MODEL FOR UPTAKE OF ORGANIC CHEMICALS BY PLANTS

L. BOERSMA, F. T. LINDSTROM, C. MCFARLANE

AUTHORS: F. T. Lindstrom and L. Boersma, Department of Soil Science, Oregon State University; C. McFarlane, Research Scientist, Corvallis Environmental Research Laboratory, United States Environmental Protection Agency.

THIS PUBLICATION IS OUT OF DATE.
For most current information: http://extension.oregonstate.edu/catalog
FOREWORD

The uptake, transport, and accumulation of organic and inorganic chemicals by plants are influenced by characteristics of the plant, properties of the chemical, properties of the soil, and by prevailing environmental conditions. Complex interrelationships exist between the physical, chemical, and physiological processes that occur in specific plant tissues and the response of these processes to environmental conditions, such as the daily cycle of radiation, evaporation, and air temperature. The uptake is further influenced by the availability of the chemical at the root surface, determined in turn by transport characteristics of the soil. Also important is the behavior of the chemical in the rhizosphere and the ease with which it moves across limiting membranes at the root surface.

This report describes the development of a predictive simulator for the uptake of xenobiotic chemicals by plants from the soil solution. The model is based on definition of the plant as a set of compartments separated from each other by thin membranes. Movement of water and solutes between compartments occurs by mass flow and diffusion. The compartments represent major pools for accumulation of water and solutes. Anatomical features of the compartments and the manner in which they are connected are described by a series of equations based on conservation of mass. Experimental data are used to calibrate and then validate the model.

ACKNOWLEDGMENTS

This publication reports results of studies supported, in part, by Research Grant CR 811940-01A, "A Mathematical Model of the Bioaccumulation of Xenobiotic Organic Chemicals in Plants" from the Corvallis Environmental Research Laboratory of the United States Environmental Protection Agency to the Department of Soil Science at Oregon State University and by the Oregon Agricultural Experiment Station.

THIS PUBLICATION IS OUT OF DATE. For most current information: http://extension.oregonstate.edu/catalog
## CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>FOREWORD</td>
<td>i</td>
</tr>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>i</td>
</tr>
<tr>
<td>FIGURES</td>
<td>iv</td>
</tr>
<tr>
<td>TABLES</td>
<td>viii</td>
</tr>
<tr>
<td>SUMMARY</td>
<td>1</td>
</tr>
</tbody>
</table>

### DEVELOPMENT OF THE MODEL
- Introduction                                 | 3    |
- Structure of the Model                       | 4    |
- Sequence of Compartments                    | 7    |
- Mass Balance Equations                      | 13   |
  - Soil Compartment                           | 14   |
  - Free Space of the Roots                    | 15   |
  - Storage Volume of Root Cortex              | 18   |
  - Root Xylem Compartment                     | 19   |
  - Root Storage Compartment                   | 21   |
  - System of Equations                        | 22   |
- Solution Method                              | 23   |
- Effective Concentrations                    | 26   |

### APPLICATION TO EXPERIMENTS
- Introduction                                | 29   |
- Experimental Procedures                     | 36   |
- Qualitative Overview of Results             | 39   |
- Calibration                                 | 43   |
- Volumes of Compartments                     | 45   |
- Chemical and Physical Parameters            | 46   |
- Phloem Transport                            | 47   |
- Concentration of Bromacil in Bathing Solution | 48   |
- Transpiration Rates                         | 50   |
- Storage Coefficients                        | 50   |

### DISCUSSION
- Introduction                                | 61   |
- Roots                                       | 64   |
- Stems                                       | 64   |
- Leaves                                      | 64   |

**This publication is out of date. For most current information:**
[http://extension.oregonstate.edu/catalog](http://extension.oregonstate.edu/catalog)
## CONTENTS (continued)

<table>
<thead>
<tr>
<th>CONTENTS</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>SENSITIVITY ANALYSIS</td>
<td></td>
</tr>
<tr>
<td>Introduction</td>
<td>67</td>
</tr>
<tr>
<td>Transpiration Rate</td>
<td>67</td>
</tr>
<tr>
<td>Ratio: Phloem Transport Rate/Xylem Transport Rate</td>
<td>67</td>
</tr>
<tr>
<td>Diffusion Coefficient of the Casparian Strip</td>
<td>70</td>
</tr>
<tr>
<td>Reflection Coefficient of the Casparian Strip</td>
<td>72</td>
</tr>
<tr>
<td>Reflection Coefficients in the Leaf Membranes Separating Xylem and Phloem Pathway</td>
<td>73</td>
</tr>
<tr>
<td>Storage Coefficient</td>
<td>76</td>
</tr>
<tr>
<td>Change in the Ratio $Q_b/Q_f$</td>
<td>76</td>
</tr>
<tr>
<td>Sorption Coefficients in the Root Storage Compartments</td>
<td>80</td>
</tr>
<tr>
<td>Rate of First Order Losses</td>
<td>84</td>
</tr>
<tr>
<td>Combined Effects</td>
<td>84</td>
</tr>
</tbody>
</table>

<p>| CONCLUSIONS | 89 |
| LITERATURE CITED | 91 |
| APPENDIX 1. Definitions of the non-zero coefficients $a_{ij}$ | 94 |</p>
<table>
<thead>
<tr>
<th>Figures</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Figure 1</td>
<td>Schematic diagram of a generic plant, with three leaves showing the hierarchy of leaves on the stem and the numbering sequence used for model compartments.</td>
</tr>
<tr>
<td>Figure 2</td>
<td>Conceptualization of the plant shown in Figure 1 in terms of compartments used for the mathematical model. Definitions of symbols are in Tables 1 and 2.</td>
</tr>
<tr>
<td>Figure 3</td>
<td>Measured bromacil concentrations in the root compartments. Details of the experimental procedures are in the text. The curves shown were drawn by hand to emphasize trends in increase in concentration. The graphs show an initial rapid rise in concentration, followed by a linear increase with time.</td>
</tr>
<tr>
<td>Figure 4</td>
<td>Measured bromacil concentrations in the stem compartments. Details of the experimental procedures are in the text. Curves were drawn by hand to emphasize trends in increase in concentration. The graphs show a linear increase in concentration during the exposure period.</td>
</tr>
<tr>
<td>Figure 5</td>
<td>Measured bromacil concentrations in the leaf compartments for the BROM1 and BROM5 experiments. Curves were drawn by hand to emphasize trends. Results suggest a linear rate of uptake in these experiments with constant transpiration rates.</td>
</tr>
<tr>
<td>Figure 6</td>
<td>Concentrations at 50 hrs of exposure as a function of solution concentration.</td>
</tr>
<tr>
<td>Figure 7</td>
<td>Concentrations in roots, stems, and leaves as a function of time for BROM5, low transpiration rate.</td>
</tr>
<tr>
<td>Figure 8</td>
<td>Concentrations in roots, stems, and leaves as a function of time for BROM5, medium transpiration rate.</td>
</tr>
<tr>
<td>Figure 9</td>
<td>Concentrations in roots, stems, and leaves as a function of time for BROM5, high transpiration rate.</td>
</tr>
<tr>
<td>Figure 10</td>
<td>Concentrations in roots, stems, and leaves as a function of time for BROM3, low transpiration rate.</td>
</tr>
<tr>
<td>Figure 11</td>
<td>Concentrations in roots, stems, and leaves as a function of time for BROM3, medium transpiration rate.</td>
</tr>
</tbody>
</table>
FIGURES (continued)

Figure 12. Concentrations in roots, stems, and leaves as a function of time for BROM3, high transpiration rate.

Figure 13. Concentrations in roots, stems, and leaves as a function of time for BROM1.

Figure 14. Ratio Qf/Qb for the root cortex and for root storage compartments as a function of transpiration rate.

Figure 15. Forward storage coefficients for stem compartments plotted as a function of volumes of stem storage compartments.

Figure 16. Forward storage coefficients for leaf compartments plotted as a function of volumes of leaf storage compartments.

Figure 17. Simulations showing the effect of changing the transpiration rates. Reference simulation was with BROM5, medium transpiration rate, Tr = 5.67 cm³/hr. Comparisons are with low transpiration rate Tr = 2.00 cm³/hr (curves A) and high transpiration rate, Tr = 7.80 cm³/hr (curves B).

Figure 18. Simulations showing the effects of changing the ratios of phloem transport rate divided by xylem transport rate. Reference simulation was with the fractions set to f₁ = 0.3; f₂ = 0.2; f₃ = 0.1. Simulation A: f₁ = 0.0; f₂ = 0.0; f₃ = 0.0, and Simulation B: f₁ = 0.15; f₂ = 0.15, and f₃ = 0.1.

Figure 19. Simulations showing the effects of changing the diffusion coefficient of the boundary representing the Casparian strip. Reference simulation was with D = 1.8 x 10⁻⁷ cm²/hr. Simulation A: D = 1.8 x 10⁻⁸ cm²/hr, simulation B: D = 1.8 x 10⁻⁸ cm²/hr.

Figure 20. Simulation showing effects of changing the reflection coefficient of the boundary representing the Casparian strip. Reference simulation was with σ = 0.0. Simulation A: α = 0.2; simulation B: σ = 0.7.
FIGURES (continued)

Figure 21. Simulations showing the effects of changing the reflection coefficients of the membranes in the leaves which separate phloem from xylem ($\sigma_{10}$, $\sigma_{14}$, and $\sigma_{18}$). Reference simulation was with the three coefficients equal to zero. Simulation A, $\sigma$'s equal to 0.2; Simulation B, $\sigma$'s equal to 0.7.

Figure 22. Simulations showing the effect of increasing or decreasing values of the forward ($Q_f$) and backward ($Q_b$) coefficients while maintaining the same ratio $Q_f/Q_b$. The reference simulation was with all $Q_f$'s and $Q_b$'s as in Table 8. For Simulation A, all coefficients were divided by two; for Simulation B, all storage coefficients were multiplied by two.

Figure 23. Simulations showing the effects of changing the ratios of forward storage coefficients to the backward storage coefficients. Reference simulation was with all storage coefficients as shown in Table 8. For Simulation A, all forward storage coefficients ($Q_f$) were divided by two while leaving the $Q_b$'s the same; for Simulation B, all forward storage coefficients were multiplied by two while leaving the $Q_b$'s the same.

Figure 24. Simulations showing the effects of changing the sorption coefficients ($B$'s) in the root compartments. These coefficients immobilize chemical so that the coefficient has an effect that is similar to that of increasing or decreasing the volume of the compartment. Reference simulation was with values of the sorption coefficients $B = 0$. Simulation A, sorption coefficients of the two root compartments, $B_1 = B_3 = 0.5$; Simulation B, sorption coefficient of the two root compartments, $B_1 = B_3 = 1.0$.

Figure 25. Simulations showing effects of changing the rates of first order loss ($\lambda$) in the leaves. Reference simulation was with all $\lambda$'s equal to zero. Simulation A: $\lambda_{15} = 0.0016$, $\lambda_{18} = 0.00175$, $\lambda_{21} = 0.0018$; simulation B: $\lambda_{15} = 0.0032$, $\lambda_{18} = 0.0035$, $\lambda_{21} = 0.0036$; simulation C: $\lambda_{15} = 0.0064$, $\lambda_{18} = 0.0070$, $\lambda_{21} = 0.0072$.  

THIS PUBLICATION IS OUT OF DATE. For most current information: http://extension.oregonstate.edu/catalog
Figure 26. Simulations showing the combined effects of changing several parameters at the same time. Reference simulation was with data set for BROM5, medium transportation rate (Table 8). Values of parameters used for this simulation are in Table 13.

Figure 27. Simulation showing the combined effects of changing several parameters. Reference simulation was with data set for BROM5, medium transpiration rate (Table 8). Values of parameters used for this simulation are in Table 13.
Tables

Table 1. Notation used in the model.
Table 2. Definitions of symbols and subscripts used to identify compartments, mass of chemical in compartments and concentrations.
Table 3. Fluid flow rules. \( Q_{11}, Q_{15}, \) and \( Q_{19} \) are specified transpiration rates (cm\(^3\)/h) where the fractions of total transpiration allocated to each leaf cluster are \( f_1 \) to \( Q_{11} \), \( f_2 \) to \( Q_{15} \), and \( f_3 \) to \( Q_{19} \).
Table 4. Environmental parameters and plant functions during uptake test (BROM3).
Table 5. Measured transpiration rates, leaf areas, and wet masses of roots, stems, and leaves for three experiments with different bromacil concentrations. The data shown are averages of several measurements obtained during an experimental period of 220 hrs for BROM5, 55 hrs for BROM3, and 72 hrs for BROM1. Numbers in parentheses following leaf area and mass of wet plant material is estimated standard error (ese).
Table 6. Bromacil concentrations in DPM/gram wet biomass.
Table 7. Basis for calculating the compartment volumes of the experimental plants. The example shown is BROM5, medium transpiration rate.
Table 8. Values of parameters used in UTAB 4.6 for geometric and chemical properties for each compartmental boundary and fluid flow rate.
Table 9. Simulated concentrations \( (C_{s}) \) divided by measured concentrations \( (C_{exp}) \) at three transpiration rates.
Table 10. Values of storage (forward) and mobilization (backward) transfer coefficient determined by the calibration procedure used in the text.
Table 11. Ratios \( Q_f/Q_b \) for individual plant parts. The transpiration rate for each experiment is listed at the top of each data column in the units of \( 10^{-3} \) cm\(^3\)/cm\(^2\) hr.
### Table 12.
Values of parameters used in the sensitivity simulations. The data base for BROM5, medium transpiration rate was the reference level for these simulations.

### Table 13.
Values of the parameters used for simulations in which several parameters were changed for an evaluation of combined effects.
MATHEMATICAL MODEL OF PLANT UPTAKE OF ORGANIC CHEMICALS

SUMMARY

Uptake, in-plant transport, and local accumulation of organic chemicals by plants are influenced by plant characteristics, properties of the chemical and the soil, and by environmental conditions. Evaluations of plant contamination required by regulatory agencies cannot be made experimentally for the many thousands of xenobiotic chemicals in existence or being developed. A predictive simulator in the form of a mathematical model would provide a valuable tool for such evaluations. For this reason, a mathematical model (UTAB, Uptake, Translocation, Accumulation, Biodegradation) was formulated by defining a generic plant as a set of adjacent compartments representing the major pools involved in transport and accumulation of water and solutes. The model consists of one root compartment, three stem compartments, and three leaf compartments. Each compartment is subdivided into two transport compartments, one for xylem and one for phloem, and a storage compartment. In addition, two compartments model the root volume outside the Casparian strip, one for the apparent free space and one for the cell volume. Values for the anatomical dimensions of the compartments and for physical and chemical coefficients were chosen from the literature. The complete system of equations, which describes uptake and accumulation, consists of 24 differential equations which are solved in terms of the chemical mass in each compartment as a function of time. The solution procedure is also developed and presented.

For calibration purposes, concentrations measured in roots, stems, and leaves were compared with model predictions, while model parameters were changed until no further improvement in matching model predictions
with experimental results was obtained. This exercise revealed important plant behavior that was not accounted for in the original formulation of the model and, as such, showed the value of the model for elucidating plant response.

The model satisfactorily predicted the observed uptake and distribution patterns for bromacil in soybean plants, at the stage of growth and under the environmental conditions used in the experiments, involving a range of transpiration rates. This indicates that the model is flexible enough to provide an accurate representation of uptake and the influence of transpiration rate on the uptake and translocation of this chemical. Parameter values used in the model were selected from literature and experimental observation. They functioned well in these simulations and they are appropriately applied in the model. The chemical parameters for storage, mobilization, and diffusion when used in the model also yielded satisfactory results, suggesting that they are also appropriately applied. Finally, the calibration, although of limited scope, showed that the model equations yielded an accurate picture of the actual uptake patterns for bromacil in soybeans used in these experiments. The theoretical exercise of compiling the model is shown to be a constructive step in learning how to predict the fate of xenobiotic contamination in plants. The model shows excellent promise for future use. However, additional testing and validation are needed.
DEVELOPMENT OF THE MODEL

Introduction

The processes of plant uptake, translocation, accumulation, and biodegradation (UTAB) of xenobiotic chemicals are important in assessing the environmental risks involved in the use of those chemicals. Since it is impossible to study each chemical with each plant in each environment, a mathematical model for predicting environmental behavior would be a valuable tool for risk assessment. Such a model, when used to explain experimental results, would also help clarify physiological mechanisms and, when validated, would allow extrapolation of experimental results to hypothetical scenarios. This report is the description of a model developed for these purposes and application of the model to experimental results.

Whole plant experiments, which are necessary to evaluate UTAB, do not allow discrete examination of the apoplastic and symplastic regions, nor of the biological properties of individual plant parts such as membrane permeabilities. Means are required to quantify individual transport mechanisms indirectly by employing procedures which make it possible to extract this information from experimental results obtained with accepted whole plant experimental techniques. A mathematical model would serve this goal. At present, few models of xenobiotic mobility in plants exist (Boersma et al., 1988a,b). None are currently available in which all the major plant parts function simultaneously in an integrated manner and operate under accepted mechanistic rules at the macroscale.

A few mechanistic models of translocation have been formulated based on the Münch transport theory (Eschich et al., 1972; Christy and
Ferrier, 1973; Ferrier and Christy, 1975; Goeschl et al., 1976; Tyree et al., 1979; Weir, 1981). These models consider transport from a single source region to a single sink region and the equations are limited to processes which occur in the sieve tubes. These models have served as a valuable starting point for the model presented here. Our objective was to construct a model for the transport of a trace organic solute in a plant, based on principles of conservation of mass. The model is a first approximation of solute transport through a complex set of physiological compartments. Because of the large number of processes involved, simplifying assumptions had to be made. Only average Fickian membrane and xylem/phloem transport processes are included.

**Structure of the Model**

The model defines a plant as a set of compartments, each representing pertinent plant tissues (Figures 1 and 2). The compartments are separated by boundaries of specified thickness and area and distinguished by the physical and chemical properties that determine passage of water and solutes. Movement of water and solutes between compartments occurs by mass flow (advective flow) or diffusion and is restricted by tortuosity of the path, selective permeability (reflection), and partitioning with tissue components (sorption).

Formulation of the model was based on identification of appropriate compartments and determining their physical and chemical characteristics and the manner in which they are connected. The example considered here subdivides a soybean plant-soil system into the major pools: soil solution, root, stem, and leaf. Although the soybean was selected
Figure 1. Schematic diagram of a generic plant, with three leaves showing the hierarchy of leaves on the stem and the numbering sequence used for model compartments.
Figure 2. Conceptualization of the plant shown in Figure 1 in terms of compartments used for the mathematical model. Definitions of symbols are in Tables 1 and 2.
as the test species, a choice based on availability of experimental data, the model can be parameterized for most terrestrial vascular plants.

