149
2.2	.0017	.0044	.0098	.0168	.0221	.0013	.0039	.0083	.0145	.0192	.0012	.0031	.0072	.0119	.0162	.0013	.0034	.0064	.0109	.0148	.0013	.0029	.0054	.0100	.0134
2.3	.0015	.0038	.0085	.0149	.0197	.0011	.0033	.0072	.0128	.0171	.0010	.0026	.0062	.0104	.0144	.0011	.0030	.0056	.0097	.0132	.0012	.0025	.0048	.0089	.0120
2.4	.0012	.0032	.0074	.0131	.0175	.0009	.0028	.0063	.0113	.0151	.0009	.0022	.0054	.0092	.0127	.0009	.0026	.0049	.0086	.0118	.0010	.0022	.0042	.0079	.0108
2.5	.0011	.0028	.0065	.0115	.0155	.0008	.0024	.0055	.0099	.0134	.0007	.0019	.0047	.0080	.0112	.0008	.0022	.0043	.0076	.0105	.0009	.0019	.0036	.0070	.0096
2.6	.0009	.0024	.0056	.0102	.0137	.0007	.0021	.0047	.0087	.0118	.0006	.0016	.0040	.0070	.0099	.0007	.0019	.0038	.0067	.0093	.0007	.0017	.0032	.0062	.0086
2.7	.0008	.0021	.0049	.0089	.0121	.0006	.0018	.0041	.0076	.0104	.0005	.0014	.0035	.0062	.0087	.0006	.0017	.0033	.0059	.0082	.0006	.0014	.0028	.0055	.0076
2.8	.0007	.0018	.0043	.0078	.0107	.0005	.0015	.0036	.0067	.0091	.0005	.0012	.0030	.0054	.0076	.0005	.0015	.0029	.0052	.0073	.0006	.0013	.0024	.0048	.0068
2.9	.0006	.0015	.0037	.0069	.0094	.0004	.0013	.0031	.0058	.0080	.0004	.0010	.0026	.0047	.0067	.0005	.0013	.0025	.0046	.0064	.0005	.0011	.0021	.0043	.0060
3.0	.0005	.0013	.0032	.0060	.0083	.0004	.0011	.0027	.0051	.0070	.0003	.0009	.0023	.0041	.0059	.0004	.0011	.0022	.0040	.0057	.0004	.0009	.0019	.0038	.0053

APPENDIX C

Comparison of Discrete Flow Model and Markov Model
[2, 9, 10, 11, 12, 14, 16]

A Markov model is an important type of stochastic model that is useful in the study of complex systems. The basic ideas of the Markov model are those of state of a system and state transition. When a system is completely described by the values of variables that define the state, we say that a system occupies a state. A system makes a state transition when its describing variables change from the values specified for one state to those specified for another. If the time between transitions is a constant that is of interest, then we may consider the system as a discrete time process. To study the discrete time process, we have to specify the probabilistic nature of the state transition. Suppose that there are n states (possibly including an absorbing state) in a system running from 1 to n. If the system is a simple Markov process, then the probability of a transition from state i to state j during the next time interval, is a function only of i and j and not of any history of that system before its arrival in i. In other words, we may specify a set of conditional probabilities p_{ij} that a system will occupy state j after next transition, given that the system now occupies state i. For a discrete time process, the probabilities that a system will remain in same state, i.e., p_{ii}, $i = 1, 2, \ldots, n$, are non-zero.

Since the p_{ij} are probabilities, they are non-negative and not greater than one.

The similarities and differences between discrete flow model and Markov model are listed as follows:

Similarities.

1. The fractional input matrix P (or transition matrix) is a complete description of either model.
2. The elements of matrix P in either model are non-negative and not greater than one.
3. The element of matrix P in either model, i.e., p_{ij}, is a function only of state i and state j and not of any history of that system before its arrival in i.

Differences.

1. The discrete flow model is based on the time average behavior of a very large number of particles, while Markov model applied to the stochastic meandering of a single particle.
