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TRANSPORT MODELS FOR SOIL – PLANT
SYSTEMS

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PREFACE

In the early part of this century, Dr. Bernard A. Keene, of Rothamsted Experimental Station spent some time in the laboratory of Dr. Willard Gardner, considered by many to be the father of modern soil physics. Dr. Gardner, in response to Dr. Keene's encouragement to make his writings simpler and more understandable, is reported to have said "Dr. Keene, God made physics hard, not Willard Gardner!" [Soil Sci. v 100, p 81 (1965)]. Despite Professor Gardner's disclaimer, it is probably true that he, and those who have followed his lead, have been responsible for making soil physics "hard". Any discipline becomes more difficult to master as it enters a quantitative phase where mathematical concepts are extensively used.

Some teachers, aware of the difficulties some students have with mathematical concepts, try to teach quantitative sciences without using mathematical tools. Such attempts are not usually successful. The answer is not in discarding the mathematics, but in finding ways to teach mathematically-based concepts to students who need them, but who find them difficult. The computer is an ideal tool for this purpose. Since microcomputers are now readily available, it seemed reasonable to try to teach difficult mathematical concepts in soil physics using microcomputers.

This book covers material taught in a graduate-level soil physics course at Washington State University. Many soil physics courses dwell mainly on deriving the differential equations for transport, rather than on solving them. I think that a soil physics course should teach students to understand and solve transport problems which exist in field situations, so the course was designed to focus on solutions to the differential equations. I am also convinced that most graduate students in soils and related areas need a good working knowledge of soil physics, since it is fundamental to so many other areas in soil, plant and engineering sciences. The course was therefore designed to take into account the mathematical background of typical graduate students in agricultural and biological sciences. It was assumed that the student would have a good working knowledge of algebra and calculus, but not of differential equations. The course therefore needed to teach methods for solving very difficult differential equations with difficult boundary conditions using fairly simple mathematical tools. This was accomplished by using numerical procedures on microcomputers to solve the differential equations. Numerical methods convert differential equations into algebraic equations which can be solved using conventional methods of linear algebra.

This book reflects the philosophy used in the soil physics course. Each chapter introduces soil physics concepts, generally in the conventional way. Most chapters then go on to develop simple computer programs to solve the
equations and illustrate the points made in the discussion. Problems are given at the end of each chapter to give the reader some practice in using the concepts introduced in the chapter. The problems and computer programs are an integral part of the presentation, and readers are strongly encouraged to experiment with each model until both the working of the model and the concepts it teaches are familiar. Many points which could have been made in the text are left for the reader to discover through using the models and working the problems.

The programs in this book are generally short and relatively simple. They are, however, quite suitable for use as submodels in large, general-purpose models of the soil-plant-atmosphere system, and have been used in this way by me and several of my students.

While only one person's name is given as the author of this book, many have contributed. My father taught me the practical aspects of soil physics at an early age. As a successful farmer in southern Idaho, he had to be a good self-taught soil physicist. The late Dr. S. A. Taylor first interested me in the formal study of soil physics, a study which was continued under the able guidance of Dr. W. H. Gardner, son, and student of Willard Gardner. Many of my students played key roles in the development of ideas which are presented here. Chak Tongyai first introduced me to the application of numerical methods to soil water problems. John Hammel first showed me that these problems could be solved on microcomputers. Susan Riha and Stuart Childs were instrumental in helping develop the approach used in the course, and Susan contributed to an early versions of Ch. 10. George Redinger taught me how to use the Newton-Raphson method, which is an important part of the water flow models used in this book. Many others contributed by checking and suggesting improvements in programs or in the presentation. The actual production of the book was a family project. My daughter Julia Bee had the difficult task of entering the text and equations into the word processor. She also proofread the copy, and produced the index. Another daughter, Karine drafted the figures. My wife, Judy, edited the entire manuscript. Other members of the family gave support and help without which this project could not have been completed. I would like to thank all who have contributed. This book would not have been possible without their help. Finally, this work was completed during a sabbatical leave at University of Nottingham, School of Agriculture. I would like to thank Washington State University and University of Nottingham for support during this time.

Sutton Bonington, 1985

G. S. C.
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<td>volumetric specific heat of component i</td>
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<td>diameter</td>
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<td>$D_0$</td>
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<td>void ratio</td>
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<td>$W \ m^{-2}$</td>
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<td>flux density of gas component i</td>
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<td>flux density of water</td>
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<td>value of a function</td>
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<td>mass balance error for node i</td>
<td>$kg \ m^{-2} \ s^{-1}$</td>
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<td>magnitude of gravitational constant</td>
<td>$m \ s^{-2}$</td>
</tr>
<tr>
<td>$g$</td>
<td>geometric mean</td>
<td>-</td>
</tr>
<tr>
<td>G</td>
<td>ground heat flux density</td>
<td>$W \ m^{-2}$</td>
</tr>
<tr>
<td>h</td>
<td>height of roughness elements</td>
<td>m</td>
</tr>
<tr>
<td>$h_a$</td>
<td>humidity of air</td>
<td>-</td>
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</tbody>
</table>
$h_r$  relative humidity
$h_s$  relative humidity at soil surface
$H$  sensible heat flux density  $W \cdot m^{-2}$
i  subscript to indicate node position in soil
$I$  cumulative infiltration  $kg \cdot m^{-2}$
j  superscript to indicate time
$J$  flux density
integral scale  $m$
k  hydraulic conductivity  $kg \cdot s^{-1} \cdot m^{-3}$
Langmuir constant  $kg/kg$
von Karman's constant
$k_s$  saturated hydraulic conductivity of soil  $kg \cdot s^{-1} \cdot m^{-3}$
$K$  thermal conductance  $W \cdot m^{-2} \cdot K^{-1}$
diffusive conductance  $m/s$
soil hydraulic conductance  $kg \cdot s^{-1} \cdot m^{-4}$
l  length  $m$
$L$  latent heat of vaporization for water  $J/kg$
m  power of hydraulic conductivity function
$m_i$  mass fraction of component $i$
$M$  molar mass  $kg/mol$
$M_i$  mass of component $i$  $kg$
n  upper limit in summations
power of hydraulic conductivity function
$N$  mass of adsorbed-phase solute in soil  $kg/kg$
p  iteration number in Newton-Raphson
$P$  pressure  $Pa$
$q$  mass flux density  $kg \cdot m^{-2} \cdot s^{-1}$
$Q$  Langmuir constant  $kg/kg$
flux of water  $kg/s$
r  radius  $m$
diffusive resistance for heat or water vapor  $s/m$
$r_k$  autocorrelation at lag $k$
$R$  molar gas constant  $J \cdot mol^{-1} \cdot K^{-1}$
resistance to liquid water flow  $m^4 \cdot s^{-1} \cdot kg^{-1}$
$R_{abs}$  absorbed radiation at crop or soil surface  $W \cdot m^{-2}$
degree of saturation
$s$  slope of vapor concentration function
sample standard deviation
$S$  amount of solute in soil  $kg/kg$
$S_t$  total global solar radiation  $W \cdot m^{-2}$
t  time  $s$
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tr>
<td>T</td>
<td>temperature</td>
<td>°C</td>
</tr>
<tr>
<td>u</td>
<td>wind speed</td>
<td>m/s</td>
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<tr>
<td>u*</td>
<td>friction velocity</td>
<td>m/s</td>
</tr>
<tr>
<td>v</td>
<td>mathematical coefficient</td>
<td>-</td>
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<tr>
<td>v_o</td>
<td>pore water velocity</td>
<td>m/s</td>
</tr>
<tr>
<td>v*</td>
<td>dimensionless fluid velocity</td>
<td>-</td>
</tr>
<tr>
<td>V</td>
<td>volume</td>
<td>m⁻³</td>
</tr>
<tr>
<td>V_i</td>
<td>volume of component i</td>
<td>m⁻³</td>
</tr>
<tr>
<td>w</td>
<td>mass wetness or gravimetric water content</td>
<td>kg/kg</td>
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<td>W</td>
<td>relative error in evaporative flux density</td>
<td>-</td>
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<tr>
<td>x</td>
<td>horizontal space coordinate</td>
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<td>value of a variate</td>
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<td>damping depth for heat</td>
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<td>roughness parameter for heat</td>
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<td>z_m</td>
<td>roughness parameter for momentum</td>
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<tr>
<td>a</td>
<td>production term in continuity equation</td>
<td>kg m⁻³ s⁻¹</td>
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<td>γ*</td>
<td>apparent psychrometer constant</td>
<td>g m⁻³ K⁻¹</td>
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<td>semivariance at lag k</td>
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<tr>
<td>δ</td>
<td>solar declination angle</td>
<td>radians</td>
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<td>e</td>
<td>ratio of soil to free air gas diffusivity</td>
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<td>c</td>
<td>function for convection equation</td>
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<td>weighting factor</td>
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<tr>
<td>θ</td>
<td>volumetric water content</td>
<td>m³ m⁻³</td>
</tr>
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<td>θ_s</td>
<td>saturation water content</td>
<td>m³ m⁻³</td>
</tr>
<tr>
<td>θ_fc</td>
<td>field capacity water content</td>
<td>m³ m⁻³</td>
</tr>
<tr>
<td>θ</td>
<td>absolute temperature</td>
<td>K</td>
</tr>
<tr>
<td>κ</td>
<td>solute dispersion factor</td>
<td>m⁻⁴ kg</td>
</tr>
<tr>
<td>λ</td>
<td>thermal conductivity</td>
<td>W m⁻¹ K⁻¹</td>
</tr>
<tr>
<td>μ</td>
<td>population mean</td>
<td>-</td>
</tr>
<tr>
<td>ν</td>
<td>kinematic viscosity</td>
<td>m²/s</td>
</tr>
<tr>
<td>ρ_b</td>
<td>bulk density</td>
<td>Mg m⁻³</td>
</tr>
<tr>
<td>ρ_s</td>
<td>particle density</td>
<td>Mg m⁻³</td>
</tr>
</tbody>
</table>
\( \rho_w \) density of liquid water \( \text{Mg m}^{-3} \)

\( \Pi \) product operator

\( \sigma \) surface tension \( \text{J m}^{-2} \)