Major segments of the pathway of water and solute transport through the generic plant are identified in Figure 1 and the corresponding system of compartments is in Figure 2. Symbols are defined in Tables 1 and 2. The fluid flow rules are summarized in Table 3. Each compartment is considered to be a well-stirred tank with a uniform concentration. The compartments are separated by barriers for which chemical and physical characteristics differ with respect to the ease with which water and solutes can pass. Those differences are described in terms of their reflection coefficient, partition coefficient, and hydraulic conductivity. The properties of the compartments of concern are volume, area of contact between compartments, sorption coefficient, and coefficient for first-order loss processes.

Sequence of Compartments

Water fluxes in the model (Table 3) are driven by the water potential gradients created by evaporation from the substomatal cavity and propagated throughout the plant to the soil solution. Water moves along the transpiration stream via mass flow and to storage volumes in adjoining cells via diffusion. Water also moves through the phloem pathway driven by pressure gradients. Both pathways are accounted for in the model. Solutes follow the same paths and partition into storage compartments at rates determined by physical characteristics of the particular chemical.
Table 1. Notation used in the model.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Contact area between compartments (cm²).</td>
</tr>
<tr>
<td>B</td>
<td>Sorption coefficient; describes the immobilization of the solute by reversible sorption to cell walls or large molecules in the compartment (dimensionless).</td>
</tr>
<tr>
<td>C</td>
<td>Concentration of solute in compartment (µg/cm³).</td>
</tr>
<tr>
<td>D</td>
<td>Diffusion coefficient (cm²/h).</td>
</tr>
<tr>
<td>Q₀</td>
<td>Rate of storage (cm³/h).</td>
</tr>
<tr>
<td>Q₀ᵇ</td>
<td>Rate of mobilization from storage (cm³/h).</td>
</tr>
<tr>
<td>M</td>
<td>Mass of solute in compartment (µg).</td>
</tr>
<tr>
<td>V</td>
<td>Volume of compartment (cm³).</td>
</tr>
<tr>
<td>Q</td>
<td>Water flow rate through xylem subcompartment (cm³/h).</td>
</tr>
<tr>
<td>Δx</td>
<td>Length of fluid flow path or membrane thickness connecting compartments (cm)</td>
</tr>
<tr>
<td>σ</td>
<td>Reflection coefficient for transport of chemical between compartments. The membrane is impermeable to the solute when the reflection coefficient has its maximum value of one. The membrane is nonselective; that is, it allows the solute to pass unimpeded with water when the reflection coefficient is equal to zero (dimensionless).</td>
</tr>
<tr>
<td>λ</td>
<td>Rate constant for first-order loss processes in compartment; describes immobilization of solute by incorporation into structural material or loss of solute due to metabolism (1/h).</td>
</tr>
</tbody>
</table>
Table 2. Definitions of symbols and subscripts used to identify compartments, mass of chemical in compartments, and concentrations.

<table>
<thead>
<tr>
<th>Compartment number</th>
<th>Compartment name</th>
<th>Mass in comp. (M&lt;sub&gt;i&lt;/sub&gt;)</th>
<th>Concentrations (C&lt;sub&gt;i&lt;/sub&gt;)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Root free volume</td>
<td>M&lt;sub&gt;0&lt;/sub&gt;</td>
<td>C&lt;sub&gt;0&lt;/sub&gt;</td>
</tr>
<tr>
<td>1</td>
<td>Root exterior cells</td>
<td>M&lt;sub&gt;1&lt;/sub&gt;</td>
<td>C&lt;sub&gt;1&lt;/sub&gt;</td>
</tr>
<tr>
<td>2</td>
<td>Root xylem lumen</td>
<td>M&lt;sub&gt;2&lt;/sub&gt;</td>
<td>C&lt;sub&gt;2&lt;/sub&gt;</td>
</tr>
<tr>
<td>3</td>
<td>Root storage</td>
<td>M&lt;sub&gt;3&lt;/sub&gt;</td>
<td>C&lt;sub&gt;3&lt;/sub&gt;</td>
</tr>
<tr>
<td>4</td>
<td>Root phloem lumen</td>
<td>M&lt;sub&gt;4&lt;/sub&gt;</td>
<td>C&lt;sub&gt;4&lt;/sub&gt;</td>
</tr>
<tr>
<td>5</td>
<td>Bottom stem xylem lumen</td>
<td>M&lt;sub&gt;5&lt;/sub&gt;</td>
<td>C&lt;sub&gt;5&lt;/sub&gt;</td>
</tr>
<tr>
<td>6</td>
<td>Bottom stem storage</td>
<td>M&lt;sub&gt;6&lt;/sub&gt;</td>
<td>C&lt;sub&gt;6&lt;/sub&gt;</td>
</tr>
<tr>
<td>7</td>
<td>Bottom stem phloem lumen</td>
<td>M&lt;sub&gt;7&lt;/sub&gt;</td>
<td>C&lt;sub&gt;7&lt;/sub&gt;</td>
</tr>
<tr>
<td>8</td>
<td>Mid stem xylem lumen</td>
<td>M&lt;sub&gt;8&lt;/sub&gt;</td>
<td>C&lt;sub&gt;8&lt;/sub&gt;</td>
</tr>
<tr>
<td>9</td>
<td>Mid stem storage</td>
<td>M&lt;sub&gt;9&lt;/sub&gt;</td>
<td>C&lt;sub&gt;9&lt;/sub&gt;</td>
</tr>
<tr>
<td>10</td>
<td>Mid stem phloem lumen</td>
<td>M&lt;sub&gt;10&lt;/sub&gt;</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;</td>
</tr>
<tr>
<td>11</td>
<td>Top stem xylem lumen</td>
<td>M&lt;sub&gt;11&lt;/sub&gt;</td>
<td>C&lt;sub&gt;11&lt;/sub&gt;</td>
</tr>
<tr>
<td>12</td>
<td>Top stem storage</td>
<td>M&lt;sub&gt;12&lt;/sub&gt;</td>
<td>C&lt;sub&gt;12&lt;/sub&gt;</td>
</tr>
<tr>
<td>13</td>
<td>Top stem phloem lumen</td>
<td>M&lt;sub&gt;13&lt;/sub&gt;</td>
<td>C&lt;sub&gt;13&lt;/sub&gt;</td>
</tr>
<tr>
<td>14</td>
<td>Leaf 1 xylem lumen</td>
<td>M&lt;sub&gt;14&lt;/sub&gt;</td>
<td>C&lt;sub&gt;14&lt;/sub&gt;</td>
</tr>
<tr>
<td>15</td>
<td>Leaf 1 storage</td>
<td>M&lt;sub&gt;15&lt;/sub&gt;</td>
<td>C&lt;sub&gt;15&lt;/sub&gt;</td>
</tr>
<tr>
<td>16</td>
<td>Leaf 1 phloem lumen</td>
<td>M&lt;sub&gt;16&lt;/sub&gt;</td>
<td>C&lt;sub&gt;16&lt;/sub&gt;</td>
</tr>
<tr>
<td>17</td>
<td>Leaf 2 xylem lumen</td>
<td>M&lt;sub&gt;17&lt;/sub&gt;</td>
<td>C&lt;sub&gt;17&lt;/sub&gt;</td>
</tr>
<tr>
<td>18</td>
<td>Leaf 2 storage</td>
<td>M&lt;sub&gt;18&lt;/sub&gt;</td>
<td>C&lt;sub&gt;18&lt;/sub&gt;</td>
</tr>
<tr>
<td>19</td>
<td>Leaf 2 phloem lumen</td>
<td>M&lt;sub&gt;19&lt;/sub&gt;</td>
<td>C&lt;sub&gt;19&lt;/sub&gt;</td>
</tr>
<tr>
<td>20</td>
<td>Leaf 3 xylem lumen</td>
<td>M&lt;sub&gt;20&lt;/sub&gt;</td>
<td>C&lt;sub&gt;20&lt;/sub&gt;</td>
</tr>
<tr>
<td>21</td>
<td>Leaf 3 storage</td>
<td>M&lt;sub&gt;21&lt;/sub&gt;</td>
<td>C&lt;sub&gt;21&lt;/sub&gt;</td>
</tr>
<tr>
<td>22</td>
<td>Leaf 3 phloem lumen</td>
<td>M&lt;sub&gt;22&lt;/sub&gt;</td>
<td>C&lt;sub&gt;22&lt;/sub&gt;</td>
</tr>
</tbody>
</table>
Table 3. Fluid flow rules. Q_{11}, Q_{15}, and Q_{19} are specified transpiration rates (cm^3/h) where the fractions of total transpiration allocated to each leaf cluster are f_1 to Q_{11}, f_2 to Q_{15}, and f_3 to Q_{19}.

<table>
<thead>
<tr>
<th>Flow rule</th>
<th>Region connected</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q_1 = Q_{11} + Q_{15} + Q_{19}</td>
<td>Soil-root xylem lumen</td>
</tr>
<tr>
<td>Q_2 = (1 + f_1)Q_{11} + (1 + f_2)Q_{15} + (1 + f_3)Q_{19}</td>
<td>Root xylem lumen-bottom stem xylem lumen</td>
</tr>
<tr>
<td>Q_3 = f_1 Q_{11} + f_2 Q_{15} + f_3 Q_{19}</td>
<td>Bottom stem phloem lumen-root phloem lumen</td>
</tr>
<tr>
<td>Q_4 = f_3 Q_{19}</td>
<td>Root phloem lumen-root xylem lumen</td>
</tr>
<tr>
<td>Q_5 = (1 + f_2)Q_{15} + (1 + f_3)Q_{19}</td>
<td>Bottom stem xylem lumen-mid stem xylem lumen</td>
</tr>
<tr>
<td>Q_6 = f_2 Q_{15} + f_3 Q_{19}</td>
<td>Mid stem phloem lumen-bottom stem phloem lumen</td>
</tr>
<tr>
<td>Q_7 = (1 + f_3)Q_{19}</td>
<td>Top stem xylem lumen-top stem xylem lumen</td>
</tr>
<tr>
<td>Q_8 = f_3 Q_{19}</td>
<td>Top stem phloem lumen-mid stem phloem lumen</td>
</tr>
<tr>
<td>Q_9 = (1 + f_3)Q_{19}</td>
<td>Bottom stem xylem lumen-leaf 1 xylem lumen</td>
</tr>
<tr>
<td>Q_{10} = f_1 Q_{11}</td>
<td>Leaf 1 xylem lumen-leaf 1 phloem</td>
</tr>
<tr>
<td>Q_{11} = specified +</td>
<td>Leaf 1 transpiration rate (cm^3/h)</td>
</tr>
<tr>
<td>Q_{12} = f_1 Q_{11}</td>
<td>Leaf 2 phloem lumen-bottom stem phloem lumen</td>
</tr>
<tr>
<td>Q_{13} = (1 + f_2)Q_{15}</td>
<td>Mid stem xylem lumen-mid 2 xylem lumen</td>
</tr>
<tr>
<td>Q_{14} = f_2 Q_{15}</td>
<td>Leaf 2 xylem lumen-leaf 2 phloem lumen</td>
</tr>
<tr>
<td>Q_{15} = specified +</td>
<td>Leaf 2 transpiration rate (cm^3/h)</td>
</tr>
<tr>
<td>Q_{16} = f_2 Q_{15}</td>
<td>Leaf 2 phloem lumen-mid stem phloem lumen</td>
</tr>
<tr>
<td>Q_{17} = (1 + f_3)Q_{19}</td>
<td>Top stem xylem lumen-leaf 3 xylem lumen</td>
</tr>
<tr>
<td>Q_{18} = f_3 Q_{19}</td>
<td>Leaf 3 xylem lumen-leaf 3 phloem lumen</td>
</tr>
<tr>
<td>Q_{19} = specified +</td>
<td>Leaf 3 transpiration rate (cm^3/h)</td>
</tr>
<tr>
<td>Q_{20} = f_3 Q_{19}</td>
<td>Leaf 3 phloem lumen-top stem phloem lumen</td>
</tr>
</tbody>
</table>

The open pathway for water and solute movement between the cortex cells of the root has been termed the "apparent free space" and is comprised of cellulose and open spaces which form a sponge-like material that provides structural support while allowing free water and solute movement. The apparent free space is typically about 7 percent of the tissue volume but because of its structure accounts for most of the water and solute movement from the rooting solution to the endodermis. The apparent free space is the first plant compartment in the model (0).

The next compartment (1) also lies outside the endodermis and consists primarily of the cortex cells, but also includes the epidermis and the root hairs. Solutes and water move into these cells and
migrate towards the endodermis via the symplasm. The cortex cells provide surfaces for adsorption and partitioning of the various organic chemicals with the lipoprotein membranes. They also provide a reactive environment where cytoplasmic enzymes catalyze some of the bonds of the xenobiotic chemicals of interest.

Analysis of experimental data, described later on in this paper, indicates the importance of these first two compartments in the uptake process. An extremely rapid uptake of bromacil by the roots occurred during the first hours of exposure. This was attributed to filling of the apparent free space by the bromacil containing solution as the transpiration stream was initiated. Furthermore, the apparent free space completely permeates the cortex, so that all cells are immediately bathed in the bromacil containing solution and diffusion and/or active transport into these cells can occur as soon as exposure is initiated.

Following the first two compartments are xylem, phloem, and storage compartments of roots, followed by the stem compartments and then the leaf compartments, from where water and volatile pollutants pass to the atmosphere in the vapor phase. Solutes travel the same path as water, except they may sorb to various materials in the root, stem, and leaves and they may partition between water and the cellulose lipids and proteins of the cell membranes. Many solutes do not evaporate in the stomatal cavity and are thus deposited or further translocated via the phloem to other areas in the plant.

In addition to the xylem pathway, water moves through the phloem. Connections between xylem and phloem in this model occur in the leaf compartments and in the root. Phloem also connects with the storage
compartments. Connection of leaf apoplast and leaf phloem was based on studies by Jachetta et al. (1986a,b). These connections allow water to pass from root phloem to root xylem and vice versa by either mass flow or diffusion between the two compartments.

Part of the volume of each compartment is available for storage of solute which passes through the xylem or phloem. Storage in stems was described by McCrady et al. (1987), storage in leaves by Jachetta et al. (1986a,b).

The mathematical description of rate of storage of chemical was based on the assumption that transport to and from storage involves several transport processes of which diffusion is the most important. Details of these processes are not currently known. We chose to represent the storage processes by first-order transport rates, which include diffusion-controlled processes but may also include mass flow.

Storage and mobilization coefficients were defined to lump together several transport processes occurring in plant structures of which geometric properties cannot easily be measured and where the relative contribution of each mechanism to the total process is not known. The diffusion component of the mass transport is

\[
\frac{\text{mass/unit time}}{\Delta x} = \frac{KAC}{\Delta x} \cdot A \cdot (1 - \sigma)
\]

where \(D\) is the diffusion coefficient (cm²/hr), \(K\) is the partition coefficient (dimensionless), \(A\) is the cross-sectional area (cm²), \(AC\) is the concentration (µg/cm³), \(\Delta x\) (cm) is the distance over which \(AC\) exists, and \(\sigma\) is the compound specific membrane reflection coefficient.

When \(A\) and \(\Delta x\) are not known, this may be written as
The quantity \( \frac{DK\Delta A}{\Delta x} (1 - \sigma) \) is sometimes referred to as the permeability coefficient and has the units of \( \text{cm}^3/\text{hr} \) which is also the unit of the storage and mobilization coefficients used in our model. The storage and mobilization coefficients may thus be thought of as coefficients describing the effective diffusion process where the cross-sectional area and the diffusion distance are not known. According to this interpretation the storage and mobilization coefficients are proportional to the cross-sectional area of a storage compartment and inversely proportional to the thickness of the membrane across which transport occurs. The coefficients also are proportional to \( (1 - \sigma) \). Values for the storage coefficients can only be obtained experimentally. These values are expected to vary with experimental conditions such as root temperature, water potential, rate of water flow, and properties of the chemical.

Mass Balance Equations

The mathematical model reported here is an adaptation of concepts presented in earlier reports (Boersma et al., 1988a,b). Development starts with the representation of a generic plant (Figure 1) by a system of compartments (Figure 2). Mathematical symbols in Figure 2 were defined in Tables 1 and 2. Numerical subscripts were used rather than mnemonic notations to avoid the confusion that such notations can lead to. Table 3 lists the fluid flow rules for the plant.

Development of the first five mass balance equations is now shown in detail. The remaining mass balance equations which were developed
in a similar manner are in Appendix 1. Figure 2 shows the numbering scheme of the compartments representing the various plant regions. The subscripts on the fluid flows can also be used as indicators for the intercompartmental parameter for chemical transport. In the mathematical model the term "mass transport" is used to describe the transport of chemical due to diffusion, advection, and/or active processes. This was done in accordance with concepts of transport modelling (Seagrave, 1971). The approach lumps diffusion, passive advection, and active first-order transport together in one general first-order term. Lack of knowledge generally precludes the separation of the active and passive processes, especially at the macroscale.

Soil Compartment

Beginning with the soil compartment (Figure 2) the first mass balance equation is

\[
\frac{d}{dt} \left[ \epsilon V_{-1} (1 + B_{-1} C_{-1}) \right] = \frac{d}{dt} \left[ \text{instantaneous time rate of change of free phase plus reversibly bound chemical mass (pg/h)} \right]
\]

\[-D_0 \frac{A_0}{A_{-1}} (C_{-1} - C_0) \text{rate of diffusion of chemical mass across the soil/root interface (pg/h)} \]

\[-\lambda_{-1} (C_{-1}) \text{rate of mass transport across the soil/root interface (pg/h)} \]

\[-\lambda_{-1} (C_{-1}) \text{rate of irreversible first order loss processes operating in the soil compartment (pg/h)} \]

where the subscript -1 identifies the soil compartment and 0 is the root free space.

The relationship between the concentration of chemical in the free phase and its mass in the soil compartment is
\[ M_{-1} = \epsilon(1 + B_{-1}) V_{-1} C_{-1} \quad (\text{\mu g}) \]  

(4)

and similarly in the compartment simulating the free space of the cortex.

\[ M_0 = (1 + B_0) V_0 C_0 \quad (\text{\mu g}) \]  

(5)

Solving equation (4) for \( C_{-1} \) in terms of \( M_{-1} \) and solving equation (5) for \( C_0 \) in terms of \( M_0 \) with subsequent substitution of \( C_{-1} \) and \( C_0 \) into equation (3) yields

\[ \frac{dM_{-1}}{dt} = a_{-1,-1} M_{-1} + a_{-1,0} M_0 \quad (1/h) \]  

(6)

which is the first mass balance equation. The matrix elements \( a_{-1,-1} \) and \( a_{-1,0} \) are defined by

\[ a_{-1,-1} = -\left[ \frac{D_0 A_0}{\Delta x_0} + Q_{-1} \right] \frac{1}{\epsilon V_{-1}(1 + B_{-1}) + \lambda_{-1}} \quad (1/h) \]  

(7)

\[ a_{-1,0} = -\frac{D_0 A_0}{\Delta x_0} \frac{1}{V_0(1 + B_0)} \quad (1/h) \]  

(8)

where \( a_{-1,-1} \) characterizes the total chemical transport from the soil compartment (compartment -1) to the root-free space and \( a_{-1,0} \) characterizes diffusive transport from the root-free space back to the soil compartment.