2. The p_{ij} in the discrete flow model can be interpreted as the fraction of material that will end up in the jth region that transfers in from the ith region in one step, while the p_{ij} in Markov model, from a physical viewpoint, can be interpreted as the fraction of material in the ith region that moves into the jth region in one step.

3. The columns of matrix P in the discrete flow model always sum to one if the columns include the inlet station, while the rows of matrix P in Markov model always sum to one if the rows include the absorbing state.

APPENDIX D

Computer Programs for Computation

```
      PROGRAM FIMTX
C     THIS PROGRAM USES GAUSS-JORDAN REDUCTION METHOD
C     COMBINING WITH MATRIX MULTIPLICATION TECHNIQUE
C     TO DETERMINE THE FRACTIONAL INPUT MATRIX OF FLOW SYSTEMS
      DIMENSION FAC(10,21),FRC(10,21),IFC(10,10),SC(10,10),
     *P(10,10)
      COMMON/ABC/N
      COMMON/BCD/FAC,FRC,M,EPS,DETER
      COMMON/CDE/IFC,SC,P
      REAL IFC
      IEX=TTYIN(4HIEX=    )
      DT=TTYIN(4HDT=    )
      N=TTYIN(4HN=    )
      M=TTYIN(4HM=    )
      EPS=TTYIN(4HEPS=   )
      LUN=TTYIN(4HLUN=   )
      WRITE(LUN,205)
      WRITE(LUN,210)IEX
      NPLUSM=N+M
      WRITE(LUN,200)DT,N,M,EPS
      WRITE(LUN,206)
      DO 2 I=1,N
      READ(5,101)(FAC(I,J),J=1,NPLUSM)
    2 WRITE(LUN,201)(FAC(I,J),J=1,NPLUSM)
      WRITE(LUN,207)
      DO 3 I=1,N
      READ(7,101)(SC(I,J),J=1,N)
    3 WRITE(LUN,201)(SC(I,J),J=1,N)
C     ...CALL ON GSJN TO COMPUTE THE 1ST RESULTING MATRIX...
      CALL GSJN
      WRITE(LUN,203)DETER
      WRITE(LUN,208)
      DO 4 I=1,N
    4 WRITE(LUN,202)(FRC(I,J),J=1,NPLUSM)
C     ....COMPUTE THE INVERSE OF 1ST MATRIX....
      DO 11 I=1,N
      DO 11 J=1,N
      JJ=M+J
   11 IFC(I,J)=FRC(I,JJ)
      WRITE(LUN,209)
      DO 12 I=1,N
   12 WRITE(LUN,202)(IFC(I,J),J=1,N)
C     ...CALL ON MULTI TO COMPUTE THE FRACTIONAL INPUT MATRIX...
      CALL MULTI
```

```
      WRITE(LUN,204)
      DO 13 I=1,N
   13 WRITE(LUN,201)(P(I,J),J=1,N)
C     ....FORMATS FOR INPUT AND OUTPUT STATEMENTS....
  101 FORMAT(1X,6F9.4)
  200 FORMAT(1X,'DT ='F10.5/1X,'N ='I5/1X,'M ='I5/1X,'EPS ='E10.
     *1/)
  201 FORMAT(1X,6F9.4)
  202 FORMAT(1X,6F10.4)
  203 FORMAT(/1X,'DETER ='E14.6/)
  204 FORMAT(//1X,'THUS, THE FRACTIONAL INPUT MATRIX IS'/)
  205 FORMAT(///1X,'****************************************'
     1'********************'/1X,'  MAINLY;USE GAUSS-JORDAN'
     2' REDUCTION ALGORITHM FOR DETERMINING'/1X,'      THE'
     3' FRACTIONAL INPUT MATRIX'/1X,'**********************'
     4'**********************************'/1X,'WITH,'//)
  206 FORMAT(/1X,'THE 1ST AUGMENTED MATRIX IS')
  207 FORMAT(/1X,'THE 2ND MATRIX IS')
  208 FORMAT(/1X,'THE 1ST RESULTING MATRIX IS')
  209 FORMAT(/1X,'THE INVERSE OF 1ST MATRIX IS')
  210 FORMAT(1X,'EXAMPLE'I3/)
      STOP
      END
C     ....SUBROUTINE FOR MAIN PROGRAM....