\( \sigma_{\text{st}} \) population standard deviation

\( \sigma_{\text{Stefan-Boltzmann}} \) Stefan-Boltzmann constant \( \text{W m}^{-2} \text{K}^{-4} \)

\( \sigma_g \) geometric standard deviation of particle diameter \( \text{mm} \)

\( \sigma_s \) reflection coefficient

\( \Sigma \) summation operator

\( \tau \) tortuosity factor

\( \phi \) porosity or volume fraction of a phase \( \text{m}^3 \text{m}^{-3} \)

\( \Phi \) matric flux potential \( \text{kg m}^{-1} \text{s}^{-1} \)

\( \chi \) osmotic coefficient

\( \psi \) potential of soil water \( \text{J/kg} \)

\( \psi_a \) pneumatic potential \( \text{J/kg} \)

\( \psi_g \) gravitational potential \( \text{J/kg} \)

\( \psi_e \) air entry potential \( \text{J/kg} \)

\( \psi_m \) matric potential \( \text{J/kg} \)

\( \psi_o \) osmotic potential \( \text{J/kg} \)

\( \Psi_h \) temperature profile stability correction

\( \Psi_m \) wind profile stability correction

\( \omega \) angular frequency \( \text{s}^{-1} \)

Variable names in computer programs

A(I) sub-diagonal element in tridiagonal matrix

B power of moisture release function

B(I) diagonal element in tridiagonal matrix

BD soil bulk density \( \text{Mg m}^{-3} \)

BZ(I) \( B_1 \) from eq. 11.12

C(I) super-diagonal element in tridiagonal matrix

C(K) autocovariance at lag \( k \)

CD cosine of solar declination angle

CH volumetric specific heat of air \( \text{J m}^{-3} \text{K}^{-1} \)

CL cloud cover

CO(I) concentration at node i \( \text{g m}^{-3} \)

CP(I) node capacity

CVA atmospheric vapor concentration

D zero plane displacement \( \text{m} \)

D(I) right hand side of matrix equations

DA day number \( \text{days} \)

DF(I) gas diffusivity at node i \( \text{m}^2/\text{s} \)

DJ(I) derivative of vapor flux with potential
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>DP(I)</td>
<td>change in potential in an iteration step</td>
<td>J/kg</td>
</tr>
<tr>
<td>DS</td>
<td>daily global solar radiation</td>
<td>W m⁻²</td>
</tr>
<tr>
<td>DT</td>
<td>time step</td>
<td>s</td>
</tr>
<tr>
<td>DZ</td>
<td>depth increment</td>
<td>m</td>
</tr>
<tr>
<td>E(I)</td>
<td>root water uptake from node i</td>
<td>kg m⁻² s⁻¹</td>
</tr>
<tr>
<td>EA</td>
<td>atmospheric emissivity</td>
<td>-</td>
</tr>
<tr>
<td>EP</td>
<td>potential evaporation rate</td>
<td>mm/day</td>
</tr>
<tr>
<td>F</td>
<td>weighting factor for forward difference etc.</td>
<td>-</td>
</tr>
<tr>
<td>F(I)</td>
<td>mass balance at node i</td>
<td>kg m⁻² s⁻¹</td>
</tr>
<tr>
<td>FG</td>
<td>air filled porosity</td>
<td>-</td>
</tr>
<tr>
<td>FL</td>
<td>water flux at soil surface</td>
<td>kg m⁻² s⁻¹</td>
</tr>
<tr>
<td>FR</td>
<td>atmospheric transmission coefficient</td>
<td>-</td>
</tr>
<tr>
<td>G</td>
<td>1 - F</td>
<td>-</td>
</tr>
<tr>
<td>G(K)</td>
<td>semivariance at lag k</td>
<td>-</td>
</tr>
<tr>
<td>GR</td>
<td>gravitational constant</td>
<td>m s⁻²</td>
</tr>
<tr>
<td>H(I)</td>
<td>humidity at node i</td>
<td>-</td>
</tr>
<tr>
<td>HA</td>
<td>humidity of air</td>
<td>-</td>
</tr>
<tr>
<td>INF</td>
<td>rain to be infiltrated in a time step</td>
<td>kg m⁻² s⁻¹</td>
</tr>
<tr>
<td>JD</td>
<td>day of year</td>
<td>day</td>
</tr>
<tr>
<td>JV(I)</td>
<td>vapor flux through element i</td>
<td>kg m⁻² s⁻¹</td>
</tr>
<tr>
<td>K(I)</td>
<td>element conductance</td>
<td>-</td>
</tr>
<tr>
<td>KH</td>
<td>conductance of boundary layer for heat</td>
<td>W m⁻² K⁻¹</td>
</tr>
<tr>
<td>KS</td>
<td>saturated hydraulic conductivity</td>
<td>kg s m⁻³</td>
</tr>
<tr>
<td>XV</td>
<td>vapor conductance</td>
<td>-</td>
</tr>
<tr>
<td>L(I)</td>
<td>root density at node i</td>
<td>m m⁻³</td>
</tr>
<tr>
<td>M</td>
<td>number of elements</td>
<td>-</td>
</tr>
<tr>
<td>M(I)</td>
<td>hourly potential solar radiation</td>
<td>W m⁻²</td>
</tr>
<tr>
<td>MW</td>
<td>molar mass of water</td>
<td>kg/mol</td>
</tr>
<tr>
<td>N</td>
<td>power for hydraulic conductivity function</td>
<td>-</td>
</tr>
<tr>
<td>P(I)</td>
<td>matric potential at node i</td>
<td>J/kg</td>
</tr>
<tr>
<td>PB</td>
<td>weighted mean soil water potential</td>
<td>J/kg</td>
</tr>
<tr>
<td>PC</td>
<td>critical leaf water potential for stomatal closure</td>
<td>J/kg</td>
</tr>
<tr>
<td>PE</td>
<td>air entry potential</td>
<td>J/kg</td>
</tr>
<tr>
<td>PH</td>
<td>temperature profile stability correction</td>
<td>-</td>
</tr>
<tr>
<td>PL</td>
<td>leaf water potential</td>
<td>J/kg</td>
</tr>
<tr>
<td>PM</td>
<td>wind profile stability correction</td>
<td>-</td>
</tr>
<tr>
<td>PR</td>
<td>precipitation</td>
<td>mm</td>
</tr>
<tr>
<td>PR(I)</td>
<td>water potential at the root surface</td>
<td>J/kg</td>
</tr>
<tr>
<td>PSR</td>
<td>potential daily solar radiation</td>
<td>W m⁻²</td>
</tr>
<tr>
<td>R</td>
<td>gas constant</td>
<td>J mol⁻¹ K⁻¹</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
</tr>
<tr>
<td>---------</td>
<td>------------------------------------------------------------------------------</td>
<td>--------------------</td>
</tr>
<tr>
<td>R(K)</td>
<td>autocorrelation at lag k</td>
<td></td>
</tr>
<tr>
<td>RB</td>
<td>weighted mean root soil-root resistance</td>
<td>m$^4$ s$^{-1}$ kg$^{-1}$</td>
</tr>
<tr>
<td>RND(I)</td>
<td>random number between 0 and 1 (computer function)</td>
<td></td>
</tr>
<tr>
<td>RNI</td>
<td>isothermal net radiation</td>
<td>W m$^{-2}$</td>
</tr>
<tr>
<td>RR(I)</td>
<td>root resistance in layer i</td>
<td>m$^4$ s$^{-1}$ kg$^{-1}$</td>
</tr>
<tr>
<td>RS(I)</td>
<td>soil resistance in layer i</td>
<td>m$^4$ s$^{-1}$ kg$^{-1}$</td>
</tr>
<tr>
<td>SD</td>
<td>sine of solar declination angle</td>
<td></td>
</tr>
<tr>
<td>SE</td>
<td>total mass balance error</td>
<td>kg m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>SL</td>
<td>power of stomatal closure function</td>
<td></td>
</tr>
<tr>
<td>SP</td>
<td>stability parameter, $\zeta$</td>
<td>m</td>
</tr>
<tr>
<td>SW</td>
<td>profile water content change</td>
<td>kg m$^{-3}$</td>
</tr>
<tr>
<td>T(I)</td>
<td>temperature at start of time step</td>
<td>°C</td>
</tr>
<tr>
<td>TA</td>
<td>air temperature</td>
<td>°C</td>
</tr>
<tr>
<td>TI</td>
<td>time</td>
<td>hrs or min</td>
</tr>
<tr>
<td>TN(I)</td>
<td>temperature at end of time step</td>
<td>°C</td>
</tr>
<tr>
<td>TP</td>
<td>potential transpiration rate</td>
<td>kg m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>TX</td>
<td>maximum daily temperature</td>
<td>°C</td>
</tr>
<tr>
<td>TY</td>
<td>minimum daily temperature</td>
<td>°C</td>
</tr>
<tr>
<td>U(I)</td>
<td>source term in mass balance equations</td>
<td></td>
</tr>
<tr>
<td>USTAR</td>
<td>friction velocity</td>
<td>m/s</td>
</tr>
<tr>
<td>V(I)</td>
<td>bulk density x volume per unit area at node i</td>
<td>kg m$^{-2}$</td>
</tr>
<tr>
<td>VK</td>
<td>von Karman's constant</td>
<td></td>
</tr>
<tr>
<td>W</td>
<td>wind speed</td>
<td>m/s</td>
</tr>
<tr>
<td>W(I)</td>
<td>volumetric water content at beginning of time step</td>
<td>m$^3$ m$^{-3}$</td>
</tr>
<tr>
<td>WD</td>
<td>density of water</td>
<td>kg m$^{-3}$</td>
</tr>
<tr>
<td>WN(I)</td>
<td>volumetric water content at end of time step</td>
<td>m$^3$ m$^{-3}$</td>
</tr>
<tr>
<td>X(I)</td>
<td>value of variate</td>
<td></td>
</tr>
<tr>
<td>Z</td>
<td>measurement height</td>
<td>m</td>
</tr>
<tr>
<td>Z(I)</td>
<td>node depth</td>
<td>m</td>
</tr>
<tr>
<td>ZH</td>
<td>heat roughness parameter</td>
<td>m</td>
</tr>
<tr>
<td>ZM</td>
<td>momentum roughness parameter</td>
<td>m</td>
</tr>
</tbody>
</table>
Chapter 1

INTRODUCTION

Soil physics deals with the state and movement of energy and material in soil. The areas of study include structure and texture of the solid matrix, retention and flow of water, the movement of solutes, soil temperature and the flow of heat, and the diffusion of gases. Consideration of any of these subjects is difficult, however, without knowing how quickly plants are withdrawing water or nutrients from the soil, or how much energy is being supplied or removed at the soil surface. Cycling of nutrients and exchange of gases are also affected by microbial processes in the soil. This book will deal mainly with physical processes in soil, but it will also be necessary to include plant-water relations, uptake of nutrients by plants, heat and mass transport at the soil surface, and activity of microbes. Since the term "soil" implies a living body in which microbes and roots grow and which acts as a reservoir of water for plants, soil physics cannot be restricted to a consideration of the flow of water in porous materials.