Free Space of the Roots

The second mass balance equation defines the time rate of change of the chemical mass in the free space of the root cortex. The transport pathways into and out of this region are shown in Figure 2.
Compound is assumed to be brought into this region by advective flow due to the transpiration stream and by diffusion which occurs in response to gradients which exist between the soil solution, or nutrient solution, and the free space of the cortex. The compound may be either passively (diffusion) or actively taken up by the cells of the cortex which make up compartment 1. Forward and backward transport coefficients with dimensions of volume rate of flow (cm$^3$/hr) define transport into and out of storage. If the uptake of compound by the exterior root cell stem compartment is by diffusion only, then $Q_{ST}$ is the product of a membrane diffusion coefficient (cm$^2$/hr) and an effective interfacial area (cm$^2$) divided by a characteristic membrane thickness (cm). The result may be multiplied by a partition coefficient and a transmission coefficient to allow gradients to exist across the cortex cells and free space at equilibrium conditions. Backward transport coefficients are similarly defined.

Putting the currently recognized process and transport rules together in a linear model obtains

$$\frac{dm}{dt} = \frac{D_0 A_0}{\Delta x_0} \frac{\Delta x_{1-1} - C_1}{C_0} + \frac{Q_{ST} C_1}{Q_{b0} C_0}$$

- $\frac{dm}{dt}$: instantaneous time rate of change of free phase plus reversibly bound chemical mass in the free space of the cortex (µg/h)
- $D_0 A_0/\Delta x_0$: rate of diffusion of chemical mass across the soil/root interface (µg/h)
- $\Delta x_{1-1}$: rate of mass transport across the soil/root interface (µg/h)
- $C_0$: rate of first-order loss due to storage (µg/h)
- $Q_{ST} C_1$: rate of first-order gain due to mobilization from storage (µg/h)
- $Q_1(1 - \sigma_1)C_0$ rate of mass transport across the endodermis (µg/h)

- $\frac{D_1 A_1}{\Delta x_1} (C_0 - C_2)$ rate of diffusion of chemical mass across the cortex/root xylem interface (µg/h)

- $\lambda_0 M_0$ rate of all other first-order irreversible processes in the free space of the cortex (µg/h)

Define chemical masses in the compartments as follows:

\[
M_1 = (1 + B_1) V_1 C_1, \quad (\text{g})
\]

\[
M_2 = (1 + B_2) V_2 C_2, \quad (\text{µg})
\]

Solving equations (10) and (11) for $C$ in terms of $M$ and substituting for $C_1$, $C_0$, $C_1$, and $C_2$ into equation (9) yields the second mass balance equation

\[
\frac{dM_0}{dt} = a_{0,1} M_1 + a_{0,0} M_0 + a_{0,1} M_1 + a_{0,2} M_2, \quad (\text{µg})
\]

where the "matrix elements" are defined by

\[
a_{0,1} = \frac{D_0 A_0 + Q_{ST}}{(1 + B_0) V_1}, \quad (1/\text{h})
\]

\[
a_{0,0} = \frac{\left[\frac{D_0 C_0}{V_0} + \frac{D_1 A_1}{\Delta x_1} + Q_{ST} + Q_{fo} + Q_1(1 - \sigma_1)}{(1 + B_0) V_0} + \lambda_0\right]}{(1/\text{hr})}
\]

\[
a_{0,2} = \frac{D_1 A_1}{(1 + B_2) V_2}, \quad (1/\text{h})
\]
Storage Volume of Root Cortex

The third mass balance equation defines the time rate of change of chemical mass in the cells of the root cortex. Uptake of compound may be by diffusion and/or active mass transport. The balance equation is made up of three first-order processes:

\[ \frac{dM_1}{dt} = \text{instantaneous time rate of change of free phase plus reversibly bound chemical mass in the root cortex storage compartment (µg/h)} \]

- \[ Q_{ST}^{ST} C_0 \] rate of first-order loss due to storage (µg/h)

+ \[ Q_{b0} C_1 \] rate of first-order gain due to mobilization from storage (µg/h)

- \[ \lambda_1 M_1 \] rate of all other first-order irreversible processes, including metabolism, in the cell volume of the cortex (µg/h)

Chemical masses in the compartments were defined earlier as follows:

\[ M_0 = (1 + B_0)V_0 C_0 \] (5)

\[ M_1 = (1 + B_1)V_1 \] (10)

Substitution for the two indicated concentrations yields

\[ \frac{dM_1}{dt} = a_{1,0} M_0 + a_{1,1} M_1 \] (18)

where the matrix elements are defined by

\[ a_{1,0} = \frac{Q_{ST}}{(1 + B_0)V_0} \] (19)

\[ a_{1,1} = -\left(\frac{Q_{b0}}{(1 + B_1)V_1} + \lambda_1\right) \] (20)
**Root Xylem Compartment**

The fourth mass balance equation defines the time rate of change of mass in the compartment simulating the root xylem. The transport pathways and processes into and out of this compartment are shown in Figure 2. The flows are self explanatory.

The mass balance equation for the root xylem compartment is:

\[
\frac{dM_2}{dt} = \text{instantaneous time rate of change of free phase plus reversibly bound chemical mass in the root xylem compartment (µg/h)}
\]

\[
\frac{D_1 A_1}{\Delta x_1} (C_0 - C_2)
\]

\[
+ Q_1 (1 - \sigma_1) C_0
\]

\[
\frac{D_4 A_4}{\Delta x_4} (C_4 - C_2)
\]

\[
+ Q_4 (1 - \sigma_4) C_4
\]

\[
\frac{D_2 A_2}{\Delta x_2} (C_2 - C_5)
\]

\[
- Q_2 (1 - \alpha_2) C_2
\]

\[
\lambda_2 \tau T C_2
\]

\[
+ \sigma T \tau \tau T C_3
\]

\[
\lambda_2 \alpha_2 C_3
\]

\[
\]
\[ M_4 = (1 + B_4) V_4 C_4, \quad (\mu g) \]  
\[ M_5 = (1 + B_5) V_5 C_5. \quad (\mu g) \]

The fourth mass balance equation for the time rate of change of mass \( \frac{dM_2}{dt} \) is obtained by solving each of equations (22), (23), and (24) for its compartment concentration \( C_1 \) in terms of its compartment mass \( M_1 \), substituting the result into equation (21), and collecting common terms. The result is:

\[
\frac{dM_2}{dt} = -a_{2,0} M_0 + a_{2,2} M_2 + a_{2,3} M_3 + a_{2,4} M_4 + a_{2,5} M_5, \quad (25)
\]

where

\[
a_{2,0} = \frac{D_1 A_1}{\Delta x_1} + Q_1 (1 - \sigma_1) \quad (26)
\]

\[
a_{2,2} = -\left[ \frac{D_1 A_1}{\Delta x_1} \frac{D_4 A_4}{\Delta x_4} + \frac{D_2 A_2}{\Delta x_2} + \frac{Q_2 (1 - \sigma_2)}{V_2 (1 + B_2)} + Q_{f1} \right] \quad (27)
\]

\[
a_{2,3} = \frac{a_{2,3}^{ST}}{V_3 (1 + B_3)}, \quad (28)
\]

\[
a_{2,4} = \frac{a_{2,4}^{ST}}{V_4 (1 + B_4)} \quad (29)
\]

\[
a_{2,5} = \frac{D_2 A_2}{\Delta x_2} + Q_1 \quad (30)
\]
Root Storage Compartment

The equation for the time rate of change of mass in the root storage compartment yields the fifth mass balance equation:

\[
\frac{dM_3}{dt} = \text{instantaneous time rate of change of free plus reversibly bound chemical mass in the root storage compartment (µg/h)} \\
Q_{f1}^{ST} C_2 \\
+ Q_{f2}^{ST} C_4 \\
- Q_{b1}^{ST} C_3 \\
- Q_{b2}^{ST} C_3 \\
- \lambda_3 M_3.
\]

ST

\[Q_{f1}^{ST} = \frac{V_2(l + B_2)}{a_{2,3}} \]  
\[Q_{f2}^{ST} = \frac{V_3(l + B_3)}{a_{3,3}} \]  
\[Q_{b1}^{ST} + Q_{b2}^{ST} = \lambda_3 \]  
\[a_{3,3} = \frac{Q_{b1}^{ST} + Q_{b2}^{ST}}{V_3(l + B_3)} + \lambda_3 \]

M_2, M_3, and M_4 were defined by equations (11), (23), and (24).

Solving each for concentrations C_2, C_3, and C_4, respectively, and substituting the results in equation (31) yields,

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4,
\]

where

\[
a_{2,3} = \frac{V_2(l + B_2)}{a_{2,3}}, \quad a_{3,3} = \frac{Q_{b1}^{ST} + Q_{b2}^{ST}}{V_3(l + B_3)} + \lambda_3.
\]
System of Equations

The remaining 19 mass balance equations with corresponding matrix elements were derived in a similar manner. The complete listing of all 24 mass balance equations is given in Appendix 1. The total chemical mass in each compartment is defined for $i = 6, 7, ..., 22$, by

$$M_i = (1 + B_i) V_i C_i.$$  \hfill (36)

The possibility of loss of mass due to volatilization from leaves is included by stating:

$$\text{rate of loss via volatilization} = \frac{DCH}{\Delta x_{11}} (\text{mg/hr}) (18 - C_{air_{11}}).$$  \hfill (37)

where $H_C$ is the dimensionless Henry law constant for the chemical compound being modeled, $DCH$ (cm$^2$/h) is the effective chemical diffusion coefficient of the compound in the boundary layer over the leaf surface, $C_{air_{11}}$ (mg/g) is the concentration of the chemical compound in the mixed air outside the boundary layer, $\Delta x_{11}$ (cm) is the thickness of the boundary layer, and $A_{11}$ (cm$^2$) is the effective area of volatilization.

Rules, similar to equation (37), were also written for leaves 2 and 3. Equation (37) allows communication with the atmosphere and incorporation of atmospheric conditions such as wind speed, and air temperature, and relative humidity.
Solution Method

The complete system of 24 differential equations in 24 unknowns can be written in matrix form as

\[ \frac{dM}{dt} = AM + S, \]  

(38)

with initial conditions summarized as

\[ M(0) = M_0, \]  

(39)

where \( M \) is the 24 x 1 vector of unknown masses at time \( t \), \( S \) is the 24 x 1 vector of sources which may have nonzero entries at positions 14, 17, and 20, \( A \) is the 24 by 24 irreducible transport-transfer matrix, which is real, weakly diagonally dominant, has negative diagonal entries, and whose off diagonal entries are either positive or zero (Varga, 1962), and \( M_0 \) is the 24 x 1 vector of initial chemical masses.

The system of equations given by equation (38) is linear and has constant coefficients, over the arbitrary slice \( T_L \) to \( T_U \) hours. As such this system has a unique continuous solution vector \( M(t) \) (Boyce and DiPrima, 1965). Each element \( M_i(t) \) of \( M(t) \) is itself a linear combination of at most 24 elementary exponential functions. Because assignment of appropriate weighting factors is not practical with current knowledge, we chose to approximate the solution numerically. The method outlined below is now enjoying a renewed interest and usage due to the availability of microcomputers with large storage, high speed, and double precision arithmetic. It is a useful method for large, sparse, arrays with constant coefficients such as frequently arise in biological and control systems.
Define the matrix exponential function, sometimes called the fundamental solution matrix, to be
\[ e^{At} = I + \sum_{k=1}^{\infty} \frac{(At)^k}{k!}. \] (40)

This series serves as the basis for the numerical solution method, although it is useful for computing only for small values of time \( \tau \) (Boyce and DiPrima, 1965), where \( I \) is the identity matrix. Boyce and DiPrima (1965) prove many important properties about this matrix exponential function, such as

i) differentiation:
\[ \frac{d}{dt} e^{At} = A e^{At}. \] (41)

ii) commutation:
\[ A e^{At} = e^{At} A. \] (42)

iii) commutation:
\[ A^{-1} e^{At} = e^{At} A. \] (43)

Rewrite equation (38) as
\[ \frac{dN}{dt} = A M. \] (44)

and matrix multiply left by \( e^{-At} \), the inverse matrix of \( e^{At} \) (Boyce and DiPrima, 1965), and recast the system into the form
\[ \frac{d(e^{-At} M)}{dt} = -A e^{-At} M. \] (45)

Next, superimpose on the time line a lattice of points \( t_0, t_1, t_2, \ldots \) so that \( t_0 = 0, t_1 = \Delta t, t_2 = 2\Delta t, t_3 = 3\Delta t, \ldots \), then multiply both sides of equation (45) by the differential \( dt \), and integrate both sides between the two time points \( t_n, t_{n+1} \), to obtain:
\[
\begin{align*}
-At_{n+1} + e^{At_n} M(t_{n+1}) - e^{At_n} M(t_n) \\
&= -A^{-1} (e^{At_{n+1}} - e^{At_n}) S \tag{46}
\end{align*}
\]

Matrix multiply left both sides of equation (46) by \(e^{At_n}\) to obtain the explicit recursion formula

\[
M(t_{n+1}) = e^{A\Delta t} M(t_n) - A^{-1} (I - e^{A\Delta t}) S \tag{47}
\]

Note that no approximation has as yet been made. Equation (47) is an exact solution of the original differential system, but the solution consists of \(M\) evaluated only on a discrete set of time points. Define the constant vector \(W\) via the formula

\[
W = -A^{-1} (I - e^{A\Delta t}) S \tag{48}
\]

Clearly, on the discrete set of time points \(t_0, t_1, t_2, \ldots\)

\[
M(t_{n+1}) = e^{A\Delta t} M(t_n) - W \tag{49}
\]

which is a 24-dimensional, first-order, nonhomogeneous, difference system (Varga, 1962; Jacquez, 1972).

Mathematical induction shows that the unique solution to system (47) is

\[
M(t_n) = (e^{A\Delta t})^n M_0 + (I - e^{A\Delta t})^{-1} (I - (e^{A\Delta t})^n) W \tag{50}
\]

for \(n = 1, 2, 3, \ldots\)

Because \(e^{A\Delta t}\) is a positive 24 x 24 array with a spectral radius (modulus of the maximum eigenvalue) less than 1, \(e^{A\Delta t}\) is said to be a convergent array since, as \(n \to \infty\), \((e^{A\Delta t})^n \to Z\), the array of zero elements (Varga, 1962). It can be shown that
\[
\lim_{n \to \infty} M(t_n) = -A^{-1} S
\]

which follows directly from equation (50).

Equation (49) is used for computational purposes. The approximation is made because \( e^{A \Delta t} \) can only be computed to the double-precision limits of the computer. A useful method for carrying out the computation is to observe that

\[
e^{A \Delta t} = (e^{N \Delta t})^{N-1} = [(e^{N \Delta t})^{N-1}]
\]

where \( N \) is chosen to be a power of 2, just large enough so that

\[
\max_{1 \leq i \leq 24} \left\{ \left| -a_{ii} \Delta t \right| \right\} < 1
\]


The key to computing \( \exp[A \Delta t] \) to high precision is to first compute \( \exp[-A \Delta t/N] \) using the matrix exponential function definition 40 to the double-precision limits of the computer. Next, compute \( (\exp[-A \Delta t/N])^{N-1} \), the inverse-scaled exponential matrix function via the classical LU factorization method. Lastly, raise \( \exp[-A \Delta t/N]^{N-1} \) to the power \( N \). Other scaling methods exist (Golub and Van Loan, 1983). Time-marching scheme (49) is a stable scheme in that any small perturbation introduced into the data at some time \( t_k > 0 \), propagates in a bounded fashion as time exceeds \( t_k \), arbitrarily large (Varga, 1962).

**Effective Concentrations**

In most experimental situations it is difficult, if not impossible, to sample the phloem, xylem, or storage compartments individually.
to determine concentrations (µg/cm³) at points in time. For example, when evaluating accumulation by leaves it is usually most convenient to harvest groups of leaves and obtain an average concentration (DPM/g) or (µg/g) for the group. An average or "effective tissue concentration" can then be obtained by dividing the chemical mass present by the wet mass of tissue (µg/g). An effective volume-based concentration (µg/cm³) can be obtained when the density is known. Assuming that the density of most plant parts of young soybean plants is 1/cm³, effective concentrations (µg/cm³) are defined as below. In the definition, (t) indicates concentration at time t and OA indicates the overall average concentration for the indicated plant part:

i) in the roots,

\[ C_{\text{roots}}(t) = \frac{\sum_{i=0}^{4} M_i}{\sum_{i=0}^{4} V_i} \]  

(53)

ii) in the individual stem parts.

\[ C_{\text{stem b}}(t) = \frac{\sum_{i=5}^{7} M_i}{\sum_{i=5}^{7} V_i} \]  

(54)

\[ C_{\text{stem m}}(t) = \frac{\sum_{i=8}^{10} M_i}{\sum_{i=8}^{10} V_i} \]  

(55)

\[ C_{\text{stem l}}(t) = \frac{\sum_{i=11}^{12} M_i}{\sum_{i=11}^{12} V_i} \]  

(56)

iii) in the stem,

\[ C_{\text{stem OA}}(t) = \frac{\sum_{i=5}^{12} M_i}{\sum_{i=5}^{12} V_i} \]  

(57)

iv) in the individual leaf clusters,
\[ c_{\text{leaf } 1}(t) = \frac{16}{\sum_{i=14}^{16} M_i} / \sum_{i=14}^{16} V_i; \]  
\[ c_{\text{leaf } 2}(t) = \frac{19}{\sum_{i=17}^{19} M_i} / \sum_{i=17}^{19} V_i; \]  
\[ c_{\text{leaf } 3}(t) = \frac{22}{\sum_{i=20}^{22} M_i} / \sum_{i=20}^{22} V_i; \]  
\[ c_{\text{leaf } 0A}(t) = \frac{22}{\sum_{i=14}^{22} M_i} / \sum_{i=14}^{22} V_i. \]  

\( v \) in the leaves,
APPLICATION TO EXPERIMENTS

Introduction

This part of the manuscript describes the application of the model to previously obtained experimental data on uptake of the herbicide Bromacil® by soybean plants (Glycine max) (McFarlane and Pfleeger, 1987). The purpose of this exercise was to calibrate the model.

Calibration of mathematical models generally consists of using the model in a parameter estimation or system identification mode for application to a set of experimentally obtained data sets. Convergence on the values of parameters is guided by some measure or criterion of "goodness of fit," e.g. mean square error or mean square deviation. Several different system driving variables may be involved (Godfrey and diSteffano, 1987). Ideally, the model is developed first, then experiments are designed and carried out to test the assumptions on which the model is based (Box et al., 1978). The lack of fit between model prediction and experimental measurement is assessed and the model may be changed to obtain improved matching between model prediction and experiment. Additional sets of experiments are then designed for testing the model. In the present case, previously obtained data were used and the model was adapted to allow for peculiar experimental differences. Results of seven uptake experiments involving three bromacil concentrations and three transpiration rates were available.