      SUBROUTINE GSJN
      DIMENSION A(10,21),R(10,21)
      COMMON/ABC/N
      COMMON/BCD/A,R,M,EPS,DETER
      NPLUSM=N+M
C     ....BEGIN ELIMINATION PROCEDURE....
      DETER=1.
      DO 2 K=1,N
C     ....UPDATE THE DETERMINANT VALUES....
      DETER=DETER*A(K,K)
C     ....CHECK FOR PIVOT ELEMENT TOO SMALL....
      IF(ABS(A(K,K)).GT.EPS)GO TO 3
      WRITE(61,202)
  202 FORMAT(1X,'SMALL PIVOT - MATRIX MAY BE SINGULAR')
C     ....NORMALIZE THE PIVOT ROW....
    3 KP1=K+1
      DO 4 J=KP1,NPLUSM
    4 A(K,J)=A(K,J)/A(K,K)
      A(K,K)=1.
C     ...ELIMINATE K(TH) COLUMN ELEMENTS EXCEPT FOR PIVOT...
      DO 2 I=1,N
      IF(I.EQ.K.OR.A(I,K).EQ.0.)GO TO 2
      DO 5 J=KP1,NPLUSM
    5 A(I,J)=A(I,J)-A(I,K)*A(K,J)
      A(I,K)=0.
    2 CONTINUE
      DO 1 I=1,N
      DO 1 J=1,NPLUSM
    1 R(I,J)=A(I,J)
```

```
      RETURN
      END
C     ....SUBROUTINE FOR MAIN PROGRAM....
      SUBROUTINE MULTI
      DIMENSION B(10,10),C(10,10),D(10,10)
      COMMON/ABC/N
      COMMON/CDE/B,C,D
      DO 1 I=1,N
      DO 1 J=1,N
      D(I,J)=0.
      DO 2 K=1,N
  2   D(I,J)=D(I,J)+B(I,K)*C(K,J)
  1   CONTINUE
      RETURN
      END
```

```
      PROGRAM VOLQ
C     THIS PROGRAM USES GAUSS-JORDAN REDUCTION METHOD
C     TO DETERMINE THE SIZE OF THE REGIONS AND THEN
C     FIND THE FLOW RATE CONNECTING THE;REGIONS OF
C     FLOW SYSTEMS
      DIMENSION APMI(10,21),P(10,10),Q(10,10),RPMI(10,21),V(10)
      COMMON APMI,RPMI,N,M,EPS,DETER
      IEX=TTYIN(4HIEX=    )
      DT=TTYIN(4HDT=    )
      N=TTYIN(4HN=    )
      M=TTYIN(4HM=    )
      EPS=TTYIN(4HEPS=   )
      LUN=TTYIN(4HLUN=   )
      WRITE(LUN,205)
      WRITE(LUN,210)IEX
      NPLUSM=N+M
      WRITE(LUN,200)DT,N,M,EPS
      WRITE(LUN,207)
      DO 2 I=1,N
      READ(5,101)(APMI(I,J),J=1,NPLUSM)
  2   WRITE(LUN,201)(APMI(I,J),J=1,NPLUSM)
      WRITE(LUN,208)
      DO 3 I=1,N
      READ(7,101)(P(I,J),J=1,N)
  3   WRITE(LUN,201)(P(I,J),J=1,N)
C     ...CALL ON GSJN TO COMPUTE (P-I) RESULTING MATRIX...
      CALL GSJN
      WRITE(LUN,203)DETER
      WRITE(LUN,209)
      DO 10 I=1,N
 10   WRITE(LUN,201)(RPMI(I,J),J=1,NPLUSM)
C     ....FIND ALL V(I) I=1,2,...N  ....