Early soil physicists were concerned mainly with a physical description of soil. They attempted to characterize soil in terms of particle size distribution, water content, water potential, pore space and temperature. To aid in these descriptions, a number of terms were defined, particularly with regard to soil water. Such expressions as hygroscopic water, capillary water, gravitational water etc. were used to represent the state of soil water. As the science progressed, these qualitative representations of the physical state of the soil system gave way to more quantitative expressions, and the dynamics of the system began to be considered. The first step in the description of transport in soil was to write the differential equations which represent transport and to determine the appropriate driving forces. A large fraction of soil physics research during the last three decades has been devoted to these problems. Writing the correct equations is a necessary first step in solving transport problems, but unless the equations are solved, they have little practical value. Because of this, a lot of effort has been and is being expended on finding methods for solving the differential equations which describe transport in soil. Early work concentrated on analytic solutions, but these are possible only for a few very simple systems. Analytic solutions tend to be complicated and often are not understood by (and therefore not used by) soil scientists and others who need to use them. When digital computers became available, numerical solutions to differential equations were attempted. Numerical solutions have the advantage that they are not restricted to simple system geometry or simple boundary conditions.
Another advantage of using numerical techniques and a computer to solve differential equations is that the numerical method converts a differential equation into a set of algebraic equations. The algebraic equations are much easier to solve than the differential equation. The availability of microcomputers, combined with the power and simplicity of numerical methods should allow soil scientists, plant scientists, hydrologists and other who need to solve transport problems to understand the procedures and use the methods for practical purposes. The intent of this book is to present the basic equations which describe transport in soil, show how to solve them using simple numerical methods, and then show how to apply them to a sample of problems. To aid in this, computer programs, written in BASIC are given for each calculation, and problems are given which will require the use of the programs. This approach will help the student to become familiar with the power as well as the simplicity of numerical methods for solving soil physics problems.

1.1 UNITS

Throughout the book units consistent with the International System will be used. The basic units in this system are the meter (m) for length, the second (s) for time, the kilogram (kg) for mass, the Ampere (A) for electric current and the kelvin (K) for temperature. Celsius temperature can also be used. The celsius temperature is $C = K - 273.15$. Other units, which can be derived from these units, are shown in Table 1.1. We will try to use those marked preferred throughout the book. Some of the units may seem unfamiliar at first, but the increased efficiency which results from using a consistent set of units easily offsets the small inconvenience associated with learning the new values. Conversion factors for other sets of units are given in the Appendix.

1.2 TRANSPORT EQUATIONS

This book will be concerned primarily with the transport of water, gases, heat, and nutrients in soil and plants. Any steady transport problem can be described (in one dimension) by a differential equation of the form

$$ J = -k \frac{dC}{dx} \quad (1.1) $$

where $J$ represents the flux density of energy or material, $k$ is a conductivity, and $dC/dx$ is a gradient in "concentration" or potential. The potential gradient is the driving force for flow. If $k$ and $J$ are constant,
### TABLE 1.1 Examples of SI units.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Unit</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>length</td>
<td>meter</td>
<td>m</td>
</tr>
<tr>
<td>area</td>
<td>square centimeter</td>
<td>( \text{cm}^2 )</td>
</tr>
<tr>
<td></td>
<td>square meter</td>
<td>( \text{m}^2 )</td>
</tr>
<tr>
<td>volume</td>
<td>cubic meter</td>
<td>( \text{m}^3 )</td>
</tr>
<tr>
<td>water content</td>
<td>kilogram water per kilogram dry soil</td>
<td>( \text{kg kg}^{-1} )</td>
</tr>
<tr>
<td></td>
<td>kilogram dry soil</td>
<td>( \text{kg kg}^{-1} )</td>
</tr>
<tr>
<td></td>
<td>cubic meter water per cubic meter soil</td>
<td>( \text{m}^3 \text{ m}^{-3} )</td>
</tr>
<tr>
<td>density</td>
<td>megagram per cubic meter</td>
<td>( \text{Mg m}^{-3} )</td>
</tr>
<tr>
<td>electrical conductivity</td>
<td>decisiemens per meter</td>
<td>( \text{dS m}^{-1} )</td>
</tr>
<tr>
<td>resistance</td>
<td>second per meter</td>
<td>( \text{s m}^{-1} )</td>
</tr>
<tr>
<td>specific heat</td>
<td>joule per kilogram kelvin</td>
<td>( \text{J kg}^{-1} \text{ K}^{-1} )</td>
</tr>
<tr>
<td>heat flux density</td>
<td>watts per square meter</td>
<td>( \text{W m}^{-2} )</td>
</tr>
<tr>
<td>gas flux density</td>
<td>gram per square meter second (p)</td>
<td>( \text{g m}^{-2} \text{ s}^{-1} )</td>
</tr>
<tr>
<td></td>
<td>mole per square meter second (a)</td>
<td>( \text{mol m}^{-2} \text{ s}^{-1} )</td>
</tr>
<tr>
<td>water flux density</td>
<td>kilogram per square meter second (p)</td>
<td>( \text{kg m}^{-2} \text{ s}^{-1} )</td>
</tr>
<tr>
<td></td>
<td>cubic meter per square meter second (a)</td>
<td>( \text{m}^3 \text{ m}^{-2} \text{ s}^{-1} )</td>
</tr>
<tr>
<td>thermal conductivity</td>
<td>watt per meter kelvin</td>
<td>( \text{W m}^{-1} \text{ K}^{-1} )</td>
</tr>
<tr>
<td>diffusivity</td>
<td>square meter per second</td>
<td>( \text{m}^2 \text{ s}^{-1} )</td>
</tr>
<tr>
<td>hydraulic conductivity</td>
<td>kilogram second per cubic meter (p)</td>
<td>( \text{kg s m}^{-3} )</td>
</tr>
<tr>
<td></td>
<td>cubic meter per kilogram (a)</td>
<td>( \text{m}^3 \text{ s kg}^{-1} )</td>
</tr>
<tr>
<td></td>
<td>meter per second (a)</td>
<td>( \text{m s}^{-1} )</td>
</tr>
<tr>
<td>water potential</td>
<td>joule per kilogram (p)</td>
<td>( \text{J kg}^{-1} )</td>
</tr>
<tr>
<td></td>
<td>kilopascal (a)</td>
<td>( \text{kPa} )</td>
</tr>
<tr>
<td></td>
<td>meter of water (a)</td>
<td>( \text{m} )</td>
</tr>
</tbody>
</table>

(p) preferred, (a) alternate
eq. 1.1 is easily integrated to obtain a difference equation. Separation of variables and integration gives

\[ J = -k \frac{(C_2 - C_1)}{(z_2 - z_1)} \]  

(1.2)

where the subscripts 2 and 1 indicate the potentials or concentrations at positions \( z_2 \) and \( z_1 \). If \( J \) and \( k \) are not constant, the integration can still be performed on eq. 1.1, though it is more complicated than the one used to get 1.2. The result of the integration is an equation like 1.2, but with \( k \) replaced by an appropriate average value over the distance \( z_2 - z_1 \). Several examples of integrations which involve non-constant \( k \)'s or \( J \)'s will be given later in the book.

Equation 1.2 is a simple algebraic equation which can be used to describe the steady flux density of matter or energy in soil. If we divide a soil column into several layers, and know the conductance \((k/Az)\) of each layer as well as the flux density of heat or material through the column, we can use eq. 1.2 to find the value for \( C \) at each depth in the soil. Each layer has one equation in two unknowns, but one of the unknowns can be eliminated between each two equations except the ones at the top and bottom of the column. These values must be supplied in order to solve the problem. These values are called boundary conditions; they supply the connection between the column and its environment. Once boundary conditions are supplied, it is an easy matter to solve for all of the \( C \)'s.

One might also be interested in using eq. 1.2 to find the flux if the potentials or concentrations are known. Again, conductances would be found experimentally, concentrations or potentials would be measured, and the flux calculated.

These examples illustrate how simple it is to solve differential equations that are not time-dependent. Solutions in more dimensions involve more equations and more unknowns, but, in principle, are no more complicated than eq. 1.2.

Time-dependent equations are much more interesting, but are also more complicated since they involve the storage of energy or material. Storage occurs throughout the soil, but to deal with storage in a discrete numerical model it must be assumed that all of the storage in each layer of soil is at the boundary between layers (the node) so that the flow within any layer is steady. The rate of storage of heat or material is the capacity of the node multiplied by the change in concentration or potential at the node and divided by the time period over which the storage occurs (called the time-step). For storage at discrete nodes to reasonably approximate the continuous system, nodes must be spaced at fairly close intervals, especially in locations where
rapid changes occur (such as at the soil surface). As we formulate numerical models, we will check the adequacy of the numerical approximations by comparisons with analytical solutions to simple problems, and by changing node spacing and time step size to see what effect this has on the solution.

The approach just outlined for solving flow equations differs somewhat from the finite difference or finite element approaches which are usually used to solve these equations. This approach is more like an analysis of a resistor - capacitor network in electronics, with the integrated conductances being the conductors connecting the nodes, and the storage represented by capacitors. The results obtained by this approach are always as good as would be obtained by finite difference or finite element approaches, and often are better. In the network analysis approach the physics of the system is more apparent, and, when taken into account, often produces more accurate results than are obtained by blind application of mathematics to the problem. The student is encouraged to understand and compare the finite difference and finite element methods to those presented here.