Experimental Procedures

Soybean [Glycine max (L.) Merr. dwarf cultivar Fiskeby v] plants were grown in a hydroponic nursery (McFarlane and Pfleeger, 1986) in a greenhouse until leaves at the eleventh or twelfth node were just
starting to develop. All lateral stems were removed as they initiated. The nutrient solution was a modified, half-strength, Hoagland solution (Berry, 1978) with a pH of 6.0 and electrical conductivity of 1.2 dS/m. Plants of similar size were transferred to the exposure chambers described by McFarlane and Pfleeger (1987). Plants were acclimated for three days to the conditions of the controlled environment prior to adding $^{14}$C-labeled bromacil (U-$^{14}$C$_6$H$_{13}$BrN$_2$O$_2$) to the nutrient solution. The specific activity of the treatment stock was $6.16 \times 10^6$ Bq/mmole bromacil as measured by liquid scintillation analysis and gas/liquid chromatography. The treatment was started by the addition of the amount of bromacil stock solution needed to obtain the desired concentration in each plant exposure chamber. The concentrations used in each of the three experiments are in Table 4 in addition to other environmental parameters. Root exposure was monitored by periodically sampling the hydroponic solution and analyzing for $^{14}$C activity. Each sample was analyzed in triplicate and the analytical variation in counting replicate samples was never larger than 3 percent of the mean.

The solution volume was maintained automatically at 6.5 liters by replacing transpired water with nutrient solution but without bromacil. Since bromacil uptake was approximately proportional to the transpiration rate, chemical was lost at a faster rate from the solution with a high transpiration rate than from one with a low transpiration rate.

Bromacil uptake was measured by periodically removing plants from each chamber for determination of $^{14}$C concentration of the plant parts. The stems were cut at the crown, the leaves removed, and fresh weights were determined for leaves, stems, and roots. The tissues were freeze dried. Roots and leaf tissues were ground to a powder, then subsamples
Table 4. Environmental parameters and plant functions during uptake test (BROM3).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Value</th>
<th>CV%</th>
</tr>
</thead>
<tbody>
<tr>
<td>BROM1</td>
<td>BROM3</td>
<td>BROM5</td>
<td></td>
</tr>
<tr>
<td>Photosynthetic Photon flux (PPF)*</td>
<td>μmol/s m²</td>
<td>350</td>
<td>350</td>
</tr>
<tr>
<td>Air Temperature</td>
<td>°C</td>
<td>23</td>
<td>23</td>
</tr>
<tr>
<td>Specific humidity</td>
<td>g/m³</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(low tr.)</td>
<td></td>
<td>20</td>
<td>16</td>
</tr>
<tr>
<td>(medium tr.)</td>
<td></td>
<td>16</td>
<td>12</td>
</tr>
<tr>
<td>(high tr.)</td>
<td></td>
<td>12</td>
<td>12</td>
</tr>
<tr>
<td>Windspeed</td>
<td>m/s</td>
<td>0.6</td>
<td>1.5</td>
</tr>
<tr>
<td>CO₂</td>
<td>mmol/m³</td>
<td></td>
<td>15.6</td>
</tr>
<tr>
<td>Transpiration</td>
<td>cm³/h plant</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(low)</td>
<td></td>
<td>4.4</td>
<td>1.2</td>
</tr>
<tr>
<td>(medium)</td>
<td></td>
<td>7.6</td>
<td>5.7</td>
</tr>
<tr>
<td>(high)</td>
<td></td>
<td>7.0</td>
<td>7.3</td>
</tr>
<tr>
<td>Bromacil concentration of bathing solution</td>
<td>μg/cm³</td>
<td>0.528</td>
<td>0.180</td>
</tr>
</tbody>
</table>

*Light cycle on/off was 24/0 hours.

were obtained and burned in a Packard 306 sample oxidizer. The CO₂ was collected and analyzed for ¹⁴C activity by liquid scintillation counting. Stem material was not easily ground because of its fibrous nature, therefore segments were selected from the lower, middle, and top portions of each plant and oxidized without powdering. Attention was given to the possibility of chemical loss during drying and as a result of incomplete combustion in the oxidation step. Quality assurance tests confirmed that less than 1 percent was lost in either procedure.
Transformation of bromacil was tested by evaluation of thin-layer chromatographs made from plant extracts and from the hydroponic solution. Only bromacil was found in the nutrient solution and roots, but about 5 percent of the $^{14}C$ activity in the leaves was determined to be associated with another chemical. This result was also found in other studies (McFarlane et al., 1987). Since this was a small contribution to the total $^{14}C$ activity, and since all the bromacil was accounted for in this study, it was assumed that the results presented on the basis of DPM are an accurate description of the movement patterns of bromacil in the test plants.

Three experiments with bromacil uptake were conducted, each with some different aspect in timing, dosing concentration, or experimental conditions (Table 4). The knowledge gained from the first experiment (BROM1) led to the design of the second (BROM3), which included three exposure chambers, each with a different transpiration rate. In the final experiment (BROM5) bromacil was periodically added to each chamber so that the concentration in the nutrient solutions remained approximately constant throughout the exposure. In the first two tests, individual leaves, stems, and root segments were analyzed. In the last test, samples were pooled and subsamples representing plant regions were analyzed.

Since two types of experiments were conducted, namely, one with decreasing bromacil concentration and one with constant bromacil concentration, the mathematical model was formulated in a manner which allowed either condition to exist in the simulation.

Results of the three experiments include measurements of transpiration rates, leaf areas, wet mass of harvested plant parts (Table 5),
Table 5. Measured transpiration rates, leaf areas, and wet masses of roots, stems, and leaves for three experiments with different bromacil concentrations. The data shown are averages of several measurements obtained during an experimental period of 220 hrs for BROM5, 55 hrs for BROM3, and 72 hrs for BROM1. Number in parenthesis following leaf area and mass of wet plant material is estimated standard error (ese).

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Leaf area cm²</th>
<th>Transp rate cm³/cm² hr</th>
<th>Wet mass of plant parts g</th>
<th>Roots g</th>
<th>Stems g</th>
<th>Leaves g</th>
</tr>
</thead>
<tbody>
<tr>
<td>BROM5</td>
<td>765 (103)</td>
<td>2.61 x 10⁻³</td>
<td>24.7 (3.5)</td>
<td>4.5 (0.8)</td>
<td>16.7 (1.4)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>725 (122)</td>
<td>7.82 x 10⁻³</td>
<td>31.1 (9.3)</td>
<td>6.5 (1.4)</td>
<td>17.3 (7.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>825 (116)</td>
<td>8.85 x 10⁻³</td>
<td>31.5 (6.0)</td>
<td>6.6 (1.1)</td>
<td>19.3 (3.7)</td>
<td></td>
</tr>
<tr>
<td>BROM3</td>
<td>1578 (250)</td>
<td>2.77 x 10⁻³</td>
<td>47.5 (6.1)</td>
<td>71.2 (7.8)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1761 (261)</td>
<td>4.32 x 10⁻³</td>
<td>56.5 (9.3)</td>
<td>114 (9.9)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1794 (160)</td>
<td>5.26 x 10⁻³</td>
<td>47.9 (7.8)</td>
<td>77.0 (8.2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>BROM1</td>
<td>845 (110)</td>
<td>8.61 x 10⁻³</td>
<td>30.0 (6.3)</td>
<td>6.1 (0.6)</td>
<td>21.3 (2.1)</td>
<td></td>
</tr>
</tbody>
</table>

and concentrations of radio-labeled bromacil in the separately harvested plant parts as a function of exposure time (Table 6). The transpiration rates shown in Table 5 were obtained by measuring the volume of water lost during measurement intervals. Table 5 indicates that the plants of the BROM3 experiment were about twice as large as those of BROM1 and BROM5.

The BROM5 experiment had the lowest bromacil concentration. The measured concentration of radio-labeled bromacil in the tank was 3250 DPM/cm³, which corresponds to 0.058 μg bromacil/cm³ solution (Table 4). The BROM3 experiment used an initial bromacil concentration which was 3.1 times higher (0.180 μg/cm³) and BROM1 used an initial bromacil concentration which was 9.1 times higher (0.528 μg/cm³).
Table 5 lists the average biomass of plant parts present during each experiment. The question of growth was of concern with these experiments, particularly with BROM5 which lasted eight days. Measurement showed that there was not a systematic increase in biomass during the time of the experiments. This was confirmed by means and estimated standard errors (ese) of leaf areas and wet masses which were calculated for each measurement sequence. The decision was made that all experiments could be treated as steady-state experiments with respect to plant growth.

Measurements of radioactivity in each harvested plant part in DPM per unit of wet mass (Table 6) shows the increase in radio-labeled bromacil with time. The C\textsuperscript{14}-labeled bromacil was counted and reported as DPM per whole tissue region. This is an aggregate value for a region and does not give the concentration of the individual leaf or stem compartments.

The model was designed to allow evaluation of three separate stem and leaf compartments in each plant and simulations were run in this mode. For output the compartments were summed, because measurements were made in this manner. The effective bromacil concentration of the wet tissue in DPM/g was defined to be the total DPM measured in the wet tissue divided by the wet mass of this tissue in grams. This assumes that the mass of wet tissue can be equated to the volume of that tissue, i.e., the density of wet tissue, excluding air spaces, is 1 g/cm\textsuperscript{3}. The definitions follow from equations (53-61). Measurements of DPM concentration can be converted into mg per cm\textsuperscript{3} by using the conversion factor of $1.82 \times 10^{-5}$ mg of bromacil per DPM. The factor
Table 6. Bromacil concentrations in DPM per gram wet biomass.

<table>
<thead>
<tr>
<th></th>
<th>BROM5</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Low</td>
<td>Medium</td>
<td>High</td>
</tr>
<tr>
<td>Time (hr)</td>
<td>Roots</td>
<td>Stems</td>
<td>Leaves</td>
</tr>
<tr>
<td>8</td>
<td>5,149</td>
<td>3,654</td>
<td>507</td>
</tr>
<tr>
<td>26</td>
<td>7,058</td>
<td>11,864</td>
<td>3,473</td>
</tr>
<tr>
<td>50</td>
<td>8,315</td>
<td>18,634</td>
<td>7,262</td>
</tr>
<tr>
<td>122</td>
<td>36,793</td>
<td>26,293</td>
<td>3,473</td>
</tr>
<tr>
<td>145</td>
<td>16,094</td>
<td>35,815</td>
<td>30,148</td>
</tr>
<tr>
<td>169</td>
<td>18,041</td>
<td>36,512</td>
<td>35,009</td>
</tr>
<tr>
<td>193</td>
<td>19,876</td>
<td>60,699</td>
<td>33,155</td>
</tr>
<tr>
<td>218</td>
<td>51,010</td>
<td>42,686</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>BROM3</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Low</td>
<td>Medium</td>
<td>High</td>
</tr>
<tr>
<td>Time (hr)</td>
<td>Roots</td>
<td>Shoots</td>
<td>Roots</td>
</tr>
<tr>
<td>3.0</td>
<td>12,616</td>
<td>536</td>
<td>15,462</td>
</tr>
<tr>
<td>7.0</td>
<td>15,651</td>
<td>2,723</td>
<td>17,799</td>
</tr>
<tr>
<td>15.0</td>
<td>14,550</td>
<td>6,098</td>
<td>14,641</td>
</tr>
<tr>
<td>23.0</td>
<td>16,218</td>
<td>17,257</td>
<td>21,452</td>
</tr>
<tr>
<td>31.0</td>
<td>16,614</td>
<td>14,790</td>
<td>21,728</td>
</tr>
<tr>
<td>39.0</td>
<td>20,542</td>
<td>28,926</td>
<td>19,013</td>
</tr>
<tr>
<td>47.0</td>
<td>21,382</td>
<td>35,527</td>
<td>26,271</td>
</tr>
<tr>
<td>55.0</td>
<td>17,725</td>
<td>29,815</td>
<td>**</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>BROM1</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Time (hr)</td>
<td>Tank</td>
<td>Roots</td>
<td>Bottom</td>
</tr>
<tr>
<td>0.0</td>
<td>31,165</td>
<td>40,000</td>
<td>0.0</td>
</tr>
<tr>
<td>1.0</td>
<td>29,186</td>
<td>24,737</td>
<td>11,158</td>
</tr>
<tr>
<td>4.0</td>
<td>27,848</td>
<td>32,007</td>
<td>32,563</td>
</tr>
<tr>
<td>8.0</td>
<td>28,168</td>
<td>47,592</td>
<td>42,421</td>
</tr>
<tr>
<td>24.0</td>
<td>30,530</td>
<td>62,247</td>
<td>64,403</td>
</tr>
<tr>
<td>48.0</td>
<td>24,200</td>
<td>86,676</td>
<td>86,590</td>
</tr>
<tr>
<td>72.0</td>
<td>22,175</td>
<td>85,225</td>
<td>81,675</td>
</tr>
</tbody>
</table>

THIS PUBLICATION IS OUT OF DATE. For most current information: http://extension.oregonstate.edu/catalog
follows from:
\[
0.05834 \, (\mu g/cm^3)/3200 \, (DPM/cm^3) = 1.82 \times 10^{-5} \, (mg/DPM).
\]

**Qualitative Overview of Results**

An initially very rapid increase in concentration occurred in the roots (Figure 3) with all experiments, followed by a slower rate of increase which remained nearly constant with time. The rapid increase during the first few hours of exposure was attributed to the filling of the free space of the root cortex with the bathing solution, with a concurrent rapid entry of solute into the cortex cells. The rapid permeation occurred as the transpiration stream drew in the bathing solution immediately upon exposure to the solution. This rapid increase indicates a large value for the storage coefficient during the early part of the uptake process with smaller values during the time following the initial loading.

Concentrations of the stem compartments of the BROM5 and BROM3 experiments (Figure 4) did not show the rapid initial increase that was found in the root compartments. However, a rapid increase in concentration did occur with the BROM1 experiment, with plants exposed to the high concentration of bromacil in the bathing solution (Table 4). The increase in stem concentrations was nearly linear for all three experiments during the first 50 hours of exposure. Concentrations in the stem compartments were higher than in the root compartments, suggesting that storage coefficients for the stem compartments were higher than for the root compartments and that the ratio of forward storage coefficient \(Q_b\) to backward storage coefficient \(Q_f\) was higher.
Measure bromacil concentrations in the root compartments. Details of the experimental procedures are in the text. The curves shown were drawn by hand to emphasize trends in increase in concentration. The graphs show an initial rapid rise in concentration, followed by a linear increase with time.
Figure 4. Measured bromacil concentrations in the stem compartments. Details of the experimental procedures are in the text. Curves were drawn by hand to emphasize trends in increase in concentrations. The graphs show a linear increase in concentration during the exposure period.
Results for the leaf compartments show a delayed arrival of the bromacil when compared to the root and stem compartments (Figure 5). Results for the BROM3 experiment are not shown because stems and leaves were analyzed together. Concentrations in the leaf compartments were still low after 10 hours of exposure. Storage in the leaf compartments continued in an apparent linear manner. This linear increase persisted over the entire 200-hour exposure period of the BROM3 experiment.

Concentrations at the end of 50 hours of exposure plotted as functions of solution concentrations (Figure 6) show that concentration effects may occur with bromacil uptake. The concentrations increased in a nonlinear manner with increasing exposure concentration for all three plant parts. The relationship had a weakly negative exponent for roots and stems, but a strong positive exponent for leaves.

Calibration

The purpose of the modeling exercise was to develop procedures for describing, by means of mathematical models, plant uptake of organic chemicals, or more specifically, bromacil uptake by soybean seedlings. Uptake behavior is embedded in the storage and mobilization coefficients and the calibration of the model was therefore with respect to these coefficients.

Calibration of mathematical models ideally consists of using the model in a parameter estimation mode. Numerical procedures are used to find the parameter values which provide simulation results closely approximating experimental results. Convergence on the values of the parameters is guided by some measure or criterion of "goodness of fit," e.g. mean square error or mean square deviation. For this study the
Figure 5. Measured bromacil concentrations in the leaf compartments for the BROM1 and BROM5 experiments. Curves were drawn by hand to emphasize trends. Results suggest a linear rate of uptake in these experiments with constant transpiration rates.
Figure 6. Concentration at 50 hrs of exposure as a function of solution concentration.
number of data points was not sufficient to follow this ideal procedure. Since model development is a recent activity, this circumstance is not unusual. Godfrey and diSteefano (1987) recently addressed the problem and describe procedures for finding parameters using incomplete data sets.

According to recommended procedures, the data of the uptake experiments were first used to gain insight into the process to be modeled. This was initiated earlier in the manuscript with a qualitative analysis of the experimental results. This analysis was also used to set initial values of the parameters. Thus an iterative procedure, guided at each step by comparison of simulation and experimental data, was used to systematically adjust $Q_{bi}$ and $Q_{bj}$ values until agreement between simulation and measured results was obtained. About 50 sets of simulations were needed to arrive at the set of storage coefficients which gave acceptable agreement with experimental results. Providing mathematical proof that the storage coefficients obtained in this manner are unique is not possible. Another set of values, different from those shown which would give an equally good fit to the data, may exist.

UTAB 4.6 is a medium-resolution model. As such, it requires values for a large number of geometric and physiologic parameters which must be obtained before calibration with respect to storage coefficients can begin. Values of the parameters were chosen on the basis of a "normalized" plant with a total leaf area of 1000 cm$^2$ and then scaled according to measured plant sizes. Leaf areas were in the range 800 to 1,800 cm$^2$ (Table 2). This approach was used in earlier reports.
(Boersma et al., 1988a,b,c) and values for anatomical features of soybean plants were derived from these reports.

**Volumes of Compartments**

Literature data and experimental results indicated that the generic soybean plant with a leaf area of 1,000 cm² would have a root volume of 25 cm³, a stem volume of 6 cm³, and a leaf volume of 25 cm³ (Boersma, 1988a). The experimental plants corresponded approximately to these values in terms of ratios and absolute values (Table 1). The next step in setting up the data base for simulation was to obtain volumes of all compartments of the model for each experiment. The procedure for doing so is detailed by Table 7. The example shown in Table 7 is for BROM5, medium transpiration rate. The first step was to change from wet mass to volume, based on the assumption of a tissue density excluding air spaces equal to 1 g/cm³. The first column in Table 7 shows the aggregate volume for each plant part of the normalized plant, i.e. 25 cm³ for the roots, 6 cm³ for the stems, and 25 cm³ for the leaves. The second column shows the percent of each of these volumes occupied by sub compartments. These percentages were chosen from literature reports. The root was divided into the region outside the endodermis (cortex) and the region inside the endodermis (xylem + phloem + storage). Seventy-five percent was allocated to the cortex and 25 percent to the stele. Then volumes of cortex and stele were further subdivided. Of the cortex volume, 85 percent was allocated to cell volume and 15 percent to apparent free space. The stele was subdivided into 4 percent xylem, 93 percent storage, and 3 percent phloem.
Table 7. Basis for calculating the compartment volumes of the experimental plants. The example shown is BROM5, medium transpiration rate.