```

```
      WRITE(LUN,204)
      DO 11 I=1,N
      V(I)=RPMI(I,M)
 11   WRITE(LUN,201)V(I)
C     ....FIND ALL Q(I,J)  I,J=1,2,....N  ....
      DO 12 I=1,N
      DO 12 J=1,N
  12  Q(I,J)=P(I,J)*V(J)/DT
      WRITE(LUN,206)
      DO 14 I=1,N
  14  WRITE(LUN,201)(Q(I,J),J=1,N)
C     ....FORMATS FOR INPUT AND OUTPUT STATEMENTS....
 101  FORMAT(1X,6F9.4)
 200  FORMAT(1X,'DT ='F10.5/1X,'N ='I5/1X,'M ='I5/1X,'EPS ='
     *E10.1/)
 201  FORMAT(1X,6F9.4)
 203  FORMAT(/1X,'DETER ='E14.6/)
 204  FORMAT(//1X,'THE SIZE OF THE REGIONS V(1),V(2),...ARE'/)
 205  FORMAT(///1X,'*****************************************'
     1'*******************'/1X,'  USE GAUSS-JORDAN REDUCTION'
     2' ALGORITHM FOR DETERMING'/1X,'THE SIZE OF THE REGIONS'
     3' AND FLOW RATE CONNECTING THEM'/1X,'*****************'
     4'****************************************'/1X,'WITH,'
     5//)
 206  FORMAT(//1X,'FLOW RATE CONNECTING THE REGIONS Q(1,1)'
     1',Q(1,2),....ARE'/)
 207  FORMAT(/1X,'THE (P-I) AUGMENTED MATRIX IS')
 208  FORMAT(/1X,'THE TRANSITION MATRIX IS')
 209  FORMAT(/1X,'THE (P-I) RESULTING MATRIX IS')
 210  FORMAT(1X,'EXAMPLE'I3/)
      STOP
      END
C     ....SUBROUTINE FOR MAIN PROGRAM....
      SUBROUTINE GSJN
      DIMENSION A(10,21),R(10,21)
      COMMON A,R,N,M,EPS,DETER
      NPLUSM=N+M
C     ....BEGIN ELIMINATION PROCEDURE....
      DETER=1.
      DO 2 K=1,N
C     ....UPDATE THE DETERMINANT VALUES....
      DETER=DETER*A(K,K)
C     ....CHECK FOR PIVOT ELEMENT TOO SMALL....
      IF(ABS(A(K,K)).GT.EPS)GO TO 3
      WRITE(61,202)
 202  FORMAT(1X,'SMALL PIVOT - MATRIX MAY BE SINGULAR')
C     ....NORMALIZE THE PIVOT ROW....
   3  KP1=K+1
      DO 5 J=KP1,NPLUSM
   5  A(K,J)=A(K,J)/A(K,K)
      A(K,K)=1.
C     ...ELIMINATE K(TH) COLUMN ELEMENTS EXCEPT FOR PIVOT...
```

```
      DO 2 I=1,N
      IF(I.EQ.K.OR.A(I,K).EQ.0.)GO TO 2
      DO 6 J=KP1,NPLUSM
 6    A(I,J)=A(I,J)-A(I,K)*A(K,J)
      A(I,K)=0.
 2    CONTINUE
      DO 4 I=1,N
      DO 4 J=1,NPLUSM
 4    B(I,J)=A(I,J)
      RETURN
      END
```

```
      PROGRAM EIGEN
C     THIS PROGRAM USES THE POWER METHOD TO FIND THE
C     EIGENVALUES AND EIGENVECTORS OF MATRICES
      REAL L,LZERO,LAMDA,IDENT
      DIMENSION A(10,10),B(10,10),U(10,10),LAMDA(10),V(10)
     *,Y(10),VZERO(10),C(10,10)
      N=TTYIN(4H N= )
      MMX=TTYIN(4HMMX=    )
      MFQ=TTYIN(4HMFQ=    )
      EPS=TTYIN(4HEPS=    )
      LUN=TTYIN(4HLUN=    )
      WRITE(LUN,205)
      READ(6,100)(VZERO(I),I=1,N)
      READ(6,100)((A(I,J),J=1,N),I=1,N)
  100 FORMAT(6F9.4)
      WRITE(LUN,203)