1.3 A NOTE ON BASIC

The Microsoft MBASIC interpreter was used for the programs in this book. It is probably the most popular and widely used BASIC for microcomputers. If your computer does not use Microsoft's MBASIC, the programs should still run, with a little modification. Points to understand in adapting programs are:

1. MBASIC allows multiple statements per line with statements separated by a colon. Some BASIC's allow only one statement per line; others use a different statement separator. If yours allows only a single statement on a line, you must rewrite the program with a separate line number for each statement.

2. MBASIC allows a prompt to be printed within an input statement. Some BASIC's may require that this be a separate print statement.

3. Some BASIC's may require the LET statement. MBASIC does not, and it is not used in this book.

4. MBASIC allows long variable names. Variable names in this book have been restricted to 2 letters to be compatible with early Radio Shack computers, but some more restrictive BASIC's may require changing variable names to a letter and a number.

5. An apostrophe in MBASIC has the same meaning as REM. Everything after the apostrophe, in a given line, is a comment. The apostrophe, rather than REM has been used throughout this book.

6. MBASIC strips off leading zero's in constants, and lists some floating point constants with a trailing exclamation mark. You should therefore be careful, when entering a program from the listings, to look for leading decimal points and ignore trailing exclamation marks.
Chapter 2

PHYSICAL PROPERTIES OF SOIL

Soil is a three-phase system made up of solids, liquids and gases. The solid phase, or soil matrix, contains mineral particles and organic materials. The liquid phase, or soil solution, consists of water and dissolved minerals, and the gas phase, or soil atmosphere, is composed of about 80 percent nitrogen, with oxygen and carbon dioxide making up most of the remaining 20 percent. In this chapter we will give a brief overview of equations used to describe this system. A more complete treatment can be found in Hillel (1980).

2.1 BULK DENSITY, WATER CONTENT, AND POROSITY

It is useful to define several variables which describe the physical condition of the three-phase soil system. In a given amount of soil, the total mass (kg or Mg), \( M_t \), is divided between mass of gases, \( M_g \) (usually taken to be zero), mass of liquid, \( M_l \), and mass of solids, \( M_s \). The total volume, \( V_t \) (m\(^3\)), is divided between volume of gases, \( V_g \), volume of liquid, \( V_l \), and volume of solids, \( V_s \). The volume of fluid, \( V_f \), is the sum of \( V_g \) and \( V_l \).

Using these variables, the following definitions can be developed:

Particle Density (Mg m\(^{-3}\)):

\[
\rho_s = \frac{M_s}{V_s}
\]  \hspace{1cm} (2.1)

Dry Bulk Density (Mg m\(^{-3}\)):

\[
\rho_b = \frac{M_s}{V_t}
\]  \hspace{1cm} (2.2)

Total porosity (m\(^3\) m\(^{-3}\)):

\[
\phi_f = \frac{V_f}{V_t} = \frac{V_g + V_l}{V_t}
\]  \hspace{1cm} (2.3)

Gas filled porosity (m\(^3\) m\(^{-3}\)):

\[
\phi_g = \frac{V_g}{V_t}
\]  \hspace{1cm} (2.4)

Void ratio (m\(^3\) m\(^{-3}\)):

\[
e = \frac{V_f}{V_s} = \frac{V_g + V_l}{V_t} = \frac{V_f}{(V_t - V_f)}
\]  \hspace{1cm} (2.5)
Mass wetness or mass basis water content (kg/kg): 

\[ w = \frac{M_1}{M_S} \]  

(2.6)

Volume wetness or volumetric water content (m\(^3\) m\(^{-3}\)): 

\[ \theta = \frac{\phi_1}{V_t} = \frac{V_1}{V_t} \]  

(2.7)

Degree of saturation (m\(^3\) m\(^{-3}\)): 

\[ s = \frac{V_1}{V_f} = \frac{V_1}{(V_g + V_1)} \]  

(2.8)

2.2 RELATIONSHIPS BETWEEN VARIABLES

It is useful to derive relationships among the variables defined in Section 2.1. For example, it can be shown that

\[ \phi_f = 1 - \frac{\rho_b}{\rho_S} \]  

(2.9)

\[ \phi_g = \phi_f - \theta = 1 - \frac{\rho_b}{\rho_S} - \theta \]  

(2.10)

and

\[ \theta = \frac{\phi_f}{(1 - \phi_f)} \]  

(2.11)

Mass wetness and volume wetness are related by

\[ \theta = w \frac{\rho_b}{\rho_1} \]  

(2.12)

and

\[ w = \theta \frac{\rho_1}{\rho_b} \]  

(2.13)

where \(\rho_1\) is the density of the liquid phase (usually taken as the density of liquid water).

A final useful relationship is

\[ s = \theta/\theta_s \]  

(2.14)

where \(\theta_s\) is the volumetric water content at saturation. If the soil does not swell, so that \(\rho_b\) is not a function of water content, the degree of
saturation could also be expressed as the ratio of mass water content to saturation mass water content.

2.3 TYPICAL VALUES OF PHYSICAL PROPERTIES

The ranges of the variables defined in Section 2.1 can now be explored using a few simple examples. Table 2.1 gives particle densities of typical soil constituents. The mineral soil particle density used in most calculations is \( \rho_s = 2.65 \text{ Mg m}^{-3} \). Table 2.1 indicates, however, that some soils have particle densities substantially different from this, depending on the composition and parent material of the soil.

Table 2.1 Densities of soil constituents

<table>
<thead>
<tr>
<th>Component</th>
<th>Density Mg m(^{-3})</th>
<th>Component</th>
<th>Density Mg m(^{-3})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartz</td>
<td>2.66</td>
<td>Orthoclase</td>
<td>2.5 - 2.6</td>
</tr>
<tr>
<td>Clay Minerals</td>
<td>2.65</td>
<td>Mica</td>
<td>2.8 - 3.2</td>
</tr>
<tr>
<td>Organic Matter</td>
<td>1.30</td>
<td>Limonite</td>
<td>3.4 - 4.0</td>
</tr>
<tr>
<td>Water</td>
<td>1.00</td>
<td>Fe(OH)(_3)</td>
<td>3.73</td>
</tr>
<tr>
<td>Air (20°C)</td>
<td>0.0012</td>
<td>Ice</td>
<td>0.92</td>
</tr>
</tbody>
</table>

Typical bulk densities for mineral soils range from around 1 Mg m\(^{-3}\) for recently tilled loam and clay soils to around 1.6 Mg m\(^{-3}\) or higher for sands. A mid-range value of \( \rho_b = 1.3 \text{ Mg m}^{-3} \) would give a total porosity of 0.5 and a void ratio of 1.0.

Water content is usually measured on a mass basis by drying a sample at 105°C, and then computing the ratio of mass of water lost to dry mass of the sample (eq. 2.6). Oven-dry soil is assumed to be at zero water content though structural water may still be present. Air-dry soil is in equilibrium with atmospheric moisture, and therefore has a water content greater than zero. Typical water contents for air-dry soil range from 0.01 to 0.04 kg/kg, depending on texture and atmospheric humidity.

At the other extreme, the saturation water content for a soil with 0.5 m\(^3\) m\(^{-3}\) pore space is 0.5 m\(^3\) m\(^{-3}\). Using eq. 2.13, the mass wetness is \( w = 0.38 \text{ kg/kg} \) for a bulk density of 1.3 Mg m\(^{-3}\). The highest water contents attained under field conditions are somewhat below the saturation value. Some pores always remain air filled. A typical maximum water content in the field would be 0.45 - 0.48 m\(^3\) m\(^{-3}\). Near-saturation conditions are usually of short duration in well-drained soils. Following rain or irrigation, the soil quickly approaches a water content termed field capacity, which will be discussed in detail in Chapter 8. Field capacity water contents vary greatly, but often are roughly half of saturation. A typical field capacity for a uniform loam soil might therefore be 0.25 m\(^3\) m\(^{-3}\) or 0.19 kg/kg.
2.4 PARTICLE SIZE DISTRIBUTION

The textural triangle is used for determining soil texture from measured fractions of sand, silt and clay. Soil texture can also be determined quite reliably by a trained person in the field, and is the one bit of physical data that is almost always available for any soil of interest.

Soil scientists use textural information to make qualitative judgments about a number of other physical properties, but, until recently, quantitative use of textural data has been difficult. Textural data represent ranges of fractions of sand, silt, and clay. Such a representation results in too many variables for convenient correlations. It is not easy to determine how much silt it takes to equal a unit of clay, or whether the silt and sand fractions have any effect at all on a particular property of interest.

Shirazi and Boersma (1984) recently produced a new texture diagram that is much more useful for obtaining physical data from soil texture. The diagram is reproduced in Fig. 2.1. It is based on the U.S.D.A. classification scheme, where equivalent diameters are:

- Clay: $d < 0.002 \text{ mm}$
- Silt: $0.002 \leq d < 0.05 \text{ mm}$
- Sand: $0.05 \leq d < 2.0 \text{ mm}$

The new diagram is based on the assumption that particle size distribution in soil is approximately log-normal (a plot of number of particles having a given diameter vs. log diameter would approximate a Gaussian distribution function). With this assumption, any combination of sand, silt and clay can be represented by a geometric (or log) mean particle diameter ($d_g$) and a geometric standard deviation ($\sigma_g$). Values for $d_g$ and $\sigma_g$ are calculated from

\[
d_g = \exp a \quad (2.15)
\]
\[
\sigma_g = \exp b \quad (2.16)
\]

where

\[
a = \sum m_i \ln d_i \quad (2.17)
\]
\[
b = [\sum m_i (\ln d_i)^2 - a^2]^{1/4} \quad (2.18)
\]

$m_i$ is the mass fraction of textural class $i$, and $d_i$ is the arithmetic mean diameter of class $i$. The summation is taken over the three texture classes,
Fig. 2.1. A new representation of the soil texture diagram using USDA particle size limits. (after Shirazi and Boersma, 1984)

sand, silt, and clay. For the three classes normally used in determining texture, \( d_{\text{clay}} = 0.001 \text{ mm} \), \( d_{\text{silt}} = 0.026 \text{ mm} \), and \( d_{\text{sand}} = 1.025 \text{ mm} \).