<table>
<thead>
<tr>
<th>Compartment name and number</th>
<th>Base volume</th>
<th>Fraction to compartment Base volumes</th>
<th>Volumes BROM5 (med.)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>ROOT</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Root apparent free space (0)</td>
<td>0.75</td>
<td>0.15</td>
<td>2.813</td>
</tr>
<tr>
<td>Root cortex cells (1)</td>
<td>0.85</td>
<td></td>
<td>15.938</td>
</tr>
<tr>
<td>Root xylem (2)</td>
<td>0.25</td>
<td>0.01</td>
<td>0.250</td>
</tr>
<tr>
<td>Root storage (3)</td>
<td>0.93</td>
<td>5.813</td>
<td>5.813</td>
</tr>
<tr>
<td>Root phloem (4)</td>
<td>0.03</td>
<td>0.188</td>
<td>0.233</td>
</tr>
<tr>
<td><strong>STEM</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bottom stem xylem (5)</td>
<td>0.73</td>
<td>0.04</td>
<td>0.176</td>
</tr>
<tr>
<td>Bottom stem storage (6)</td>
<td>0.93</td>
<td>4.101</td>
<td>4.443</td>
</tr>
<tr>
<td>Bottom stem phloem (7)</td>
<td>0.03</td>
<td>0.132</td>
<td>0.143</td>
</tr>
<tr>
<td>Mid stem xylem (8)</td>
<td>0.182</td>
<td>0.04</td>
<td>0.044</td>
</tr>
<tr>
<td>Mid stem storage (9)</td>
<td>0.93</td>
<td>1.016</td>
<td>1.100</td>
</tr>
<tr>
<td>Mid stem phloem (10)</td>
<td>0.03</td>
<td>0.033</td>
<td>0.035</td>
</tr>
<tr>
<td>Top stem xylem (11)</td>
<td>0.083</td>
<td>0.04</td>
<td>0.020</td>
</tr>
<tr>
<td>Top stem storage (12)</td>
<td>0.93</td>
<td>0.463</td>
<td>0.5047</td>
</tr>
<tr>
<td>Top stem phloem (13)</td>
<td>0.03</td>
<td>0.015</td>
<td>0.0162</td>
</tr>
<tr>
<td><strong>LEAF</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Leaf cluster 1 xylem (14)</td>
<td>0.5</td>
<td>0.01</td>
<td>0.125</td>
</tr>
<tr>
<td>Leaf cluster 1 storage (15)</td>
<td>0.98</td>
<td>12.250</td>
<td>8.477</td>
</tr>
<tr>
<td>Leaf cluster 1 phloem (16)</td>
<td>0.01</td>
<td>0.125</td>
<td>0.087</td>
</tr>
<tr>
<td>Leaf cluster 2 xylem (17)</td>
<td>0.3</td>
<td>0.01</td>
<td>0.075</td>
</tr>
<tr>
<td>Leaf cluster 2 storage (18)</td>
<td>0.98</td>
<td>7.350</td>
<td>5.086</td>
</tr>
<tr>
<td>Leaf cluster 2 phloem (19)</td>
<td>0.01</td>
<td>0.075</td>
<td>0.052</td>
</tr>
<tr>
<td>Leaf cluster 3 xylem (20)</td>
<td>0.2</td>
<td>0.01</td>
<td>0.050</td>
</tr>
<tr>
<td>Leaf cluster 3 storage (21)</td>
<td>0.98</td>
<td>4.900</td>
<td>3.391</td>
</tr>
<tr>
<td>Leaf cluster 3 phloem (22)</td>
<td>0.01</td>
<td>0.050</td>
<td>0.035</td>
</tr>
</tbody>
</table>

44
Stem volume was allocated as follows: 73.5 percent to bottom stem segment, 18.2 percent to middle stem segment, and 8.3 percent to upper stem segment. The volume of each stem segment was divided into 3 percent for phloem, 4 percent for xylem, and 93 percent for storage. Total leaf volume was divided into 50 percent, 30 percent, and 20 percent to lower, middle, and upper leaf, respectively. Each of these volumes was divided into 1 percent phloem, 1 percent xylem, and 95 percent storage.

The volumes used for simulation were then calculated by scaling the base values from Table 7 in proportion to volumes derived from measured plant mass (Table 5) using linear scaling. For example, with the medium transpiration rate of BROM5 the mean root mass was 31.1 g (Table 5). The volumes of root compartments (labeled 0 through 4) were obtained by multiplication of the base volume of root compartment shown in Table 7 by the quotient (31.1/25.0 = 1.244). This yielded the root compartment volumes shown in the last column in Table 4. The sum of these volumes should be 71.1 cm². The scale factor for the stem compartments was (6.5/6.0 = 1.083), and (17.3/25.0 = 0.692) for the leaf compartments. The same procedure was used to obtain volumes for the other experiments. Table 8 summarizes the other geometric parameters used in the UTAB 4.6 simulation runs.

Chemical and Physical Parameters

Information available for bromacil suggested setting sorption parameters, first-order irreversible loss process parameters, and reflection coefficients all equal to zero. This information must be
Table 8. Values of parameters used in UTAB 4.6 for geometric and chemical properties for each compartmental boundary and fluid flow rate.

<table>
<thead>
<tr>
<th>Index</th>
<th>Regions connected</th>
<th>Area</th>
<th>Thickness</th>
<th>Diffusion coeff.</th>
<th>Fluid flow rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Soil/apparent free space</td>
<td>6.350</td>
<td>0.00375</td>
<td>0.0036</td>
<td>6.671</td>
</tr>
<tr>
<td>1</td>
<td>Soil/root xylem</td>
<td>3.180</td>
<td>0.0001</td>
<td>1.8 x 10^{-7}</td>
<td>5.671</td>
</tr>
<tr>
<td>2</td>
<td>Root xylem/bottom stem xylem</td>
<td>0.00784</td>
<td>0.5</td>
<td>0.0036</td>
<td>6.975</td>
</tr>
<tr>
<td>3</td>
<td>Bottom stem phloem/root phloem</td>
<td>0.0056</td>
<td>0.5</td>
<td>0.0036</td>
<td>1.304</td>
</tr>
<tr>
<td>4</td>
<td>Root phloem/root xylem</td>
<td>1.0</td>
<td>0.001</td>
<td>3.6 x 10^{-5}</td>
<td>1.304</td>
</tr>
<tr>
<td>5</td>
<td>Bottom stem xylem/mid stem xylem</td>
<td>0.00504</td>
<td>1.0</td>
<td>0.0036</td>
<td>3.29</td>
</tr>
<tr>
<td>6</td>
<td>Mid stem phloem/</td>
<td>0.00360</td>
<td>1.0</td>
<td>0.0036</td>
<td>0.4537</td>
</tr>
<tr>
<td></td>
<td>bottom stem phloem</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Mid stem xylem/top stem xylem</td>
<td>0.00284</td>
<td>1.0</td>
<td>0.0036</td>
<td>1.249</td>
</tr>
<tr>
<td>8</td>
<td>Top stem phloem/mid stem phloem</td>
<td>0.00203</td>
<td>1.0</td>
<td>0.0036</td>
<td>0.8505</td>
</tr>
<tr>
<td>9</td>
<td>Bottom stem xylem/leaf 1 xylem</td>
<td>0.00784</td>
<td>1.0</td>
<td>0.0036</td>
<td>0.8505</td>
</tr>
<tr>
<td>10</td>
<td>Leaf 1 xylem/leaf 1 phloem</td>
<td>5.0</td>
<td>0.001</td>
<td>3.6 x 10^{-5}</td>
<td>8.8505</td>
</tr>
<tr>
<td>11</td>
<td>Leaf 1 xylem/atmosphere</td>
<td>10.0</td>
<td>1.0</td>
<td>0.0036</td>
<td>2.835</td>
</tr>
<tr>
<td>12</td>
<td>Leaf 1 phloem/bottom stem phloem</td>
<td>0.0056</td>
<td>1.0</td>
<td>0.0036</td>
<td>0.8505</td>
</tr>
<tr>
<td>13</td>
<td>Mid stem xylem/leaf 2 xylem</td>
<td>0.00204</td>
<td>1.0</td>
<td>0.0036</td>
<td>2.041</td>
</tr>
<tr>
<td>14</td>
<td>Leaf 2 xylem/leaf 2 phloem</td>
<td>6.0</td>
<td>0.001</td>
<td>3.6 x 10^{-5}</td>
<td>0.3402</td>
</tr>
<tr>
<td>15</td>
<td>Leaf 2 xylem/atmosphere</td>
<td>6.0</td>
<td>1.0</td>
<td>0.0036</td>
<td>1.701</td>
</tr>
<tr>
<td>16</td>
<td>Leaf 2 phloem/mid stem phloem</td>
<td>0.00204</td>
<td>1.0</td>
<td>0.0036</td>
<td>0.3402</td>
</tr>
<tr>
<td>17</td>
<td>Top stem xylem/leaf 3 xylem</td>
<td>0.00804</td>
<td>5.0</td>
<td>0.0036</td>
<td>1.249</td>
</tr>
<tr>
<td>18</td>
<td>Leaf 3 xylem/leaf 3 phloem</td>
<td>0.00804</td>
<td>5.0</td>
<td>0.0036</td>
<td>0.1135</td>
</tr>
<tr>
<td>19</td>
<td>Leaf 3 xylem/atmosphere</td>
<td>4.0</td>
<td>1.0</td>
<td>0.0036</td>
<td>1.135</td>
</tr>
<tr>
<td>20</td>
<td>Leaf 3 phloem/mid stem phloem</td>
<td>0.00203</td>
<td>1.0</td>
<td>0.0036</td>
<td>0.1135</td>
</tr>
</tbody>
</table>

*Fluid flow rates were calculated using formulas in Table 3, with f1 = 0.3, f2 = 0.2, and f3 = 0.1. QTR = 5.67 (cm^3/hr/leaf), secured outside of the model. Initial concentrations of bromacil were zero in all compartments except in the "soil compartment."

Phloem Transport

The model contains a parameter for the ratio of xylem flow to phloem flow. In order to run the model, it was necessary to choose this ratio for each leaf. The rate of water transport in xylem and phloem depends on environmental conditions and vigor of growth. Under
the constant environmental conditions of the experimental chambers the xylem and phloem flow rates could be assumed to remain constant. The ratio of xylem to phloem flow has been measured in many experiments (Noble, 1983). Based on these reports the ratio was set highest in the oldest leaf and smallest in the youngest leaf, as follows: $f_1 = 0.3$, $f_2 = 0.2$, and $f_3 = 0.1$, respectively.

**Concentration of Bromacil in Bathing Solution**

In the BROM3 experiment the concentration of bromacil in the bathing solution was maintained to be approximately constant. This condition was simulated in the model by setting the volume of the soil compartment very large ($1.0 \times 10^{10}$ cm$^3$). The initial mass of bromacil set at $3.2 \times 10^{13}$ DPM so that the initial concentration was 3,200 DPM/cm$^3$ which is equal to the experimental condition of 0.058 µg/cm$^3$. The amount of bromacil taken up by plants during the 200-hour simulation time was negligible relative to the mass of bromacil remaining in the soil compartment. For BROM3 and BROM1 the soil volume was set equal to 6,400 cm$^3$, which was the volume of the root chambers, and the initial concentrations were those of the experiments (Table 4).

**Transpiration Rates**

The total rate of transpiration measured experimentally (Table 5). Measured rates were allocated to the three leaves in approximate proportion of leaf area, i.e. 50 percent to leaf 1, 30 percent to leaf 2, and 20 percent to leaf 3.
Storage Coefficients

The objective of the calibration procedure was to find plausible values of the storage coefficients. Important qualitative observations may be derived from Figures 3 through 5 and from literature reports. The value of storage coefficients for molecules such as glycine may be approximated from the relationship \( Q = (DKA/\Delta x) \) (equation 2 with \( \sigma = 0 \)). For such molecules \( D = 0.036 \text{ cm}^2/\text{hr} \). Assuming \( \sigma = 0, \Delta x = 0.1 \text{ cm} \), and \( A = 1.0 \text{ cm}^2 \) obtains \( Q = 0.360 \text{ cm}^3/\text{hr} \) for a surface area of 1 cm². There are many uncertainties with this estimate. The value for \( D \) is for a dilute solution. Furthermore, only part of the surface of cells are available for diffusion, making it smaller than shown. Diffusion may be limited by partitioning at the membrane surfaces. In the experiments, the surface area of compartments could be much larger than 1 cm². However, the value of 0.360 cm³/hr provides a useful estimate for the initial simulation.

In the leaves, the rate of increase in bromacil concentration at the medium-transpiration rate and low-exposure concentration (BROM5) was approximately 0.100 x 10³ DPM/g-hr (Figure 5). This corresponds to

\[
(0.100 \times 10^3 \text{ DPM/g-hr}) / (1.82 \times 10^{-5} \text{ mg/DPM}) = 1.82 \times 10^{-3} \mu g/\text{g-hr} = 0.00182 \mu g/\text{g-hr}.
\]

This is the rate that would apply to 1 cm³ of storage volume. For a storage volume of 10 cm³ the rate would be 0.0182 µg/hr. The increase in concentration is the consequence of \( Q_f \) and \( Q_b \), thus with \( Q_b = 0.5 Q_f \) the necessary \( Q_f \) should be 0.036 cm³/hr. Based on these considerations, the initial guesses of \( Q_f = 0.10 \text{ cm}^3/\text{hr} \) and \( Q_b = 0.05 \text{ cm}^3/\text{hr} \) were used for stems and leaves.

Other considerations were that bromacil moves readily from transport vessels to surrounding tissues as indicated by the rapid increase
in concentrations in roots and stems following exposure. Storage coefficients for phloem and xylem may therefore be assumed to be equal to each other for a given tissue. Finally, we assumed that the storage and mobilization coefficients are proportional to storage volume. This proportionality derives from the volume to surface area relationship indicated in equation 1.
DISCUSSION

Introduction

Simulations rapidly achieved the condition where the correct total mass of chemical was stored in the plant as a function of time, indicating that the overall process was correctly described and that physical and chemical parameters were correct. However, the measured distribution between the three plant parts was not immediately simulated. This distribution is determined by storage coefficients. Progress with obtaining agreement between simulations and experiments was judged from tabulation of the ratio of simulated concentration ($C_s$) divided by experimentally measured concentration ($C_{exp}$) (Table 9).

The quotients shown in Table 9 are those of the final run in the "eyeball" curve-fitting calibration procedure. The storage coefficients which resulted from the calibration procedure are in Table 10.

Figures 7 through 13 show simulated (solid lines) and measured (data points) concentrations for BROM5 (Figures 7, 8, and 9 for low, medium, and high transpiration rates, respectively), BROM3 (Figures 10, 11, and 12), and BROM1 (Figure 13). Ratios of simulated concentrations divided by measured concentrations (Table 9), indicate that experimental results of all experiments were simulated with equal success. The model simulated all the important features of the uptake behavior revealed by the experiments.

An additional step in the analysis was the effort to find structure in the storage coefficients found by the calibration procedure. Important considerations were to look for the relationship between storage coefficients and size of compartments, possible effects of concentration and/or transpiration rates, and differences, if any,
Figure 7. Concentrations in roots, stems, and leaves as a function of time for BROM5, low transpiration rate.
Figure 8. Concentrations in roots, stems, and leaves as a function of time for BROM5, medium transpiration rate.
Figure 9. Concentrations in roots, stems, and leaves as a function of time for BROM5, high transpiration rate.
Figure 10. Concentrations in roots, stems, and leaves as a function of time for BROM3, low transpiration rate.
Figure 11. Concentrations in roots, stems, and leaves as a function of time for BROM3, medium transpiration rate.
Figure 12. Concentrations in roots, stems, and leaves as a function of time for BROM3, high transpiration rate.
Figure 13. Concentrations in roots, stems, and leaves as a function of time for BROM1.
Table 9. Simulated concentrations (Cs) divided by measured concentrations (Cexp) at three transpiration rates.

<table>
<thead>
<tr>
<th>BROM5</th>
<th>Low</th>
<th>Medium</th>
<th>High</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Roots</td>
<td>Stems</td>
<td>Leaves</td>
</tr>
<tr>
<td>Time (hr)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>-0.93</td>
<td>1.37</td>
<td>3.15</td>
</tr>
<tr>
<td>26</td>
<td>-0.88</td>
<td>1.21</td>
<td>1.54</td>
</tr>
<tr>
<td>50</td>
<td>-0.97</td>
<td>1.26</td>
<td>1.47</td>
</tr>
<tr>
<td>122</td>
<td>0.00</td>
<td>1.05</td>
<td>1.06</td>
</tr>
<tr>
<td>145</td>
<td>-0.95</td>
<td>1.15</td>
<td>1.10</td>
</tr>
<tr>
<td>169</td>
<td>-0.94</td>
<td>1.20</td>
<td>1.11</td>
</tr>
<tr>
<td>193</td>
<td>-0.94</td>
<td>0.00</td>
<td>1.34</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>BROM3</th>
<th>Low</th>
<th>Medium</th>
<th>High</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Roots</td>
<td>Shoots</td>
<td>Roots</td>
</tr>
<tr>
<td>Time (hr)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.0</td>
<td>-0.88</td>
<td>3.49</td>
<td>0.67</td>
</tr>
<tr>
<td>7.0</td>
<td>-0.89</td>
<td>1.98</td>
<td>0.91</td>
</tr>
<tr>
<td>15.0</td>
<td>1.06</td>
<td>1.32</td>
<td>-0.84</td>
</tr>
<tr>
<td>23.0</td>
<td>1.04</td>
<td>1.21</td>
<td>-0.76</td>
</tr>
<tr>
<td>31.0</td>
<td>1.10</td>
<td>1.10</td>
<td>-0.76</td>
</tr>
<tr>
<td>39.0</td>
<td>-0.95</td>
<td>-0.74</td>
<td>-0.30</td>
</tr>
<tr>
<td>47.0</td>
<td>-0.95</td>
<td>-0.92</td>
<td>-0.78</td>
</tr>
<tr>
<td>55.0</td>
<td>1.07</td>
<td>0.99</td>
<td>0.00</td>
</tr>
</tbody>
</table>

This publication is out of date. For most current information: http://extension.oregonstate.edu/catalog
Table 10. Values of storage (forward) and mobilization (backward) transfer coefficient determined by the calibration procedure used in the text.