      DO 1 I=1,N
 1    WRITE(LUN,204)(A(I,J),J=1,N)
      DO 2 I=1,N
      DO 2 J=1,N
    2 B(I,J)=0.
      DO 3 I=1,N
    3 B(I,I)=1.
      DO 11 I=1,N
      DO 102 II=1,N
  102 V(II)=0.
      SUM=0.
      DO 104 II=1,N
      DO 103 JJ=1,N
  103 V(II)=B(II,JJ)*VZERO(JJ)+V(II)
  104 SUM=SUM+V(II)*V(II)
      LZERO=SQRT(SUM)
      DO 5 M=1,MMX
      IF((M/MFQ)*MFQ.NE.M)GOTO 4
      SUM=0.
      DO 105 II=1,N
```

```
105 Y(II)=0.
    DO 107 II=1,N
    DO 106 JJ=1,N
106 Y(II)=B(II,JJ)*V(JJ)+Y(II)
107 SUM=SUM+Y(II)*Y(II)
    L=SQRT(SUM)
    DO 108 IJ=1,N
108 V(IJ)=1./L*Y(IJ)
  4 SUM=0.
    DO 109 II=1,N
    Y(II)=0.
    DO 110 JJ=1,N
110 Y(II)=A(II,JJ)*V(JJ)+Y(II)
109 SUM=SUM+Y(II)*Y(II)
    L=SQRT(SUM)
    DO 111 II=1,N
111 V(II)=1./L*Y(II)
    IF(ABS((L-LZERO)/LZERO).LT.EPS)GOTO 7
    IF(M.GE.(MMX-2))WRITE(LUN,210)L,LZERO
210 FORMAT(5X'L ='F9.4,15X'LZERO ='F9.4)
  5 LZERO=L
    IM1=I-1
    WRITE(LUN,200)(LAMDA(K),K=1,IM1)
200 FORMAT(//5X'NO CONVERGENCE . EIGENVALUES ARE'//(7X,6F9.4))
    GOTO 12
  7 CONTINUE
    DO 112 II=1,N
    Y(II)=0.
    DO 112 JJ=1,N
112 Y(II)=A(II,JJ)*V(JJ)+Y(II)
    DO 8 K=1,N
    IF(ABS(V(K)).LT.1.E-3)GOTO 8
    IF(V(K)*Y(K).LT.0.)L=-L
    GOTO 9
  8 CONTINUE
  9 LAMDA(I)=L
    WRITE(LUN,199)I,LAMDA(I)
199 FORMAT(//5X'LAMBDA('I3') ='F9.4)
    DO 10 K=1,N
 10 U(K,I)=V(K)
    IF(I.GT.N)GOTO 11
    DO 114 II=1,N
    DO 114 IJ=1,N
    C(II,IJ)=0.
    DO 114 IK=1,N
    IDENT=0.
    IF(IK.EQ.II)IDENT=1.