In later chapters, the hydraulic properties of soils will be inferred from textural data. We will then find that the information given by Fig 2.1 is much more useful than the data one obtains from a textural triangle.
2.5 REFERENCES


2.6 PROBLEMS

2.1 Write a program in BASIC which takes $P_b$ and $w$ as input and computes and prints $\phi_f$, $\phi_g$, $e$, $\theta$, and $s$.

2.2 Using eqs. 2.1 - 2.8, derive eqs. 2.9 - 2.14.

2.3 Write a program in BASIC to find geometric mean particle diameter and $c_g$ for any combination of sand, silt, and clay.
Chapter 3

GAS DIFFUSION IN SOIL

Oxygen is consumed and carbon dioxide is generated by the metabolic activity of microorganisms and plant roots in the soil. Oxygen, carbon dioxide and water vapor all diffuse into and out of the soil. Soil air is typically around 79 percent N₂. The remaining 21 percent is mostly CO₂ and O₂, which vary reciprocally. In well aerated soil, the CO₂ content of the air is around 0.25 percent and O₂ is 20.73 percent. In poorly aerated soil, O₂ levels can approach zero.

The absorption of nutrients by roots, and the beneficial activity of microorganisms depend on an adequate supply of oxygen. Soils should therefore be managed to provide adequate aeration. Data presented by Taylor and Ashcroft (1972), show that O₂ levels below 10-15 percent can inhibit plant growth.

The rate of respiration of living organisms in the soil depends primarily on the availability of oxygen and carbon in the soil, and on soil temperature and soil moisture. Oxygen consumption is greatest when organic matter is incorporated into moist, warm soil. Respiration rates in winter are often suppressed because of low temperature and low oxygen concentration. In the summer, low soil water potential may inhibit respiration. Respiration rates are usually highest in spring months when roots are growing rapidly, root exudates are plentiful for microorganism growth, and moisture and temperature conditions are favorable.

In this chapter, gas exchange for individual roots or microorganism colonies in the soil, as well as gas exchange between the soil profile and the atmosphere, will be modeled. Only steady state exchange will be considered since exchange is usually rapid enough to make storage unimportant.

3.1 TRANSPORT EQUATIONS

Diffusion of gases in soil follows Fick's law:

\[ f_g = Q/A = -D \frac{dc}{dx} \] (3.1)

where \( Q \) is the flux (g/s), \( A \) is area, \( f_g \) is the flux density (g m\(^{-2}\) s\(^{-1}\)), \( D \) is the diffusion coefficient (m\(^2\)/s), \( c \) is concentration (g m\(^{-3}\)), and \( x \) is distance.

Equation 3.1 is easily integrated, giving

\[ Q = K (c_2 - c_1) \] (3.2)
where \( K \) is a conductance (reciprocal of a resistance), and the subscript following the concentration indicates a location where concentration is measured.

Under steady conditions the flux of gas, \( Q \), across any surface is constant, though the flux density may change if the area available for flow changes. Equation 3.1 can therefore be rearranged and integrated to obtain

\[
\frac{Q}{[1/A(x)]dx} = \frac{D}{dc} = D(c_2 - c_1)
\]  

(3.3)

Using eq. 3.2

\[
K = \frac{D}{[1/A(x)]dx}
\]  

(3.4)

For simple geometries the integration can be done and the conductances determined. When diffusion is purely one dimensional, the area available for flow remains constant with distance, so \( A(x) = \text{1 m}^2 \). The conductance is therefore

planar diffusion: \( K = \frac{D}{(x_2 - x_1)} \)  

(3.5)

When diffusion is spherical, as it might be from a microorganism colony in soil, \( A(x) = 4\pi x^2 \), where \( x \) is the radial distance from the center of the sphere. Integration of eq. 3.4 gives

spherical diffusion: \( K = \frac{4\pi D r_1 r_2}{(r_2 - r_1)} \)  

(3.6)

Diffusion to a root or cylindrical surface is a third interesting case. Here \( A(x) = 2\pi x \), per meter of root, where \( x \) is the distance from the center of the cylinder. Again, using 3.4, we obtain

cylindrical diffusion: \( K = \frac{2\pi D}{\ln(r_2/r_1)} \)  

(3.7)

Note that the units of \( K \) have been allowed to differ depending on system geometry. For planar diffusion, the flux per unit area is constant, conductance has units of \( \text{m/s} \) and \( Q \) is per unit area. For cylindrical systems, the flux per unit length is constant, so \( K \) has units of \( \text{m}^2/\text{s} \) and flux is per meter of length. For spherical systems, \( K \) has units of \( \text{m}^3/\text{s} \) and flux is per sphere.

It is interesting to note that, for a spherical organism, the conductance becomes independent of \( r_2 \) when \( r_2 \) is large compared to the radius of the organism. In other words when \( r_2 >> r_1 \), eq. 3.6 becomes \( K = 4\pi D r_1 \).
3.2 THE DIFFUSIVITY OF GASES IN SOIL

Gas diffusivity in the gas phase of a porous medium is usually expressed as the product of two terms, the binary diffusion coefficient for the gas in air, and some function of air-filled porosity:

\[ D = D_0 \varepsilon(\phi_B) . \]  

(3.8)

The diffusivity of a gas in air depends on the diffusing species, as well as the temperature and pressure of the air. Some binary diffusion coefficients for gases in air under standard conditions are given in Table 3.1. Others can be calculated using the theory in Bird et al. (1960). Diffusivity increases at a rate of about 0.7 percent per kelvin with temperature, and decreases at a rate of around 1 percent per kilopascal with increasing atmospheric pressure. The following relationship is often used to express pressure and temperature dependence of diffusivity:

\[ D_0(T,P) = D_0(NT) \left( \frac{T}{T_0} \right)^n \left( \frac{P}{P_0} \right) \]  

(3.9)

where \( R \) is in Kelvins, and the superscript, ° indicates temperature and pressure at NTP (101.3 kPa, 273.16 K). The exponent, \( n \) has a value of 2 for \( H_2O \) and \( O_2 \), and a value of 1.75 for \( CO_2 \).

Over some part of the diffusion path, \( O_2 \) and \( CO_2 \) usually must diffuse through liquid water. Diffusivities in water are much smaller than those in air. Typical values are around \( 2 \times 10^{-9} \) \( m^2/s \) for both \( CO_2 \) and \( O_2 \) at 20°C. Diffusivity of gases in water increases with temperature at about the same rate as viscosity decreases with temperature (Bird et al., 1960). The temperature correction can be made using \( D_w = D_{wo} \left( \frac{T}{T_0} \right)^6 \) where \( T \) is the Kelvin temperature.

The fact that diffusivities in the liquid phase are four orders of magnitude smaller than those in the gas phase indicates that gas exchange in a
soil profile without a continuous air phase is, for practical purposes, zero. Gas transport in moist soil profiles will therefore be assumed to occur only through the gas phase. Gas transport through the liquid phase will only be considered when dealing with gas exchange of microorganisms and roots.

The diffusion rate of a gas in a porous medium is reduced relative to that in free space because some of the space is occupied by solid particles and liquids and because the path the molecule must follow is more tortuous than that of the molecule in free space. For dry porous materials, Currie (1965) has shown that an equation of the form

$$
\varepsilon(\phi) = b\phi^m
$$

(3.10)

fits data reasonably well. The constant, \( m \) has a value which depends on the shape of the soil particles, but generally falls between 1 and 2, for dry materials. The constant, \( b \) ranges from 0.5 to 1.0 and depends on the value chosen for \( m \). Penman found \( b = 0.66 \) and \( m = 1 \) provided a good fit to data. Marshall (1959) found \( b = 1 \) and \( m = 1.5 \).

When water is added to the porous material, the cross-section for flow is reduced and the tortuosity of the flow path is increased. As water content approaches saturation, dead-end pores may be formed that contribute to air-filled porosity, but do not aid gas diffusion. Equation 3.10 can still be used, but the constants \( b \) and \( m \) may not be the ones which work best for dry materials. Table 3.2 gives values for \( b \) and \( m \) from several data sets. In spite of some variation, it appears that values of \( b \) around 0.9 and \( m \) around 2.3 are good approximations for undisturbed cores, especially at high water content.

Troeh et al. (1982) proposed an equation of the form

$$
\varepsilon(\phi) = [(\phi - u)/(1 - u)]^v
$$

(3.11)

where \( u \) and \( v \) are empirical constants. The constant \( u \) represents the porosity at which diffusion becomes zero. Such an equation does give reasonable extrapolations at high air-filled porosity, approaching unity as \( \phi \rightarrow 0 \).

Table 3.2. Values for the constants \( b \) and \( m \) (eq 3.10) from non-linear least squares fits to data from the indicated source.

<table>
<thead>
<tr>
<th>material</th>
<th>( b )</th>
<th>( m )</th>
<th>data source</th>
</tr>
</thead>
<tbody>
<tr>
<td>aggregated Yolo silt loam</td>
<td>0.90</td>
<td>2.36</td>
<td>Sallam et al. (1984)</td>
</tr>
<tr>
<td>Riverton soil (1.4&lt;p_b&lt;1.8)</td>
<td>0.92</td>
<td>1.70</td>
<td>Rogers et al. (1982)</td>
</tr>
<tr>
<td>Hamble silt loam (undist. cores)</td>
<td>0.81</td>
<td>2.29</td>
<td>Ball (1981)</td>
</tr>
<tr>
<td>sandy loam (sieved, repacked)</td>
<td>1.30</td>
<td>1.70</td>
<td>Lai et al. (1976)</td>
</tr>
</tbody>
</table>
approaches unity. However low porosity conditions (which usually are of greatest interest in modeling) are not as well represented. Several data sets in Table 3.2 contain diffusivity data at very low air-filled porosity. Here eq. 3.10 appears to give the best predictions. Equation 3.10 will therefore be used for diffusivity calculations throughout the book.

3.3 COMPUTING CONCENTRATIONS

The composition of air is generally reported in terms of percent of the total volume which would be occupied by each gas in its pure state, or the partial pressure of that gas. The following equations will convert the concentration to a mass of gas per unit volume of air. These values can be found by using the gas law:

\[ c_i = \frac{M_i P_i}{R \theta} \]  

(3.12)

where \( P_i \) is the partial pressure of the gas (Pa), \( M_i \) is the molecular weight, \( R \) is the gas constant (8.3143 J mole\(^{-1}\) K\(^{-1}\)) and \( \theta \) is kelvin temperature. The partial pressure of the gas is the volume fraction (0.21 for \( O_2 \), 0.79 for \( N_2 \), etc.) multiplied by atmospheric pressure (1.013 \times 10^5 Pa at sea level). Concentrations of \( O_2 \), \( CO_2 \), and \( N_2 \) in air are therefore \( c_o = 279 \text{ g/m}^3 \), \( c_c = 0.59 \text{ g/m}^3 \), and \( c_n = 920 \text{ g/m}^3 \).