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Volume cm³</th>
<th>Q-f cm³/hr</th>
<th>Q-b cm³/hr</th>
<th>Ratio Q_f/Q_b</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>BROM5-low</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Root cortex</td>
<td>15.75</td>
<td>26.000</td>
<td>13.000</td>
<td>2.0</td>
</tr>
<tr>
<td>Root storage</td>
<td>5.743</td>
<td>0.190</td>
<td>0.009</td>
<td>21.1</td>
</tr>
<tr>
<td>Stem bottom</td>
<td>3.076</td>
<td>0.100</td>
<td>0.015</td>
<td>6.6</td>
</tr>
<tr>
<td>Stem middle</td>
<td>0.762</td>
<td>0.045</td>
<td>0.006</td>
<td>7.1</td>
</tr>
<tr>
<td>Stem top</td>
<td>0.347</td>
<td>0.106</td>
<td>0.013</td>
<td>8.0</td>
</tr>
<tr>
<td>Leaf bottom</td>
<td>8.183</td>
<td>0.050</td>
<td>0.009</td>
<td>7.8</td>
</tr>
<tr>
<td>Leaf middle</td>
<td>4.910</td>
<td>0.048</td>
<td>0.006</td>
<td>8.0</td>
</tr>
<tr>
<td>Leaf top</td>
<td>3.273</td>
<td>0.048</td>
<td>0.006</td>
<td>8.0</td>
</tr>
<tr>
<td><strong>BROM5-medium</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Root cortex</td>
<td>19.83</td>
<td>26.000</td>
<td>12.000</td>
<td>2.2</td>
</tr>
<tr>
<td>Root storage</td>
<td>7.231</td>
<td>0.162</td>
<td>0.023</td>
<td>7.6</td>
</tr>
<tr>
<td>Stem bottom</td>
<td>4.447</td>
<td>0.065</td>
<td>0.009</td>
<td>2.7</td>
</tr>
<tr>
<td>Stem middle</td>
<td>1.160</td>
<td>0.058</td>
<td>0.027</td>
<td>2.5</td>
</tr>
<tr>
<td>Stem top</td>
<td>0.402</td>
<td>0.030</td>
<td>0.012</td>
<td>3.2</td>
</tr>
<tr>
<td>Leaf bottom</td>
<td>8.477</td>
<td>0.108</td>
<td>0.013</td>
<td>8.3</td>
</tr>
<tr>
<td>Leaf middle</td>
<td>5.086</td>
<td>0.071</td>
<td>0.009</td>
<td>7.9</td>
</tr>
<tr>
<td>Leaf top</td>
<td>3.391</td>
<td>0.049</td>
<td>0.006</td>
<td>8.2</td>
</tr>
<tr>
<td><strong>BROM5-high</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Root cortex</td>
<td>20.81</td>
<td>1.000</td>
<td>13.000</td>
<td>2.4</td>
</tr>
<tr>
<td>Root storage</td>
<td>7.326</td>
<td>0.130</td>
<td>0.025</td>
<td>5.2</td>
</tr>
<tr>
<td>Stem bottom</td>
<td>4.511</td>
<td>0.250</td>
<td>0.095</td>
<td>2.6</td>
</tr>
<tr>
<td>Stem middle</td>
<td>1.114</td>
<td>0.065</td>
<td>0.0215</td>
<td>2.6</td>
</tr>
<tr>
<td>Stem top</td>
<td>0.410</td>
<td>0.028</td>
<td>0.011</td>
<td>2.6</td>
</tr>
<tr>
<td>Leaf bottom</td>
<td>8.051</td>
<td>0.118</td>
<td>0.015</td>
<td>7.9</td>
</tr>
<tr>
<td>Leaf middle</td>
<td>5.851</td>
<td>0.0880</td>
<td>0.010</td>
<td>8.0</td>
</tr>
<tr>
<td>Leaf top</td>
<td>3.900</td>
<td>0.055</td>
<td>0.007</td>
<td>7.9</td>
</tr>
<tr>
<td><strong>BROM3-low</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Root cortex</td>
<td>29.01</td>
<td>25.000</td>
<td>13.000</td>
<td>1.9</td>
</tr>
<tr>
<td>Root storage</td>
<td>10.579</td>
<td>0.270</td>
<td>0.027</td>
<td>12.1</td>
</tr>
<tr>
<td>Stem bottom</td>
<td>9.440</td>
<td>0.264</td>
<td>0.027</td>
<td>3.2</td>
</tr>
<tr>
<td>Stem middle</td>
<td>2.338</td>
<td>0.146</td>
<td>0.074</td>
<td>2.0</td>
</tr>
<tr>
<td>Stem top</td>
<td>1.066</td>
<td>0.065</td>
<td>0.022</td>
<td>2.0</td>
</tr>
<tr>
<td>Leaf bottom</td>
<td>28.155</td>
<td>0.217</td>
<td>0.027</td>
<td>8.0</td>
</tr>
<tr>
<td>Leaf middle</td>
<td>16.893</td>
<td>0.168</td>
<td>0.021</td>
<td>8.0</td>
</tr>
<tr>
<td>Leaf top</td>
<td>11.262</td>
<td>0.130</td>
<td>0.016</td>
<td>8.1</td>
</tr>
<tr>
<td>Compartment</td>
<td>Volume</td>
<td>Q-f</td>
<td>Q-b</td>
<td>Ratio Qf/Qb</td>
</tr>
<tr>
<td>--------------------</td>
<td>--------</td>
<td>-------</td>
<td>-------</td>
<td>-------------</td>
</tr>
<tr>
<td><strong>BROM3-medium</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Root cortex</td>
<td>36.02</td>
<td>25.000</td>
<td>13.000</td>
<td>1.9</td>
</tr>
<tr>
<td>Root storage</td>
<td>13.136</td>
<td>0.320</td>
<td>0.021</td>
<td>15.2</td>
</tr>
<tr>
<td>Stem bottom</td>
<td>10.793</td>
<td>0.657</td>
<td>0.084</td>
<td>2.0</td>
</tr>
<tr>
<td>Stem middle</td>
<td>2.673</td>
<td>0.077</td>
<td>0.036</td>
<td>2.0</td>
</tr>
<tr>
<td>Stem top</td>
<td>1.219</td>
<td>0.077</td>
<td>0.036</td>
<td>2.0</td>
</tr>
<tr>
<td>Leaf bottom</td>
<td>32.188</td>
<td>0.230</td>
<td>0.029</td>
<td>13.5</td>
</tr>
<tr>
<td>Leaf middle</td>
<td>19.313</td>
<td>0.179</td>
<td>0.022</td>
<td>9.1</td>
</tr>
<tr>
<td>Leaf top</td>
<td>12.875</td>
<td>0.140</td>
<td>0.018</td>
<td>7.8</td>
</tr>
<tr>
<td><strong>BROM3-high</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Root cortex</td>
<td>30.54</td>
<td>215.000</td>
<td>13.000</td>
<td>1.9</td>
</tr>
<tr>
<td>Root storage</td>
<td>11.137</td>
<td>0.260</td>
<td>0.026</td>
<td>13.0</td>
</tr>
<tr>
<td>Stem bottom</td>
<td>10.212</td>
<td>0.621</td>
<td>0.310</td>
<td>2.0</td>
</tr>
<tr>
<td>Stem middle</td>
<td>2.529</td>
<td>0.158</td>
<td>0.080</td>
<td>2.0</td>
</tr>
<tr>
<td>Stem top</td>
<td>1.213</td>
<td>0.070</td>
<td>0.036</td>
<td>2.0</td>
</tr>
<tr>
<td>Leaf bottom</td>
<td>30.449</td>
<td>0.225</td>
<td>0.028</td>
<td>8.0</td>
</tr>
<tr>
<td>Leaf middle</td>
<td>18.269</td>
<td>0.170</td>
<td>0.022</td>
<td>7.9</td>
</tr>
<tr>
<td>Leaf top</td>
<td>12.179</td>
<td>0.134</td>
<td>0.017</td>
<td>8.1</td>
</tr>
<tr>
<td><strong>BROM1</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Root cortex</td>
<td>19.14</td>
<td>16.000</td>
<td>11.000</td>
<td>1.5</td>
</tr>
<tr>
<td>Root storage</td>
<td>5.975</td>
<td>0.120</td>
<td>0.027</td>
<td>4.4</td>
</tr>
<tr>
<td>Stem bottom</td>
<td>4.170</td>
<td>0.085</td>
<td>0.018</td>
<td>4.7</td>
</tr>
<tr>
<td>Stem middle</td>
<td>1.132</td>
<td>0.032</td>
<td>0.027</td>
<td>1.2</td>
</tr>
<tr>
<td>Stem top</td>
<td>0.433</td>
<td>0.017</td>
<td>0.015</td>
<td>1.1</td>
</tr>
<tr>
<td>Leaf bottom</td>
<td>14.277</td>
<td>0.220</td>
<td>0.020</td>
<td>11.0</td>
</tr>
<tr>
<td>Leaf middle</td>
<td>6.262</td>
<td>0.170</td>
<td>0.017</td>
<td>10.0</td>
</tr>
<tr>
<td>Leaf top</td>
<td>4.175</td>
<td>0.100</td>
<td>0.010</td>
<td>10.0</td>
</tr>
</tbody>
</table>
between the three plant parts. To prepare for this analysis the ratios Qf/Qb shown in Table 10 were reordered as shown in Table 11.

**Roots**

Root concentrations increased rapidly during the first hours of exposure (Figures 7 through 13). The duration of this period of rapid uptake decreased with increasing concentration of the bathing solution. This uptake pattern was reproduced by the model by using large storage coefficients during this initial period. The large storage coefficients were changed to lower values after 10 hours of simulation for BROM5, 8 hours for BROM3, and 6 hours for BROM1. The uptake behavior reflected the rapid uptake which occurred upon the initial entry of solution into the root-free space. The medium transpiration rate for BROM5 was 5.7 cm$^3$/hr per plant; the root volume was 23.3 cm$^3$, consisting of 3.5 cm$^3$ apparent free space and 19.8 cm$^3$ cortex volume. At the indicated transpiration rate, the water in the 3.5 cm$^3$ of apparent free space would be flushed out in 0.6 hour. Uptake after that time represents rapid storage in the cortex cells.

The instantaneous exposure would not occur under field conditions, except where a spill of contaminant occurred so that contaminated water would reach the root zone over a short period of time. For such conditions, the model should be run as done here. More likely is the scenario with low-level, chronic exposure such as occurs where plants are growing in contaminant soil water. The chronic exposure should be modeled using the smaller storage coefficients. Following the rapid initial uptake, storage continued in the root cortex and storage compartment of the root stele at a lower rate.
Table 11. Ratios $Q_f/Q_b$ for individual plant parts. The transpiration rate for each experiment is listed at the top of each data column in the units of $10^{-3}$ cm$^3$/cm$^2$ hr.

<table>
<thead>
<tr>
<th>Compartment</th>
<th>BROM5</th>
<th>BROM3</th>
<th>BROM1</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(2.61)</td>
<td>(7.82)</td>
<td>(8.85)</td>
</tr>
<tr>
<td>Roots cortex</td>
<td>16.1</td>
<td>9.0</td>
<td>5.3</td>
</tr>
<tr>
<td>Roots storage</td>
<td>21.1</td>
<td>7.6</td>
<td>5.2</td>
</tr>
<tr>
<td>Stems bottom</td>
<td>8.1</td>
<td>2.7</td>
<td>2.6</td>
</tr>
<tr>
<td>middle</td>
<td>6.7</td>
<td>2.5</td>
<td>2.6</td>
</tr>
<tr>
<td>top</td>
<td>7.5</td>
<td>2.5</td>
<td>2.6</td>
</tr>
<tr>
<td>Leaves bottom</td>
<td>8.0</td>
<td>8.3</td>
<td>7.9</td>
</tr>
<tr>
<td>middle</td>
<td>7.8</td>
<td>7.9</td>
<td>8.0</td>
</tr>
<tr>
<td>top</td>
<td>8.0</td>
<td>8.2</td>
<td>7.9</td>
</tr>
</tbody>
</table>

A relationship between storage coefficients of the root cortex and the root storage compartments was not apparent. The storage coefficients decreased with transpiration rate for the BROM5 and BROM3 experiments, but a clear relationship was not found. However, when the ratio of $Q_f/Q_b$ was evaluated as a function of transpiration rate (Figure 14) a relationship was found. This ratio is a measure of storage rate, a higher ratio indicating more rapid storage. A similar transpiration rate dependency was not found with the storage coefficients of stem or leaf compartments (Table 11). These results indicate that the rate of storage was higher at the low transpiration rate. While the number of data points is small, the decreasing rate of storage with increasing rate of transpiration was observed with all experiments where the comparison could be made. Reasons for this relationship are not clear to us at this time. Other reports have suggested that uptake is independent of transpiration rate.
Figure 14. Ratio $Q_f/Q_b$ for the root cortex and for root storage compartments as a function of transpiration rate.
Stems

The relationship between storage coefficients and stem volumes was found to be linear (Figure 15). The same relationship applied to all experiments except BROM5, low transpiration rate. The proportionality in the absence of a transpiration or concentration effect reflects the proportionality of storage with surface area, as was previously discussed.

Leaves

Storage coefficients of leaves were related to leaf volume in an exponential manner (Figure 16). The relationship was the same for BROM5 and BROM3 experiments, but had a higher exponent for the BROM1 experiment. The difference between the BROM1 and the other two experiments may indicate a concentration effect. Storage coefficients did not increase with the increase of concentration from BROM5 to BROM3, but increased about 50 percent by increasing the concentration from BROM3 to BROM1. This concentration effect may result from an affect of bromacil on plant tissue which occurs at the much higher concentrations in the leaf with the BROM1 experiment. This effect was also shown earlier in Figure 6.
Figure 15. Forward storage coefficients for stem compartments plotted as a function of volumes of stem storage compartments.
Figure 16. Forward storage coefficients for leaf compartments plotted as a function of volumes of leaf storage compartments.
SENSITIVITY ANALYSIS

Introduction

One of the best methods for choosing the parameters in a sensitivity study of a mathematical model is the factorial design (Box et al., 1978). This "experimental design" is practical when the number of independent parameters is less than or equal to 10. However, UTAB 4.6 contains more than 200 independent parameters. It is therefore not practical to choose a factorial design for varying the parameters. It is also nearly impossible to set up and solve, in closed form, a set of sensitivity equations as described by Bard (1974). For purposes of this report only some of the individual parameters which are important to the uptake, accumulation, and translocation processes were varied. The results of changing these parameters are compared with BROM5 medium transpiration rate as the reference simulation. Nineteen sets of simulations were made. The parameters which were evaluated and their values are in Table 12. Results are shown in Figures 17 through 27.

Transpiration Rate

The transpiration rate used for the reference simulation was that of the BROM5 medium transpiration rate (Table 12). The curves labeled Ref in Figure 17 correspond to this transpiration value. The curve labeled A corresponds to the simulation with the low transpiration rate, while the curve labeled B corresponds to the simulation with the high transpiration rate. Simulations show an increase in concentration in all three plant parts as a result of increasing the transpiration rate and a decrease in all three plant parts as a result of decreasing the transpiration rates. On a relative basis, the effect of increasing
Table 12. Values of parameters used in the sensitivity simulations. The data base for BROM5 medium transpiration rate was the reference level for these simulations.

<table>
<thead>
<tr>
<th>Parameter changed</th>
<th>Curve</th>
<th>Values used</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transpiration rate</td>
<td>Ref</td>
<td>BROM5 Med Trans (2.61 x 10^{-3} cm³/cm² hr)</td>
</tr>
<tr>
<td></td>
<td>A</td>
<td>BROM5 Low Trans (7.82 x 10^{-3} cm³/cm² hr)</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>BROM5 High Trans (8.85 x 10^{-3} cm³/cm² hr)</td>
</tr>
<tr>
<td>Ratio (phloem/xylem)</td>
<td>Ref</td>
<td>f₁=0.3, f₂=0.2, f₃=0.1</td>
</tr>
<tr>
<td></td>
<td>A</td>
<td>f₁=0.15, f₂=0.15, f₃=0.1</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>f₁=0, f₂=0, f₃=0</td>
</tr>
<tr>
<td>Diffusion coefficient</td>
<td>Ref</td>
<td>DIFFU[1] = 1.8 x 10^{-7} cm²/hr</td>
</tr>
<tr>
<td>across Casparian strip</td>
<td>A</td>
<td>DIFFU[1] = 1.8 x 10^{-6} Gm²/hr</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>DIFFU[1] = 1.8 x 10^{-6} Gm²/hr</td>
</tr>
<tr>
<td>Reflection coefficient</td>
<td>Ref</td>
<td>SIGMA[1] = 0.0</td>
</tr>
<tr>
<td>for Casparian strip</td>
<td>A</td>
<td>SIGMA[1] = 0.2</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>SIGMA[1] = 0.7</td>
</tr>
<tr>
<td>Reflection coefficient</td>
<td>Ref</td>
<td>SIGMA[10;14;18] = 0.0</td>
</tr>
<tr>
<td>of leaf membrane</td>
<td>A</td>
<td>SIGMA[10;14;18] = 0.2</td>
</tr>
<tr>
<td>separating phloem and xylem</td>
<td>B</td>
<td>SIGMA[10;14;18] = 0.7</td>
</tr>
<tr>
<td>Constant (Qf/Qb) ratio</td>
<td>Ref</td>
<td>All Qf's and Qb's as in Table 8</td>
</tr>
<tr>
<td></td>
<td>A</td>
<td>All Qf's and Qb's ÷ by 2</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>All Qf's and Qb's times 2</td>
</tr>
<tr>
<td>Variable (Qf/Qb) ratio</td>
<td>Ref</td>
<td>All Qf's and Qb's as in Table 8</td>
</tr>
<tr>
<td></td>
<td>A</td>
<td>All Qf's and Qb's ÷ by 2</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>All Qf's and Qb's times 2</td>
</tr>
<tr>
<td>Sorption Coefficients</td>
<td>Ref</td>
<td>All B's = 0.0</td>
</tr>
<tr>
<td>in root compartments</td>
<td>A</td>
<td>B(1)-B(3)=0.5</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>B(1)-B(3)=1.0</td>
</tr>
<tr>
<td>First-order loss rates</td>
<td>Ref</td>
<td>All λ's = 0.0 (1/hr)</td>
</tr>
<tr>
<td></td>
<td>A</td>
<td>λ₁₅=0.0016, λ₁₈=0.00175, λ₂₁=0.0018</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>λ₁₅=0.0032, λ₁₈=0.0035, λ₂₁=0.0036</td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>λ₁₅=0.0064, λ₁₈=0.0070, λ₂₁=0.0072</td>
</tr>
</tbody>
</table>
Figure 17. Simulations showing the effect of changing the transpiration rate. Reference simulation was with BROM5 medium transpiration rate, $T_r = 5.67 \text{ cm}^3/\text{hr}$. Comparisons are with low transpiration rate $T_r = 2.00 \text{ cm}^3/\text{hr}$ (curves A) and high transpiration rate, $T_r = 7.80 \text{ cm}^3/\text{hr}$ (curves B).
the transpiration rate was much smaller than the effect of decreasing
the transpiration rate. The decrease in the transpiration rate by 67
percent decreased the concentration at 200 hours in the leaves
(curve A) from $1.57 \times 10^6$ to $8.09 \times 10^5$ dpm/g, in the stems from
$2.23 \times 10^5$ to $1.14 \times 10^5$ dpm/g, and in the roots from $5.21 \times 10^5$ to
$3.26 \times 10^5$ dpm/g. On the other hand, increasing the transpiration
rate by 13 percent (curve B) produced a corresponding increase in the
concentrations of the three plant regions. The increases in concentra-
tions were from $1.57 \times 10^6$ to $1.93 \times 10^6$ dpm/g in the leaves, from
$2.23 \times 10^5$ to $2.78 \times 10^5$ dpm/g in the stems, and from $5.21 \times 10^5$ to
$6.31 \times 10^5$ dpm/g in the roots. These simulations show that the effects
of increasing transpiration rates are not linear. The increase in
concentrations diminishes as concentrations become higher.