114 C(II,IJ)=C(II,IJ)+(A(II,IK)-L*IDENT)*B(IK,IJ)
    DO 115 II=1,N
    DO 115 IJ=1,N
115 B(II,IJ)=C(II,IJ)
 11 CONTINUE
    WRITE(LUN,201)(LAMDA(K),K=1,N)
```

```
 201 FORMAT(////5X,'EIGENVALUES ARE'//(6F9.4))
     WRITE(LUN,202)((U(I,J),J=1,N),I=1,N)
 202 FORMAT(////5X,'EIGENVECTORS ARE'//(6F9.4))
 203  FORMAT(5X,'THE STARTING MATRIX IS'/)
 204  FORMAT(1X,6F9.4)
 205  FORMAT(//1X,'*************************************'
     1'*******************'/1X,'USE THE POWER METHOD;FOR '
     2'DETERMINING EIGENVALUES AND'/1X,'      EIGENVECTORS'
     3/1X,'*******************************************'
     4'***********'//)
  12 CONTINUE
     END
```

```
      PROGRAM SODE
C    THIS PROGRAM USES 4TH-ORDER RKM METHOD TO FIND THE
C    TRANSIENT CONCENTRATIONS IN CONTINUOUS-TIME FLOW
C    SYSTEMS
      DIMENSION C(10),F(10)
      COMMON N,T,C,F,H,IRKM,E,TINT
      IEX=TTYIN(4HIEX=    )
      N=TTYIN(4HN=      )
      H=TTYIN(4HH=      )
      TINT=TTYIN(4HTINT    )
      TMAX=TTYIN(4HTMAX    )
      E=TTYIN(4HE=      )
      LUN=TTYIN(4HLUN=    )
      WRITE(LUN,210)
      WRITE(LUN,240)IEX
C     ....SET INITIAL CONDITIONS....
      T=0. $ C(1)=1.0 $ C(2)=0. $ C(3)=0.
      WRITE(LUN,250)N,H,TINT,TMAX,E
      WRITE(LUN,220)
      WRITE(LUN,230)
      WRITE(LUN,200)T,(C(I),I=1,N)
C     ....CALL ON RKM TO COMPUTE ALL C(J)  J=1,2,...N ....
  10  CALL RKM
      IF(IRKM.EQ.2)GO TO 5
C     ....CALCULATION OF F(J) FOR ALL EQUATIONS....
      F(1)=-2.75*C(1)+.25*C(2)+.5*C(3)
      F(2)=2.2*C(1)-4.8*C(2)+2.6*C(3)
      F(3)=1.1*C(1)+1.1*C(2)-2.2*C(3)
      GO TO 10
  5   WRITE(LUN,260)T,(C(I),I=1,N)
      IF((TMAX-T).GT.1.E-9)GO TO 10
      WRITE(LUN,230)
C     ....FORMATS FOR INPUT AND OUTPUT STATEMENTS....
 210  FORMAT(///1X,'**********************************'
     1'***********************'/1X,' USE 4TH-ORDER RKM'
```

```
     2' METHOD TO SOLVE N SIMULTANEOUS'/1X,'           1ST'
     3'-ORDER O.D.E.'/1X,'*******************************'
     4'***************************'/1X,'WITH,'//)
 240  FORMAT(1X,'EXAMPLE'I3/)
 250  FORMAT(1X,'N ='I4/1X,'H ='F10.5/1X,'TINT ='F10.5/1X,
     1'TMAX ='F10.5/1X,'E ='E10.5//)
 220  FORMAT(1X,'THE TRANSIENT CONCENTRATIONS IN THE FLOW'
     2' SYSTEM ARE :'//////)
 200  FORMAT(17X,'T(MIN)',3X,'C(1)',4X,'C(2)',4X,'C(3)'
     3/14X,'---------------------------------------'
     4//14X,4F8.4)
 260  FORMAT(14X,4F8.4)
 230  FORMAT(/14X,'-----------------------------------------')
      STOP
      END
C     ....SUBROUTINE FOR MAIN PROGRAM....
      SUBROUTINE RKM
      DIMENSION Y(10),F(10),SAVEY(10),PHI(10),K(10,5),
     *ERROR(10)
      COMMON N,X,Y,F,H,IRKM,E,XINT
      REAL K
      M=M+1
      GO TO (100,200,300,400,500,600),M
 100  IRKM=1
      IF(XINT.EQ.0.)GO TO 16
      IF(INDEX.EQ.0)13,14
  13  INDEX=1 $ ACCUM=0.
  14  ACCUM=ACCUM+H
      IF(ABS(ACCUM-XINT).LT.1.E-9)25,11
  25  INDEX=0 $ RETURN
  11  IF(ACCUM.GT.XINT)15,16
  15  INDEX=0
      HLAST=H $ IH=2
      H=H-ACCUM+XINT
      ACCUM=XINT
  16  RETURN
 200  X=X+H/3.
      DO 1 J=1,N
      SAVEY(J)=Y(J)
      K(J,1)=F(J)*H/3.