3.4 ONE DIMENSIONAL OXYGEN DIFFUSION IN A SOIL PROFILE

As a first example, oxygen flux into soil, and \( O_2 \) profiles within a soil profile are simulated. To do this, the soil is divided into layers, or elements. Within each element, it is assumed that the flux is linearly related to the concentration difference across the element. Respiratory production of \( CO_2 \) and consumption of \( O_2 \) are assumed to occur only at the nodes. Figure 3.1 shows two elements with their conductances \( (K(I)) \), nodal concentrations \( (CO(I)) \) and sink functions \( (U(I)) \).

The flux (positive downward) within element \( I \) is

\[ J(I) = -K(I) (CO(I+1) - CO(I)), \]  

(3.13)

where

\[ K(I) = DF(I)/(Z(I+1) - Z(I)). \]  

(3.14)

DF(I) is the gas diffusivity in element \( I \). Note that eq. 3.14 is the
Fig. 3.1. Elements and nodes for computing gas concentration and flux in a soil profile, showing the numbering system, concentrations, and sinks.

element conductance, defined in eq. 3.5. The mass balance at node I is

\[ J(I) - J(I-1) - U(I) = 0 \]  

(3.15)

The source term at node I, \( U(I) \) is defined as

\[ U(I) = \int_{1-1/2}^{1+1/2} a(z) \, dz \]  

(3.16)

where \( a(z) \) is the source strength \( (g \, m^{-3} \, s^{-1}) \) (+ for production, - for consumption). If the source strength is assumed constant for short distances, then eq. 3.16 becomes

\[ U(I) = a(z) (Z(I+1) - Z(I-1))/2 \]

Combining eqs. 3.13 and 3.15, and rearranging, we obtain

\[-K(I-1) \, CO(I-1) + (K(I-1) + K(I)) \, CO(I) - K(I) \, CO(I+1) - U(I) = 0 \]  

(3.17)

Equation 3.17 can be written for each node in the soil, giving \( M \) equations in \( M + 2 \) unknowns, \( CO(0) - CO(M+1) \). Boundary conditions are used to reduce the number of unknowns by two so that the system of equations can be solved. The boundary condition at the top of the soil is established by setting \( CO(0) = 280 \, g \, m^{-3} \) for \( O_2 \) or \( 0.59 \, g \, m^{-3} \) for \( CO_2 \). The node at \( Z(1) \) is at the soil surface, and the element conductance, \( K(0) \) is the atmospheric boundary layer conductance. The boundary condition at the bottom of the profile is probably best handled by setting \( K(M) = 0 \) so that there is no flow out the bottom of
the profile and the concentration, CO (M+1), has no effect on the other concentrations.

The M equations in M unknowns can now be solved using Gauss elimination (students not familiar with matrix representation of linear equations should consult an elementary linear algebra book such as Kolman, 1982). Writing eq 3.17 for each node, and then arranging the equations in matrix form for M = 4 gives:

\[
\begin{bmatrix}
B(1) & C(1) & 0 & 0 \\
A(2) & B(2) & C(2) & 0 \\
0 & A(3) & B(3) & C(3) \\
0 & 0 & A(4) & B(4)
\end{bmatrix}
\begin{bmatrix}
CO(1) \\
CO(2) \\
CO(3) \\
CO(4)
\end{bmatrix}
= 
\begin{bmatrix}
D(1) \\
D(2) \\
D(3) \\
D(4)
\end{bmatrix}
\tag{3.18}
\]

where B(I) = K(I) + K(I-1), A(I+1) = C(I) = -K(I), and D(I) = U(I) for I ≠ 1; D(1) = U(1) + K(0) CO(0). If K(M) were not zero, then D(M) would have K(M)CO(M+1) added. The coefficient matrix is symmetric and tridiagonal. The set of equations is solved very efficiently using the Thomas algorithm.

Program 3.1 is a BASIC code for determining the oxygen concentration using eq. 3.18. The Thomas algorithm goes from line 190 to line 280. Figure 3.2 shows results of the simulation for a soil column at uniform water content. Typical literature values of O_2 uptake rate for surface soil samples are 10^{-4} - 10^{-3} g m^{-3} s^{-1}. In this simulation a rate of 5 \times 10^{-4} g m^{-3} s^{-1} was used at the surface. Values were decreased with depth as indicated in line 110 in pgm 3.1. Using these values, the flux at the surface was 145 mg m^{-2} s^{-1}. Typical values from Baver et al. (1972) are 36 mg m^{-2} s^{-1} for an undisturbed sandy clay loam soil, 170 mg m^{-2} s^{-1} for a peat soil, and 36, 93, and 50 mg m^{-2} s^{-1} for potato, kale, and tobacco crops. The simulation therefore seems reasonable. From Fig. 3.2 it is seen that oxygen concentration remains near atmospheric levels when air-filled porosity is 0.2 or above, but decreases quickly with depth as \phi_g drops to 0.1 or below. Negative \text{O}_2 concentrations are indicated deep in the profile. These are an artifact of the model caused by the incorrect assumption that oxygen consumption rate is independent of \text{O}_2 concentration.

3.5 ANAEROBIC MICROsites

The fact that the soil profile itself is aerobic does not mean that all sites within the soil can support aerobic respiration. There are increasing numbers of reports of anaerobic processes, such as denitrification, or ethylene production, occurring in apparently well aerated soil. Some computations are shown which describe the possible physical characteristics of such microsites.
PROGRAM 3.1 BASIC PROGRAM FOR COMPUTING OXYGEN CONCENTRATIONS AND FLUXES IN A SOIL PROFILE

10 INPUT "NUMBER OF ELEMENTS"; M
20 INPUT "AIR FILLED POROSITY - M+3/M+3"; FG
30 INPUT "ELEMENT LENGTH, M"; X
40 DIM A(M+1), B(M), C(M), K(M), CO(M), D(M), U(M), Z(M+1), DF(M)
50 Z(1) = 0: K(0) = .01: CO(0) = 280
60 K(0) = .01
70 CO(0) = 280
80 FOR I = 1 TO M
90 Z(I+1) = Z(I) + X
100 DF(I) = .0000177* .9*FG + 2.3
110 U(I) = -.0005*EXP(-Z(I)/.3)*(Z(I+1) - Z(I-1))/2
120 IF I < M THEN K(I) = DF(I) / (Z(I+1) - Z(I)) ELSE K(I) = 0
130 A(I+1) = -K(I)
140 B(I) = K(I-1) + K(I)
150 C(I) = K(I)
160 D(I) = U(I)
170 NEXT
180 D(1) = D(1) + K(0)*CO(0)
190 FOR I = 1 TO M - 1
200 C(I) = C(I) / B(I)
210 D(I) = D(I) / B(I)
220 B(I+1) = B(I+1) - A(I+1)*C(I)
230 D(I+1) = D(I+1) - A(I+1)*D(I)
240 NEXT
250 CO(M) = D(M) / B(M)
260 FOR I = M - 1 TO 1 STEP -1
270 CO(I) = D(I) - C(I)*CO(I+1)
280 NEXT
290 PRINT "DEPTH-M","O2 CONC","K(I)","U(I)"
300 FOR I = 0 TO M
310 PRINT Z(I), CO(I), K(I), U(I)
320 NEXT
330 PRINT "OXYGEN FLUX"; K(0)*(CO(0) - CO(1))
Anaerobic microsites are usually envisioned as spherical soil aggregates or fungal masses. A microsite would not be anaerobic unless all pores were water-filled. Diffusion through air-filled pores would be much too fast to allow anaerobic conditions. It will therefore be assumed that an anaerobic microsite is a spherical mass of microbial and soil material, whose pores are water-filled. The diffusivity will be assumed to be around half that in water, to account for tortuosity and the presence of the solid matrix.

Figure 3.3 shows the subdivision of the microsites into spherical shells. It is assumed that the flux across any element is constant, and that sinks occur only at the nodes. Using eq. 3.6, element conductances for spherical diffusion can be written as

\[ K(I) = 4\pi DF(I) R(I) R(I+1)/(R(I+1) - R(I)) \]  

(3.19)

The mass balance for node I is given in eq. 3.15, but here the f's are mass per unit time, rather than mass per unit area and time. The source strength (again assuming \( \alpha(r) \) can be taken as constant over small increments in \( r \)) is

\[ U(I) = \alpha(r) (4\pi/3) (R(I+1)^3 - R(I-1)^3)/2 \]  

(3.20)
for all but $I = 1$ where an additional $(2\pi/3) R(1)^3$ must be added to account for the innermost spherical volume.

The boundary conditions for this problem differ somewhat from the planar diffusion problem. Here $K(0) = 0$ because there is no diffusion across the center of the sphere, and $K(M)$ is the boundary layer conductance for the air boundary layer around the microsite. Since conductance of the boundary layer is expected to be large compared to that of other elements, its exact value is unimportant. It could be calculated from equation 3.6 or simply set to some number, say $10^4$ times as large as the other $K$'s. The concentration, $CO(M+1)$, is the oxygen concentration in the soil air.

The respiration rate for anaerobic microsites is much greater than that for bulk soil. Small microsites may be composed almost entirely of live biological material with almost no soil. A typical respiration rate at 20°C for biological material might be 1-2 g m$^{-3}$ s$^{-1}$. The diffusivity to be used in the anaerobic microsite problem is the diffusivity for water, corrected for tortuosity and the reduced cross section for flow. Since it is assumed that the microsite is mainly organic material, these factors probably do not reduce the diffusivity, compared to that in water, by more than a factor of 2 or 3.