**Ratio:** Phloem Transport Rate / Xylem Transport Rate

The ratio (phloem transport rate/xylem transport rate) is a mea-
sure of the mobility of the chemical in the plant. A higher ratio
means that chemical accumulating in the leaves readily enters the
phloem pathway through which it is transported back to the roots. The
expectation is that a low ratio increases the concentrations in the
leaves and decrease concentrations in stems and roots, whereas a high
ratio decreases the concentrations in the leaves and increases concen-
trations in stems and roots. Results agreed with these expectations
(Figure 18). Simulation with the ratios equal to zero (curve A), i.e.
no phloem transport, showed the expected increase in concentrations in
the leaves and decrease in stems and roots. The decrease in concentra-
tions in stems and roots were large, namely from $2.23 \times 10^5$ to $5.12 \times$

THIS PUBLICATION IS OUT OF DATE. 
For most current information: 
http://extension.oregonstate.edu/catalog
Figure 18. Simulations showing the effects of changing the ratios of phloem transport rate divided by xylem transport rate. Reference simulation was with the fractions set to $f_1 = 0.3$, $f_2 = 0.2$, $f_3 = 0.1$. Simulation A: $f_1 = 0.0$, $f_2 = 0.0$, $f_3 = 0.0$, and Simulation B: $f_1 = 0.15$, $f_2 = 0.15$, and $f_3 = 0.1$. 
$10^4$ dpm/g in the stems and from $5.21 \times 10^5$ to $2.63 \times 10^5$ dpm/g in the roots. The increase in the leaves was dramatic, namely from $1.57 \times 10^6$ to $3.52 \times 10^6$ dpm/g. Simulation with the phloem/xylem ratio greater than zero showed the expected increase in the stems, namely from $2.23 \times 10^5$ to $2.52 \times 10^5$ dpm/g, but there was no change in the concentrations in the roots when compared with the reference simulation. Concentration in the leaves were lowest with the reference simulation. The fact that for ratios greater than 0.1 the concentration in the roots did not respond to the further increases indicates that this process is no longer a rate-limiting process. Compound is being recycled sufficiently fast so that storage is the rate-limiting process. The small increase in concentrations in the leaves relative to the reference curve, namely from $1.57 \times 10^6$ to $1.89 \times 10^6$ dpm/g, is attributed to the fact that the slower recycling results in a longer residence time in the leaves which thereby increases the leaf storage of bromacil.

**Diffusion Coefficient of the Casparian Strip**

For this simulation the diffusion coefficient of the Casparian strip was changed. This coefficient determines the rate at which diffusion across the Casparian strip can occur. The value of this coefficient is important with respect to diffusion from the root xylem and phloem compartments back to the root cortex. The role played by this coefficient can be learned from the mass balance equations, specifically equations (9) and (21). The expectation was that a decrease in the diffusion coefficient would increase the amount of chemical in the plant and therefore increase the concentrations in all compartments. Similarly, an increase in the diffusion coefficient at the
The Casparian strip was expected to decrease the total amount of chemical in the plant and therefore produce a decrease in the concentrations in all plant compartments. These expectations were borne out by the simulations shown in Figure 19. The effects were not linear, however. The effect of increasing the diffusion coefficient by a factor of 10 was somewhat larger than that of decreasing it by the same factor. Increasing the coefficient decreased the concentrations at 200 hours in the leaves from $1.57 \times 10^6$ to $1.18 \times 10^6$ dpm/gm, in the stems from $2.23 \times 10^5$ to $1.60 \times 10^5$ dpm/gm, and in the roots from $5.21 \times 10^5$ to $4.25 \times 10^5$ dpm/gm. Increasing the diffusion coefficient increased the concentrations in the leaves from $1.57 \times 10^6$ to $2.33 \times 10^6$ dpm/gm, in the stems from $2.23 \times 10^5$ to $3.54 \times 10^5$ dpm/gm, and in the roots from $5.21 \times 10^5$ to $7.07 \times 10^5$ dpm/gm.

**Reflection Coefficient of the Casparian Strip**

The reflection coefficient is a measure of the ease of passing across the Casparian strip. A reflection coefficient equal to zero allows the chemical to pass unimpeded, a reflection coefficient equal to one does not allow any chemical to pass this barrier. All plant parts were expected to be influenced equally by changes in the reflection coefficient of the Casparian strip. This expectation was confirmed by the results (Figure 20). With the reflection coefficient equal to 0.2, concentrations in leaves decreased from $1.57 \times 10^6$ to $1.42 \times 10^6$ dpm/gm, in the stems from $2.23 \times 10^5$ to $2.01 \times 10^5$ dpm/gm, and in the roots from $5.21 \times 10^5$ to $4.83 \times 10^5$ dpm/gm. Setting the reflection equal to 0.7 further decreased concentrations, namely from $1.57 \times 10^6$ to $1.03 \times 10^6$ dpm/gm in the leaves, from $2.23 \times 10^5$ to
Figure 19. Simulations showing the effects of changing the diffusion coefficient of the boundary representing the Casparian strip. Reference simulation was with $D = 1.8 \times 10^{-7}$ cm$^2$/hr. Simulation A: $D = 1.8 \times 10^{-6}$ cm$^2$/hr, simulation B: $D = 1.8 \times 10^{-8}$ cm$^2$/hr.
Figure 20. Simulation showing effects of changing the reflection coefficient of the boundary representing the Casparian strip. Reference simulation was with $\sigma = 0.0$.
Simulation A: $\alpha = 0.2$; simulation B: $\sigma = 0.7$. 

For most current information: 
http://extension.oregonstate.edu/catalog
Reflection Coefficients in the Leaf Membranes Separating Xylem and Phloem Pathway

The reflection coefficient of the membrane separating xylem and phloem pathways is a measure of the ease with which the chemical can enter the phloem pathway. An increase in this reflection coefficient in the leaves was expected to increase concentrations in the leaf despite the "choking-off" effect an increasing $a$ has. The concentrations in the leaf xylem increased under these conditions, thereby driving more compound into storage. Concentration in stems and roots were expected to decrease as the entry into the phloem system was decreased by the increasing reflection coefficients. These expectations were confirmed by the simulations. Figure 21 shows that concentrations increased in the leaves and decreased in stems and roots. Changes from the reference level with the reflection coefficient equal to zero to the simulation with $a = 0.2$ were small. A larger change occurred with the reflection coefficient $a = 0.7$. With these simulations the total amount of chemical in the plant was the same so that increases in leaf concentrations corresponded to decreases in stem and root concentrations.

Storage Coefficients

The role played by the storage and mobilization coefficients was discussed in detail in the text of this report. The values of the storage coefficients, $Q_f$'s, and the mobilization coefficients, $Q_b$'s,
Figure 21. Simulations showing the effects of changing the reflection coefficients of the membranes in the leaves which separate phloem from xylem ($\sigma_{10}$, $\sigma_{14}$, and $\sigma_{18}$). Reference simulation was with the three coefficients equal to zero. Simulation A, $\sigma$'s equal to 0.2; Simulation B, $\sigma$'s equal to 0.7.
were increased by a factor of 2 (curves B) in one simulation and decreased by a factor of 2 (curves A) in the second simulation. With these changes, the ratios $Q_f/Q_b$ remained the same. Figure 22 shows that the simultaneous increase of $Q_f$'s and $Q_b$'s by a factor of 2 increased the concentrations in leaves, while decreasing concentrations in the stems and increasing concentrations in the roots. The increase in the leaves was from $1.57 \times 10^6$ to $2.07 \times 10^6$ dpm/gm, the decrease in the stems was from $2.23 \times 10^5$ to $1.94 \times 10^5$ dpm/gm, and the increase in the roots was from $5.21 \times 10^5$ to $5.45 \times 10^5$ dpm/gm. The ratio $(Q_f/Q_b)$ of the leaves was higher than for the other two plant parts, so that an increase by a factor of 2 resulted in increased storage. Since more of the chemical taken up by the plant was stored in the leaves, less remained available for storage in stems and roots. In the competition for chemical to be stored, the stems were the most strongly effected, with little change in the roots.

When values of $(Q_f/Q_b)$ were decreased by a factor of 2, uptake in the leaf decreased, as did the uptake in the roots; however, uptake by the stems increased. The simulation resulted in a lower concentration in the leaves, as expected. Reasons for the increases in stems and decrease in roots are not clear. Since the ratios were not changed, the final concentrations at very long time values are the same for all simulations; however, the rate at which equilibrium concentrations are achieved depends on the ratio $(Q_f/Q_b)$.
Figure 22. Simulations showing the effect of increasing or decreasing values of the forward (Qf) and backward (Qb) coefficients while maintaining the same ratio Qf/Qb. The reference simulation was with all Qf’s and Qb’s as in Table 8. For Simulation A, all coefficients were divided by two; for Simulation B, all storage coefficients were multiplied by two.
Change in the Ratio \( Q_f/Q_b \)

When the ratio \( Q_f/Q_b \) was changed, equilibrium concentrations, as well as rates of approach to equilibrium, changed in each plant part. With the ratio increased by a factor of 2 (curves B), storage increased and the increases were similar for all three plant parts. Figure 23 shows that the increases were from \( 1.57 \times 10^6 \) to \( 2.18 \times 10^6 \) dpm/gm for leaves, from \( 2.23 \times 10^5 \) to \( 3.00 \times 10^5 \) dpm/gm for stems, and from \( 5.21 \times 10^5 \) to \( 7.78 \times 10^5 \) dpm/gm for roots. Concentrations decreased in all plant parts by decreasing the \( Q_f/Q_b \) (curves A) ratios, and the decreases were about the same for each plant part. The decreases were from \( 1.57 \times 10^6 \) to \( 1.00 \times 10^6 \) dpm/gm for leaves, from \( 2.23 \times 10^5 \) to \( 1.46 \times 10^5 \) dpm/gm for stems, and from \( 5.21 \times 10^5 \) to \( 3.28 \times 10^5 \) dpm/gm for roots.

Sorption Coefficients in the Root Storage Compartments

The sorption coefficients allow linear equilibrium sorption to occur. The effect is equivalent to that of increasing the volume of a compartment in which sorption occurs. Figure 24 shows simulations with the sorption coefficients of the root storage compartments set equal to \( 0.5 \) and \( 1.0 \). Results (Figure 24) indicate that these changes did not change the concentrations of the leaves and stems, but concentrations in the root compartments increased, as was expected. The increase was from \( 5.21 \times 10^5 \) to \( 6.47 \times 10^5 \) dpm/gm for \( B_1 = B_3 = 0.5 \), and from \( 5.21 \times 10^5 \) to \( 7.50 \times 10^5 \) dpm/gm for \( B_1 = B_3 = 1.0 \).
Figure 23: Simulations showing the effects of changing the ratios of forward storage coefficients to the backward storage coefficients. Reference simulation was with all storage coefficients as shown in Table 8. For Simulation A, all forward storage coefficients (Qf) were divided by two while leaving the Qb the same; for Simulation B, all forward storage coefficients were multiplied by two, while leaving the Qb's the same.
Figure 24. Simulations showing the effects of changing the sorption coefficients (B’s) in the root compartments. These coefficients immobilize chemical so that the coefficient has an effect that is similar to that of increasing or decreasing the volume of the compartment. Reference simulation was with values of the sorption coefficients B = 0. Simulation A, sorption coefficients of the two root compartments, B₁ = B₃ = 0.5; Simulation B, sorption coefficient of the two root compartments, B₁ = B₃ = 1.0.
Figure 25. Simulations showing effects of changing the rates of first-order loss (λ) in the leaves. Reference simulation was with all λ's equal to zero. Simulation A: λ_{15} = 0.0016, λ_{18} = 0.00175, λ_{21} = 0.0018; simulation B: λ_{15} = 0.0032, λ_{18} = 0.0035, λ_{21} = 0.0036; simulation C: λ_{15} = 0.0064, λ_{18} = 0.0070, λ_{21} = 0.0072.
Rate of First Order Losses

This simulation shows the result of allowing first-order loss processes to operate. In the reference simulation, the rate of first-order loss were zero in all compartments. For the simulation shown in Figure 25, values of the coefficient, $\lambda$, were as shown in Table 12. Appendix I, equations (15), (18), and (21), indicate the role played by this coefficient. The effects were most pronounced in the leaves, which was expected since values were not changed in stem and root compartments. An increase in the value of $\lambda$ has the effect of decreasing the concentration. As there is less and less chemical available in the leaves, the redistribution of the chemical by the phloem pathway is affected so that, increasingly, the concentration in the stem compartments shows a decrease. Concentrations in the root compartments started to show a decrease as well.

Combined Effects

In conclusion of the limited set of sensitivity simulations, two simulations were done in which several parameters were changed from the reference data set at the same time. The sets of parameters for each of these two simulations are in Table 13. Results are in Figures 26 and 27. The simulation in Figure 26 is labelled "combined high" and the simulation in Figure 27 is labelled "combined low." This terminology derives from the high concentrations with the simulation in Figure 27 and the low concentrations with the simulations in Figure 27.

The most influential parameter in these simulations was clearly the diffusion coefficient at the Casparian strip. The diffusion coefficient of the simulation labelled "combined high" was the lower of the two
simulations and that was two orders of magnitude lower than with the simulation referred to as "combined low." The diffusion coefficient at the Casparian strip determines the rate of diffusion back to the bathing solution of the root medium. With the high diffusion coefficient, the rate of backward diffusion was high. This rate increased as the concentration of the nutrient solution decreased. The concentrations in all three plant parts approached a steady state with the "combined low" simulation, whereas the concentrations of the reference simulation and the "combined high" simulation continued to increase. The lower rate of increase in the concentrations with the "combined low" simulations was also in part caused by high value of first-order loss rate in the leaves. The high concentrations in the roots with the "combined high" simulations derived in part from high value of the sorption coefficients in the root compartments. The very low concentration in the stems of the "combined low" simulations resulted from the very low value of the phloem/xylem transport rate and the high reflection coefficient at the root surface.
Table 13. Values of the parameters used for simulations in which several parameters were changed for an evaluation of combined effects.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value of parameters</th>
<th>Simulation in Fig. 26</th>
<th>Simulation in Fig. 27</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transpiration (cm³/cm²/hr)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Phloem/xylem transport rate</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Diffusion coefficient (cm²/hr)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Reflection coefficient, root</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Reflection coefficient, leaf</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ratio: Qf/Qb</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sorption coefficient, root</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>First order loss rate, leaves</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Tr = 8.85 x 10⁻³</th>
<th>Tr = 7.82 x 10⁻³</th>
</tr>
</thead>
<tbody>
<tr>
<td>f₁=0.30; f₂=0.20; f₃=0.10</td>
<td>f₁=0.30; f₂=0.20; f₃=0.10</td>
</tr>
<tr>
<td>D₁ = 1.8 x 10⁻⁸</td>
<td>1.8 x 10⁻⁸</td>
</tr>
<tr>
<td>σ₁ = 0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>σ₁₀=σ₁₄=σ₁₈=0.2</td>
<td>σ₁₀=σ₁₄=σ₁₈=0.2</td>
</tr>
<tr>
<td>Qf/Qb = 2 times reference</td>
<td>Qf/Qb = 0.5 times reference</td>
</tr>
<tr>
<td>B₁ = B₂ = 1.0</td>
<td>B₁ = B₂ = 0.5</td>
</tr>
<tr>
<td>λ₁₅ = 0.00160</td>
<td>λ₁₅ = 0.00640</td>
</tr>
<tr>
<td>λ₁₈ = 0.00172</td>
<td>λ₁₈ = 0.00700</td>
</tr>
<tr>
<td>λ₂₁ = 0.00180</td>
<td>λ₂₁ = 0.00720</td>
</tr>
</tbody>
</table>
Figure 26. Simulations showing the combined effects of changing several parameters at the same time. Reference simulation was with data set for BROM5 medium transportation rate (Table 8). Values of parameters used for this simulation are in Table 13.
Figure 27. Simulation showing the combined effects of changing several parameters. Reference simulation was with data set for BROM5 medium transpiration rate (Table 8). Values of parameters used for this simulation are in Table 13.
CONCLUSIONS

The model satisfactorily predicted the observed uptake and distribution patterns for bromacil in soybean plants at the stage of growth and under the environmental conditions used in the experiments involving a range of transpiration rates. This indicates that the model provides an accurate representation of uptake and the influence of transpiration rate on the uptake and translocation of this chemical. Parameter values used in the model for compartment size were selected from literature and experimental observation. They functioned well in these simulations and they are appropriately applied in the model. The chemical parameters for storage, mobilization, and diffusion when used in the model also yielded satisfactory results, suggesting that they are also appropriately applied. Finally, the calibration, although of limited scope, showed that the model equations yielded an accurate picture of the actual UTAB patterns for bromacil in soybeans used in these experiments. The theoretical exercise of compiling the model is shown to be a constructive step in learning how to predict the fate of xenobiotic contamination in plants.

The model shows excellent promise for future use. However, additional testing and validation are needed. Mathematical models can be used productively in combination with experimental results to obtain values of the unknown coefficients. Unfortunately, the parameters which characterize compartments usually cannot be estimated uniquely from "lumped" or "wash-out" type of experimental data when the number of compartments exceeds two (Godfrey and diSteffano, 1987). When using large system models for determination of unknown coefficients, experiments must be carefully designed so that input/output information...
(variables) can be measured over time for fixed environmental conditions. The input/output information so obtained would best be used in an optimization scheme based on a nonlinear least squares or minimum residual square error criterion to identify as many as possible of the characterizing parameters. An optimization scheme could not be used here because the data set was of the "lumped" type. Data requirements must be firmly kept in mind when contemplating use of models.
LITERATURE CITED


APPENDIX 1
DEFINITIONS OF THE NON-ZERO COEFFICIENTS, \( a_{ij} \).