      PHI(J)=K(J,1)
      ERROR(J)=K(J,1)
   1  Y(J)=SAVEY(J)+K(J,1)
      RETURN
 300  DO 2 J=1,N
      K(J,2)=F(J)*H/3.
   2  Y(J)=SAVEY(J)+.5*(K(J,1)+K(J,2))
      RETURN
 400  DO 3 J=1,N
      K(J,3)=F(J)*H/3.
      ERROR(J)=ERROR(J)-4.5*K(J,3)
   3  Y(J)=SAVEY(J)+3./8.*K(J,1)+9./8.*K(J,3)
      X=X-H/3.+H/2.
```

```
      RETURN
500   DO 4 J=1,N
      K(J,4)=F(J)*H/3.
      PHI(J)=PHI(J)+4.*K(J,4)
      ERROR(J)=ERROR(J)+4.*K(J,4)
4     Y(J)=SAVEY(J)+1.5*K(J,1)-4.5*K(J,3)+6.*K(J,4)
      X=X+H/2.
      RETURN
600   DO 5 J=1,N
      K(J,5)=F(J)*H/3.
      PHI(J)=PHI(J)+K(J,5)
      ERROR(J)=.2*(ERROR(J)-.5*K(J,5))
      IF(ABS(ERROR(J)).GT.E)GO TO 10
5     CONTINUE
      GO TO 20
10    I=I+1
      IF(I.GE.21)WRITE(61,1000)I,X,H
1000  FORMAT(1X,'RKM HALVED STEP INCREMENT'I3'TIMES. X='
     *E15.8 ' H= 'E15.6)
      X=X-H $ H=H/2.
      ACCUM=ACCUM-H
      INDEX=1
      IH=1
      DO 6 JJ=1,N
      Y(JJ)=SAVEY(JJ)
6     F(JJ)=1.5*K(JJ,1)/H
      IRKM=1 $ M=2
      GO TO 200
20    CONTINUE
      DO 8 J=1,N
      IF(ABS(ERROR(J))/E.GT.0.003)GO TO 90
8     CONTINUE
      IF(IH.EQ.2)17,26
90    IF(IH.EQ.2)17,9
17    IH=1
      IF(HLAST.LT.0.4*XINT)21,22
21    H=HLAST $ GO TO 9
22    IF(HLAST.GT.0.8*XINT)23,24
23    H=XINT $ GO TO 9
24    H=0.5*XINT $ GO TO 9
26    H=2.*H
9     DO 7 JJ=1,N
7     Y(JJ)=SAVEY(JJ)+0.5*PHI(JJ)
      M=0 $ IRKM=2
      I=0
      RETURN
      END
```

```
      PROGRAM MAD
C     TO COMPUTE TRANSIENT CONCENTRATIONS IF THE
C     INITIAL CONDITION AND THE MATRIX P ARE KNOWN
      DIMENSION C(100,30),P(30,30)
      M=TTYIN(4HM=   )
      N=TTYIN(4HN=   )
      READ(7,100)(C(1,J),J=1,N)
  100 FORMAT(10F6.3)
      DO 1 I=1,N
    1 READ(5,100)(P(I,J),J=1,N)
      DO 2 I=1,M
      II=I+1
      DO 3 J=1,N
      C(II,J)=0.
      DO 3 K=1,N
    3 C(II,J)=C(II,J)+C(I,K)*P(K,J)
    2 CONTINUE
      MM=M+1
      DO 4 I=1,MM,2
      WRITE(61,200)(C(I,J),J=1,N)
    4 WRITE(4,200)(C(I,J),J=1,N)
  200 FORMAT(10F6.4/)
      END
```