Programming the spherical diffusion problem is left as an exercise for the reader. Results of the simulation may be used to determine, for example, the size of a microsite which would have an anaerobic center, given the oxygen concentration in the air or water surrounding the site and the respiration rate. Griffin (1972) reports values of the critical radius for anaerobiosis in fungal pellets in shake culture ranging from 0.1 mm to 0.4 mm. Anaerobic
soil crumbs are larger. Figure 3.4 shows simulated oxygen concentration as a function of radius for a spherical microsite having a respiration rate of 2 g m\(^{-3}\) s\(^{-1}\). The core of the site is still aerobic, but a slight increase in respiration rate or size of the sphere, or a decrease in ambient concentration, would result in anaerobic conditions at the core.

![Graph showing oxygen concentration as a function of distance](image)

**Fig. 3.6.** Simulated oxygen concentrations within a respiring spherical or cylindrical tissue mass.

### 3.6 CYLINDRICAL DIFFUSION - ANAEROBIOSIS IN ROOTS

Anaerobic microsites in soil may not be confined to microbial colonies alone. Crawford (1978) reviews various studies which indicate that anaerobic conditions may exist in rapidly growing root tissue of plants. Tissue at the core of a root may become anaerobic, even when peripheral tissue is in contact with O\(_2\) concentrations well above zero. This is the result of the high resistance to oxygen diffusion. Oxygen diffuses to root tissue both radially from the soil and axially within special tissues in roots of some species. However, only radial diffusion will be considered here. A more complete model is given by Luxmoore et al. (1970).

From eq. 3.7

\[
K(I) = 2\pi D F(I)/\ln[R(I+1)/R(I)]
\]  

(3.21)
The sink term for cylindrical diffusion becomes

\[ U(I) = \alpha(R) \pi \frac{1}{2} (R(I+1)^2 - R(I-1)^2)/2 \]  

(3.22)

Since \( \pi \) appears in all terms of the nodal equations, it can be divided out.

The boundary conditions and solution procedure are the same for cylindrical diffusion as for spherical diffusion. Results of a simulation using a respiration (O\(_2\) consumption) rate of 2 g m\(^{-3}\) s\(^{-1}\) and \( D = 10^{-9} \) m\(^2\)/s, are compared to results for spherical diffusion under similar conditions in Fig. 3.6. For the conditions assumed here, anaerobiosis is more easily achieved with cylindrical geometry than with spherical. This is a result of the greater surface to volume ratio of the sphere. The actual programming of the cylindrical diffusion problem requires only a simple modification of the spherical diffusion program, and is also left as a reader exercise.

### 3.7 EFFECT OF OXYGEN CONCENTRATION ON RESPIRATION RATE

In all of the examples given so far, it has been assumed that the oxygen concentration has no effect on respiration rate (zero-order reactions). However, oxygen uptake is an enzyme catalyzed reaction which should respond to oxygen concentration according to the Michaelis Menten (M-M) equation:

\[ \alpha = \alpha_{\text{max}} \frac{c_0}{(K_0 + c_0)} \]  

(3.23)

where \( \alpha_{\text{max}} \) is the maximum rate of O\(_2\) uptake, and \( K_0 \) is the M-M constant. When \( c_0 >> K_0 \), the reaction is second order (no effect of \( c_0 \) on \( \alpha \)).

Griffin (1972) gives a value of \( K_0 \) for uptake of O\(_2\) by fungi and bacteria of 3 \( \times \) 10\(^{-6}\) moles/kg. The \( K_0 \) for the principal enzyme involved in the uptake, cytochrome oxidase, is 2.5 \( \times \) 1\(^{-8}\) moles/kg. The oxygen concentration of water in equilibrium with atmospheric oxygen is 2.6 \( \times \) 10\(^{-6}\) moles/kg. From these numbers, it appears that the assumption of constant respiration rate is reasonable down to O\(_2\) concentrations of at least 1-2 percent in tissue or microorganism colonies. In soil profiles, resistances to diffusion to sites of respiration may cause respiration rates to fall at higher concentrations.

From a modeling standpoint, \( \alpha \) could be made a function of \( c_0 \), using equation 3.23. This would avoid the problem of negative oxygen concentrations, but would require more difficult numerical techniques.
3.8 REFERENCES


3.9 PROBLEMS

3.1 Write a program in BASIC to determine the oxygen concentrations within a spherical microsite. Use the program to determine the effect of \( O_2 \) uptake rate on critical radius (radius at which the center of the sphere just becomes anaerobic). Plot the results.

3.2 Do problem 2 for a cylindrical site (root) and compare results to those obtained for a sphere.

3.3 Use the program from problem 3.1 or 3.2 to determine the effect of external \( O_2 \) concentration on critical radius.

3.4 Alter program 3.1 so that it computes and prints percent oxygen and percent \( CO_2 \) at each level in the soil profile. Then use the program to determine what air-filled porosity is required to keep \( CO_2 \) concentration below 5% and \( O_2 \) concentration above 15% in the root zone.
Chapter 4

SOIL TEMPERATURE AND HEAT FLOW

All of the physical, chemical, and biological processes which go on in soil are influenced by soil temperature. Biological processes such as the uptake of nutrients and water by roots, the decomposition of organic matter by microbes and the germination of seeds are strongly affected by soil temperature. Rates of some of these processes more than double for each 10°C increase in temperature. In some cases, growth of above-ground plant parts is more closely correlated with soil temperature than with air temperature. Physical processes, such as water movement and soil drying can also be strongly influenced by temperature. For these reasons, most simulations of soil processes require submodels which predict soil temperature.

The simplest model for soil temperature would be to assume that it is constant, or that it is equal to a daily, weekly, or monthly mean air temperature. Such a model may be adequate for some purposes, which will be considered in later chapters. More accurate models require analysis of heat flow within the soil and heat exchange at the soil surface to determine soil temperature.

The transport or loss of latent heat of either fusion or vaporization, and the movement of soil moisture are important in determining soil temperature. Analysis of these aspects of the problem must follow the study of moisture movement, and will be considered in Chap. 11. In this chapter, the differential equations for heat transport and the parameters needed to solve them will be given, followed by methods for solving the equations using numerical procedures.

4.1 DIFFERENTIAL EQUATIONS FOR HEAT FLOW

The relationship between heat flux density (W/m²) and temperature is the Fourier law:

\[ f_h = -\lambda \frac{dT}{dz} \quad (4.1) \]

where \( \lambda \) is thermal conductivity (W m\(^{-1}\) K\(^{-1}\)), \( T \) is temperature (°C or K), and \( z \) is vertical distance. Equation 4.1 applies to heat flow in the vertical, only, but it is easily generalized to three dimensions by adding conductivities and temperature gradients in the x and y directions.
Equation 4.1 can be combined with the continuity equation to obtain the time dependent differential equation

\[ C_h \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial z^2} \]  

(4.2)

where \( C_h \) is the volumetric specific heat of the soil (J m\(^{-3}\) K\(^{-1}\)).

Solutions to eq. 4.2 will describe soil temperature as a function of depth and time.

A closed-form solution to eq. 4.2 can only be obtained for simple sets of soil properties and boundary conditions which may not realistically represent soils under field conditions. It is useful, however, to examine at least one of these solutions in detail. If thermal conductivity and capacity do not vary with depth, then \( \lambda \) may be taken out of the derivative and combined with \( C_h \) to give

\[ \frac{\partial T}{\partial t} = D_h \frac{\partial^2 T}{\partial z^2} \]  

(4.3)

where \( D_h \) is thermal diffusivity. For a soil column which has a surface temperature given by

\[ T(0,t) = T + A(0) \sin\omega t \]  

(4.4)

and is infinitely deep, the temperature at any depth and time is given by

\[ T(z,t) = T + A(0) \exp(-z/z_d) \sin(\omega t - z/z_d). \]  

(4.5)

Here \( T \) is the mean soil temperature, \( A(0) \) is the amplitude of the temperature wave at the soil surface (difference between \( T \) and \( T_{max} \) or \( T_{min} \)), \( \omega (s^{-1}) \) is the angular frequency of the oscillation (2\( \pi \) divided by the period in seconds) and \( z_d \) is the damping depth, given by

\[ z_d = (2D_h/\omega)^{\frac{1}{2}} \]  

(4.6)

Equation 4.5 shows how temperature would vary with depth and time in a uniform soil subject to the assumed boundary conditions. Note that the amplitude is attenuated exponentially with depth, and that the phase of the wave is shifted with depth. At \( z = z_d \), the amplitude is \( e^{-1} = 0.37 \) times its value at the surface. The temperature at 2-3 damping depths would therefore be expected to be about the mean temperature for the period of oscillation because temperature fluctuations would be only 5-10% of the temperature fluctuation at the surface. Typical diurnal damping depths are 10
to 15 cm for mineral soils, and typical annual damping depths are 2-3 m. Temperatures at around 30 cm would therefore remain almost constant over a diurnal cycle, and temperatures at 5-6 m would be almost constant over an annual cycle.

4.2 NUMERICAL SOLUTION TO THE HEAT FLOW EQUATION

A numerical solution to eq. 4.2 can be applied more generally than the analytical solution which was just presented. No assumptions need to be made about constant thermal properties, and the boundary conditions can be made realistic. Setting up the equations for a numerical solution of the heat flow problem is similar to setting up the gas diffusion problem, with two exceptions. Equation 4.2 is time dependent, so solutions will need to be in both depth and time. Also heat will be stored or taken from storage within the soil. Figure 4.1 shows how the soil is divided into elements.

Fig. 4.1. Elements and nodes for computing temperature and heat flux in a soil profile, showing numbering system, conductances and storage.

Depth is indicated by Z, temperature by T, heat storage by CP and conductance by K. Note the numbering system for nodes and elements. The element number is that of the node just above it. Heat flow within any element is assumed to be steady, so that eq. 4.1 describes the heat flux density. Storage of heat is assumed to occur only at the nodes. The energy balance equation for node I is

\[ K_i(T_i+1 - T_i) - K_i(I-1)(T_i - T_i-1) = C_{hi}(T_i^{j+1} - T_i^{j})(Z_{i+1} - Z_{i-1}) / 2 \Delta t \]  

where \( \Delta t \) is the time increment and \( C_h \) is soil volumetric specific heat. The superscript \( j \) indicates the time at which temperature is determined.
The conductance, $K$ is

$$K_i = \frac{\lambda_i}{(Z_{i+1} - Z_i)}$$  \hspace{1cm} (4.8)$$

where $\lambda_i$ is the thermal conductivity of the $i$th element. The first term on the right of eq. 4.7 is the specific heat per unit volume of soil multiplied by the change in temperature of the soil and the volume of soil per unit area for node $i \left(\frac{(Z_{i+1} - Z_{i-1})}{2}\right)$, and divided by the time over which the temperature change occurs. It is therefore the rate of heat storage at node $i$.