-1) \textbf{Soil compartment}

\[
\frac{dM_{-1}}{dt} = a_{-1,-1} M_{-1} + a_{-1,0} M_0
\]

\[
a_{-1,-1} = \left[ \frac{D_0 A_0}{\Delta x_0} + Q_0 \right]
\]

\[
a_{-1,0} = \frac{D_1 A_0}{v_0(1 + B_0)} + \lambda_1
\]

0) \textbf{Root free space compartment}

\[
\frac{dM_0}{dt} = a_{0,-1} M_{-1} + a_{0,0} M_0 + a_{0,1} M_1 + a_{0,2} M_2
\]

\[
a_{0,-1} = \frac{D_0 A_0}{\Delta x_0} + Q_0
\]

\[
a_{0,0} = \frac{D_0 A_1}{\Delta x_0} + Q_0
\]

\[
a_{0,1} = \frac{D_0 A_1}{v_0(1 + B_1)}
\]

\[
a_{0,2} = \frac{D_1 A_1}{v_2(1 + B_2)}
\]

1) \textbf{Root exterior cells compartment}

\[
\frac{dM_1}{dt} = a_{1,0} M_0 + a_{1,1} M_1
\]

\[
a_{1,0} = \frac{Q_{ST}}{v_0(1 + B_0)}
\]

\[
a_{1,1} = -\left\{ \frac{Q_{ST}}{v_1(1 + B_1)} + \lambda_1 \right\}
\]
2) Root xylem compartment

\[
\frac{dM_2}{dt} = a_{2,0} M_0 + a_{2,2} M_2 + a_{2,3} M_3 + a_{2,4} M_4 + a_{2,5} M_5
\]

\[
a_{2,0} = \frac{D_1 A_1}{\Delta x_1} + Q_1(1 - \sigma_1)
\]

\[
a_{2,0} = \frac{V_0(1 + B_0)}{}
\]

\[
a_{2,2} = -\left(\frac{D_1 A_1}{\Delta x_1} + \frac{D_4 A_4}{\Delta x_4} + \frac{D_2 A_2}{\Delta x_2} + Q_2(1 - \sigma_2) + Q_3^ST + \lambda_2\right)
\]

\[
a_{2,3} = \frac{Q_{b1}^{ST}}{V_3(1 + B_3)}
\]

\[
a_{2,4} = \frac{D_4 A_4}{\Delta x_3} + Q_4(1 - \sigma_4)
\]

\[
a_{2,5} = \frac{D_2 A_2}{\Delta_2}
\]

\[
a_{2,5} = \frac{V_5(1 + B_5)}{}
\]

3) Root storage compartment

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
a_{3,2} = \frac{Q_{b1}^{ST}}{V_2(1 + B_2)}
\]

\[
a_{3,3} = \frac{D_4 A_4}{\Delta x_3} + Q_3^{ST} + Q_4^{ST}
\]

\[
a_{3,4} = \frac{Q_{b2}^{ST}}{V_4(1 + B_4)}
\]

\[
a_{3,4} = \frac{Q_{b2}^{ST}}{V_4(1 + B_4)}
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]

\[
\frac{dM_3}{dt} = a_{3,2} M_2 + a_{3,3} M_3 + a_{3,4} M_4
\]
4) **Root phloem lumen compartment**

\[
\frac{dM_4}{dt} = a_{4,2} M_2 + a_{4,3} M_3 + a_{4,4} M_4 + a_{4,7} M_7
\]

\[
a_{4,2} = \frac{D_4 A_4}{\Delta x_4} ; \quad a_{4,3} = \frac{Q_{ST}}{V_3(1 + B_3)}
\]

\[
a_{4,4} = \left( \frac{D_4 A_4}{\Delta x_4} + Q_4(1 - \sigma_4) + \frac{D_3 A_3}{\Delta x_3} + Q_{f2} \right) \frac{V_4(1 + B_4)}{V_3(1 + B_3)}
\]

\[
a_{4,7} = \frac{D_3 A_3}{\Delta x_1} + Q_3(1 - \sigma_3)
\]

\[
a_{4,7} = \frac{V_7(1 + B_7)}{V_4(1 + B_4)}
\]

5) **Bottom stem xylem compartment**

\[
\frac{dM_5}{dt} = a_{5,2} M_2 + a_{5,5} M_5 + a_{5,6} M_6 + a_{5,8} M_8 + a_{5,14} M_{14}
\]

\[
a_{5,2} = \frac{D_2 A_2}{\Delta x_2} ; \quad a_{5,5} = \frac{D_9 A_9}{\Delta x_9}
\]

\[
a_{5,5} = \left( \frac{D_5 A_5}{\Delta x_5} + Q_5(1 - \sigma_5) + \frac{D_2 A_2}{\Delta x_2} + Q_6(1 - \sigma_6) + Q_{f3} \frac{Q_{ST}}{Q_{b3}} \right) \frac{V_5(1 + B_5)}{V_6(1 + B_6)}
\]

\[
a_{5,8} = \frac{D_5 A_5}{\Delta x_5} ; \quad a_{5,8} = \frac{V_8(1 + B_8)}{V_6(1 + B_6)}
\]
6) **Bottom stem storage compartment**

\[
\begin{align*}
\frac{dM_6}{dt} &= a_{6,5} M_5 + a_{6,6} M_6 + a_{6,7} M_7 \\
a_{6,5} &= \frac{Q_{ST}^{ST}}{V_5(1 + B_5)}; \quad a_{6,6} = -\frac{Q_{b3}^{ST} + Q_{b4}^{ST}}{V_6(1 + B_6)} \lambda_6 \\
a_{6,7} &= \frac{Q_{f4}^{ST}}{V_7(1 + B_7)}
\end{align*}
\]

7) **Bottom stem phloem compartment**

\[
\begin{align*}
\frac{dM_7}{dt} &= a_{7,4} M_4 + a_{7,6} M_6 + a_{7,7} M_7 + a_{7,10} M_{10} + a_{7,16} M_{16} \\
a_{7,4} &= \frac{D_3 A_3}{\Delta x_3}; \quad a_{7,6} = \frac{D_6 A_6}{\Delta x_6} + \frac{D_{12} A_{12}}{\Delta x_{12}} + Q_{ST}^{ST} \\
a_{7,7} &= -\frac{\left[D_3 A_3 + Q_3(1 - \sigma_3) + D_6 A_6 + D_{12} A_{12} + Q_{ST}^{ST}\right]}{V_7(1 + B_7)} + \lambda_7 \\
a_{7,10} &= \frac{D_6 A_6 + Q_6(1 - \sigma_6)}{V_{10}(1 + B_{10})}; \quad a_{7,16} = \frac{D_{12} A_{12} + Q_{12}(1 - \sigma_{12})}{V_{16}(1 + B_{16})}
\end{align*}
\]
8) **Mid stem xylem lumen compartment**

\[
\frac{dM_8}{dt} = a_{8,5} M_5 + a_{8,8} M_8 + a_{8,9} M_9 + a_{8,11} M_{11} + a_{8,17} M_{17}
\]

\[
a_{8,5} = \frac{D_5 A_5}{\Delta x_5} + Q_5 (1 - \sigma_5) \quad V_5 (1 + B_5)
\]

\[
a_{8,8} = - \left[ \frac{D_3 A_3}{\Delta x_3} + \frac{D_7 A_7}{\Delta x_7} + Q_7 (1 - \sigma_7) + \frac{D_{13} A_{13}}{\Delta x_{13}} + Q_{13} (1 - \sigma_{13}) + Q_{ST}^{ST} \right] \quad V_8 (1 + B_8)
\]

\[
a_{8,9} = V_9 (1 + B_9)
\]

\[
a_{8,17} = \frac{D_{13} A_{13}}{\Delta x_{13}} \quad V_{17} (1 + B_9)
\]

9) **Mid stem storage compartment**

\[
\frac{dM_9}{dt} = a_{9,8} M_8 + a_{9,9} M_9 + a_{9,10} M_{10}
\]

\[
a_{9,8} = \frac{D_{18} A_{18}}{\Delta x_{18}} \quad V_9 (1 + B_9)
\]

\[
a_{9,9} = - \left[ \frac{Q_{ST}^{ST}}{V_9 (1 + B_9) + \lambda_9} \right]
\]

\[
a_{9,10} = V_{10} (1 + B_{10})
\]
10) **Mid stem phloem lumen compartment**

\[
\frac{dM_{10}}{dt} = a_{10,7} M_7 + a_{10,9} M_9 + a_{10,10} M_{10} + a_{10,13} M_{13} + a_{10,19} M_{19}
\]

\[
a_{10,7} = \frac{D_6 A_6}{\Delta x_6} ; \quad a_{10,9} = \frac{Q_{ST}}{V_9(1 + B_9)}
\]

\[
a_{10,10} = \frac{D_8 A_8 + Q_6(1 - \sigma_6) + D_{16} A_{16} + Q_{16}}{V_{10}(1 + B_{10})} + \lambda_{10}
\]

\[
a_{10,13} = \frac{D_8 A_8 + Q_6(1 - \sigma_8)}{V_{13}(1 + B_{13})} ; \quad a_{10,19} = \frac{Q_{ST}}{V_{16}(1 + B_{16})}
\]

11) **Top stem xylem lumen compartment**

\[
\frac{dM_{11}}{dt} = a_{11,8} M_8 + a_{11,11} M_{11} + a_{11,12} M_{12} + a_{11,20} M_{20}
\]

\[
a_{11,8} = \frac{D_7 A_7}{\Delta x_8} + \lambda_7(1 - \sigma_8)
\]

\[
a_{11,11} = \frac{D_{17} A_{17} + D_{17}(1 - \sigma_{17}) + Q_{ST}}{V_{11}(1 + B_{11})} + \lambda_{11}
\]

\[
a_{11,12} = \frac{Q_{ST}}{V_{12}(1 + B_{12})} ; \quad a_{11,20} = \frac{D_{17} A_{17}}{\Delta x_{17}} \frac{Q_{ST}}{V_{20}(1 + B_{20})}
\]
12) Top stem storage compartment

\[
\frac{dM_{12}}{dt} = a_{12,11} M_{11} + a_{12,12} M_{12} + a_{12,13} M_{13}
\]

\[
a_{12,11} = \frac{Q_{f7}^{ST}}{V_{11}(1 + B_{11})}; \quad a_{12,12} = \left( \frac{Q_{b7}^{ST} + Q_{b8}^{ST}}{V_{12}(1 + B_{12})} \right) + \lambda_{12}; \quad a_{12,13} = \frac{Q_{f8}^{ST}}{V_{13}(1 + B_{13})}
\]

13) Top stem phloem lumen compartment

\[
\frac{dM_{13}}{dt} = a_{13,10} M_{10} + a_{13,12} M_{12} + a_{13,13} M_{13} + a_{13,22} M_{22}
\]

\[
a_{13,10} = \frac{D_8 A_8}{\Delta x_8}; \quad a_{13,12} = \frac{D_{20} A_{20}}{\Delta x_8}; \quad a_{13,13} = \frac{D_8 A_8}{\Delta x_8} Q_8(1 - \sigma_8) + \frac{D_{20} A_{20}}{\Delta x_8} Q_{f8}^{ST} + \lambda_{13}; \quad a_{13,22} = \frac{D_{20} A_{20}}{\Delta x_8}
\]

14) Leaf cluster 1 xylem lumen compartment

\[
\frac{dM_{14}}{dt} = a_{14,15} M_{15} + a_{14,14} M_{14} + a_{14,16} M_{16} + a_{14,16} M_{16} + S_{16}
\]

\[
a_{14,14} = \frac{D_9 A_9}{\Delta x_9} + Q_9(1 - \sigma_9) \quad a_{14,15} = \frac{D_9 A_9}{\Delta x_9}; \quad a_{14,16} = \frac{D_{20} A_{20}}{\Delta x_9} + Q_{f9}^{ST} \quad a_{14,16} = \frac{D_{20} A_{20}}{\Delta x_9}
\]

THIS PUBLICATION IS OUT OF DATE. 
For most current information: http://extension.oregonstate.edu/catalog
\[ a_{14,14} = -\left( \frac{D_g A_g}{\Delta x_g} + \frac{D_{10} A_{10}}{\Delta x_{10}} + Q_{10}(1 - \sigma_{10}) + \frac{D_{CH} A_{11} H_c}{\Delta x_{11}} + Q^{ST}_{f9} \right) \frac{v_{14}(1 + B_{14})}{v_{15}(1 + B_{15})} + \lambda_{14} \]

\[ a_{14,15} = \frac{Q_{b9}^{ST}}{v_{15}(1 + B_{15})} ; \quad a_{14,16} = \frac{D_{10} A_{10}}{\Delta x_{10}} \frac{v_{16}(1 + B_{16})}{v_{15}(1 + B_{15})} + \lambda_{14} \]

\[ s_{14} = \frac{D_{CH} A_{11} C_{air}}{\Delta x_{11}} \]

15) Leaf cluster 1 storage compartment

\[ \frac{dm_{15}}{dt} = a_{15,14} M_{14} + a_{15,15} M_{15} + a_{15,16} M_{16} \]

\[ a_{15,14} = \frac{Q_{f9}^{ST}}{v_{14}(1 + B_{14})} ; \quad a_{15,15} = \frac{Q_{b9}^{ST} + Q_{b10}^{ST}}{v_{15}(1 + B_{15})} + \lambda_{15} \]

\[ a_{15,16} = \frac{Q_{f10}^{ST}}{v_{16}(1 + B_{16})} \]

16) Leaf cluster 1 phloem lumen compartment

\[ \frac{dm_{16}}{dt} = a_{16,14} M_{14} + a_{16,15} M_{15} + a_{16,16} M_{16} \]

\[ a_{16,14} = \frac{D_{12} A_{12}}{\Delta x_{12}} + \frac{D_{10} A_{10}}{\Delta x_{10}} + Q_{10}(1 - \sigma_{10}) \]

\[ a_{16,15} = \frac{Q_{b10}^{ST}}{v_{15}(1 + B_{15})} \]

\[ a_{16,16} = \frac{v_{14}(1 + B_{14})}{v_{15}(1 + B_{15})} \]
\[ a_{16,16} = - \left( \frac{D_{10} A_{10}}{\Delta x_{10}} + \frac{D_{12} A_{12}}{\Delta x_{12}} + Q_{12}(1 - \sigma_{12}) + Q_{f10}^{ST}}{V_{16}(1 + B_{16})} + \lambda_{16} \right) \]

17) Leaf 2 cluster xylem lumen compartment

\[
\frac{dM_{17}}{dt} = a_{17,8} M_{8} + a_{17,17} M_{17} + a_{17,18} M_{18} + a_{17,19} M_{19} + S_{17}
\]

\[
a_{17,8} = \frac{D_{13} A_{13}}{\Delta x_{13}} + Q_{13}(1 - \sigma_{13})
\]

\[
a_{17,17} = - \left( \frac{D_{13} A_{13} + D_{14} A_{14} + Q_{14}(1 - \sigma_{14}) + D_{15} A_{15}}{\Delta x_{15}} + Q_{f11}^{ST}}{V_{14}(1 + B_{14})} + \lambda_{17} \right)
\]

\[
a_{17,18} = \frac{Q_{b11}^{ST}}{V_{18}(1 + B_{18})}
\]

\[
a_{17,19} = \frac{Q_{f11}^{ST}}{V_{19}(1 + B_{19})}
\]

\[ S_{17} = \frac{D_{CH} A_{15} c_{air}}{\Delta x_{13}} \]

18) Leaf 2 cluster storage compartment

\[
\frac{dM_{18}}{dt} = a_{18,17} M_{17} + a_{18,18} M_{18} + a_{18,19} M_{19}
\]

\[
a_{18,17} = \frac{Q_{ST}^{ST}}{V_{17}(1 + B_{17})} ;
\]

\[
a_{18,18} = \frac{Q_{b11}^{ST} + Q_{b12}^{ST}}{V_{18}(1 + B_{18}) + \lambda_{18}} ;
\]

\[
a_{18,19} = \frac{Q_{f12}^{ST}}{V_{19}(1 + B_{19})}
\]
19) Leaf 2 cluster phloem lumen compartment

\[
\frac{dM_{19}}{dt} = a_{19,10} M_{10} + a_{19,17} M_{17} + a_{19,18} M_{18} + a_{19,19} M_{19}
\]

\[
a_{19,10} = \frac{D_{16} A_{16}}{\Delta x_{16}} \text{ ST}
\]

\[
a_{19,17} = \frac{D_{14} A_{14} + Q_{14}(1 - \sigma_{14})}{\Delta x_{14}} + \frac{Q_{ST}}{V_{17}(1 + B_{17})}
\]

\[
a_{19,18} = \frac{Q_{ST}}{V_{18}(1 + B_{18})}
\]

\[
a_{19,19} = -\left(\frac{D_{16} A_{16} + Q_{16}(1 - \sigma_{16}) + \frac{D_{14} A_{14} + Q_{ST}}{\Delta x_{16}}}{V_{19}(1 + B_{19})}\right) + \lambda_{19}
\]

20) Leaf 3 cluster xylem lumen compartment

\[
\frac{dM_{20}}{dt} = a_{20,11} M_{11} + a_{20,20} M_{20} + a_{20,21} M_{21} + a_{20,22} M_{22} + S_{20}
\]

\[
a_{20,11} = \frac{D_{17} A_{17}}{\Delta x_{17}} \text{ ST}
\]

\[
a_{20,20} = \frac{D_{18} A_{18} + Q_{18}(1 - \sigma_{18}) + \frac{D_{CH H_c A_{19}}}{\Delta x_{19}} + Q_{ST}}{V_{20}(1 + B_{20})} + \lambda_{20}
\]

\[
s_{20} = \frac{D_{CH H_c A_{19}}}{\Delta x_{19}} \text{ C}_{air}
\]

\[
a_{20,22} = \frac{D_{18} A_{18}}{\Delta x_{18}}
\]

\[
s_{20} = \frac{D_{CH H_c A_{19}} C_{air}}{\Delta x_{19}}
\]
21) Leaf 3 cluster storage compartment
\[ \frac{dM_{21}}{dt} = a_{21,20}M_{20} + a_{21,21}M_{21} + a_{21,22}M_{22} \]
\[ a_{21,20} = \frac{Q_{ST}}{V_{20}(1 + B_{20})} ; \quad a_{21,21} = \left( \frac{Q_{ST}}{V_{21}(1 + B_{21})} + \lambda_{21} \right) \]
\[ a_{21,22} = \frac{Q_{ST}}{V_{22}(1 + B_{22})} \]

22) Leaf 3 cluster phloem lumen compartment
\[ \frac{dM_{22}}{dt} = a_{22,13}M_{13} + a_{22,20}M_{20} + a_{22,21}M_{21} + a_{22,22}M_{22} \]
\[ a_{22,13} = \frac{D_{20}A_{20}}{\Delta x_{20}} + \frac{Q_{ST}}{V_{21}(1 + B_{21})} \]
\[ a_{22,20} = \frac{D_{20}A_{20}}{\Delta x_{20}} + \frac{Q_{ST}}{V_{22}(1 + B_{22})} \]
\[ a_{22,21} = \frac{D_{18}A_{18}}{\Delta x_{18}} + \frac{Q_{ST}}{V_{21}(1 + B_{21})} \]
\[ a_{22,22} = \frac{D_{18}A_{18}}{\Delta x_{18}} + \frac{Q_{ST}}{V_{22}(1 + B_{22})} + \lambda_{22} \]