In eq. 4.1 the heat flux between nodes is proportional to the temperature difference. When the time increment is infinitesimally small, or when temperature does not change with time, it is obvious which temperature to use in computing the heat flux through an element. However, equation 4.7 indicates that temperature does change with time, so the choice of nodal temperature to be used for computing heat flux through an element becomes more difficult. The overbar on the $T_i$'s on the left side of eq. 4.7 is to indicate that the flux is computed from an appropriate mean temperature. If superscript $j$ indicates present time and $j+1$ is one time step in the future, an appropriate mean temperature must be somewhere between $T_j$ and $T_{j+1}$.

Therefore,

$$T = \eta T_{j+1} + (1 - \eta) T_j.$$  \hspace{1cm} (4.9)$$

Here, $\eta$ is a weighting factor which may range from 0 to 1. If $\eta = 0$, the flux is determined by the temperature difference at the beginning of the time step. The numerical procedure which results from this choice is called a forward difference of explicit method, since an explicit expression for $T_{j+1}$ can be written using eq. 4.7. If $\eta = 0.5$, the average of the old and new temperatures is used to compute heat flux. This is called a time-centered, or Crank-Nicholson scheme. The equation for computing $T_{j+1}$ is implicit for this choice of $\eta$ (and any other except $\eta = 0$) since each $T_{j+1}$ depends on the values of the new temperatures at the nodes $i+1$ and $i-1$. The solution must be obtained using the tridiagonal matrix system given in Chapter 3. If $\eta = 1$, the scheme is called a backward difference. Here fluxes are computed using only the new temperatures. This scheme is also implicit. Most heat flow models use either $\eta = 0$ or $\eta = 0.5$. The best value to use for $\eta$ is determined by considerations of numerical stability and accuracy. The reader is encouraged to investigate the effect of $\eta$ on accuracy in problem 4.1 at the end of this chapter. A few general comments, however, should be given here.

The explicit scheme, with $\eta = 0$ predicts more heat transfer between nodes than would actually occur, and can therefore become unstable if time steps are
too large. Stable numerical solutions are only obtained when (Simonson, 1975)
\[ \Delta t < \frac{C_h(\Delta z)^2}{2\lambda} \]  
(4.10)

When \( \eta > 0.5 \), stable solutions to the heat flow problem will always be obtained, but if \( \eta \) is too small, the solutions may oscillate. The reason for this is that the simulated heat transfer between nodes in one time step is too large, and the new temperature overshoots. On the next time step the excess heat must be transferred back, so the predicted temperature at that node oscillates. On the other hand, if \( \eta \) is too large, the temperature difference will be too small and not enough heat will be transferred. Simulated temperatures will never oscillate under these conditions, but the simulation will underestimate the heat flux. The best accuracy is obtained with \( \eta \) around 0.4, while best stability is at \( \eta = 1 \). A typical compromise is \( \eta = 0.6 \).

Equations 4.7 and 4.9 can be combined to give a single equation for \( T_{j+1} \) in terms of the known values of \( K \) and \( C_h \), and unknown values of \( T^I_{j+1} \) and \( T^I_{j+1} \). If similar equations are written for each node in the soil, the set of equations describing the system is similar to eq. 3.18 for gas diffusion.

For four nodes

\[
\begin{bmatrix}
B(1) & C(1) & 0 & 0 \\
A(2) & B(2) & C(2) & 0 \\
0 & A(3) & B(3) & C(3) \\
0 & 0 & A(4) & B(4)
\end{bmatrix}
\begin{bmatrix}
T(1) \\
T(2) \\
T(3) \\
T(4)
\end{bmatrix}
= 
\begin{bmatrix}
D(1) \\
D(2) \\
D(3) \\
D(4)
\end{bmatrix}
\]  
(4.11)

where

\[
B(I) = \eta[K(I) + K(I-1)] + C_h[Z(I+1) - Z(I-1)]/2\Delta t
\]  
(4.12)

\[
A(I+1) = C(I) = -\eta K(I)
\]  
(4.13)

and

\[
D(I) = (1-\eta)K(I-1)T(I-1) + C_h[Z(I+1)-Z(I-1)]/2\Delta t - (1-\eta)(K(I)+K(I-1))T(I) \\
+ (1-\eta)K(I)T(I+1)
\]  
(4.14)

The new \((j+1)\) temperatures are \(T_{j+1}\); the old temperatures \((j)\) are \(T(I)\).

4.3 BOUNDARY CONDITIONS

The boundary condition at the bottom of the soil column is usually specified as remaining at some constant, measured temperature, \(T_{N(M+1)}\).
The last value for $D$ is therefore

$$D(M) = D'(M) + \eta K(M) TN(M+1)$$  \hspace{1cm} (4.15)

where $D'(M)$ is the value obtained from eq. 4.14. For a no-flux condition, $K(M) = 0$, so nothing is added.

The boundary condition at the soil surface is more complex since convection and radiation may be important. When radiative and latent heat transfer are unimportant, then

$$D(1) = D'(1) + \eta K(0) TN(0)$$  \hspace{1cm} (4.16)

where $D'(1)$ is the value computed from 4.14, $K(0)$ is the boundary layer conductance, and $TN(0)$ is the air temperature at the end of the time step. When significant radiative and/or latent heat transfer occur they are added as heat sources at node 1 to give

$$D(1) = D'(1) + \eta K(0) TN(0) - R_n + LE$$  \hspace{1cm} (4.17)

where $R_n$ is the net radiation at the soil surface and $LE$ is the latent heat flux. The net radiation will be discussed in detail in Chapter 12. The evaporation rate depends on the water content and temperature of the soil surface, the concentration of water vapor in the air, and on atmospheric boundary layer conductance. The computation of evaporation rate will be covered in Chapter 9.

4.4 HEAT STORAGE IN SOIL

Before soil heat fluxes and temperature profiles can be computed, the specific heat and thermal conductivity of the soil must be known. It is possible to obtain these values by experiment, but for modeling purposes it is better to predict them from basic physical properties of the soil.

The volumetric specific heat of the soil, which is needed to solve the heat flow problem, is the sum of the specific heats of all soil constituents:

$$C_h = C_{m}\phi_m + C_w\phi_w + C_a\phi_a + C_o\phi_o$$  \hspace{1cm} (4.18)

where $\phi$ is the volume fraction of the component indicated by the subscript, and the subscripts $m$, $w$, $a$, and $o$ indicate mineral, water, air, and organic constituents. Table 4.1 gives typical values for $C$ for each of these substances. The contribution of soil air to heat capacity is usually ignored. In mineral soils, the contribution from organic matter is also negligible.
because the volumetric specific heats of mineral and organic materials are so similar. The volumetric specific heat of mineral soil therefore becomes

\[ C_h = C_m(1 - \phi_f) + C_w \theta \quad (4.19) \]

where \( \phi_f \) is the total porosity and \( \theta \) is the volumetric water content.

### Table 4.1. Thermal properties of soil materials (after deVries, 1963).

<table>
<thead>
<tr>
<th>Material</th>
<th>Density ( \text{Mg m}^{-3} )</th>
<th>Specific heat ( \text{J g}^{-1} \text{K}^{-1} )</th>
<th>Thermal conductivity ( \text{W m}^{-1} \text{K}^{-1} )</th>
<th>Volumetric sp. heat ( \text{MJ m}^{-3} \text{K}^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartz</td>
<td>2.66</td>
<td>0.80</td>
<td>8.80</td>
<td>2.13</td>
</tr>
<tr>
<td>Clay minerals</td>
<td>2.65</td>
<td>0.90</td>
<td>2.92</td>
<td>2.39</td>
</tr>
<tr>
<td>Organic matter</td>
<td>1.30</td>
<td>1.92</td>
<td>0.25</td>
<td>2.50</td>
</tr>
<tr>
<td>Water (20°C)</td>
<td>1.00</td>
<td>4.18</td>
<td>0.025</td>
<td>4.18</td>
</tr>
<tr>
<td>Ice</td>
<td>0.92</td>
<td>1.88</td>
<td>2.18</td>
<td>1.73</td>
</tr>
</tbody>
</table>

#### 4.5 THERMAL CONDUCTIVITY OF SOIL

The thermal conductivity of soil depends on its bulk density, water content, quartz content, and organic matter content. Figure 4.2 shows typical values of thermal conductivity as a function of water content for forest litter, a silt loam soil, and a sand.

At low water content, the air space controls the thermal conductivity, and the litter, sand, and silt loam have similar thermal conductivities. At high water content, the thermal conductivity of the solid phase becomes more important. The large differences which occur in the thermal conductivity of different materials is the result of differences in bulk density and composition. The transition from low to high conductivity occurs at low water content in sands, and high water content in soils high in clay.

These relationships, which are qualitatively evident from Fig. 4.2, need to be made more quantitative if we are to use them for modeling. The curves were produced using the equation (McInnes, 1981)

\[ \lambda = A + B \theta - (A - D) \exp[-(C \theta)^E] \quad (4.20) \]

where \( \theta \) is volumetric water content, and \( A, B, C, D, \) and \( E \) are coefficients which McInnes obtained by curve fitting. They would be more useful if they could be related to soil properties. Looking at limits of \( \theta \), when \( \theta = 0, \lambda = D \). deVries (1963) gives both experimental and theoretical values for
Fig. 4.2. Typical thermal conductivity functions for sand, silt loam, and forest litter predicted using eq. 4.20 with $\phi_q=0.3$, $m=0.3$, $m_c=0.01$ for sand; $\phi_q=0$, $m=0.47$, $m_c=0.124$ for silt loam; $A=0.4$, $B=0.5$, $C=1$, $D=0.06$ for forest litter.

$\lambda$ of dry materials which are well fit by

$$D = 0.03 + 0.7\phi_s^2$$

(4.21)

where $\phi_s$ is the volume fraction of solids. For mineral soils with a particle density of 2.65 Mg m$^{-3}$, eq. 4.21 gives

$$D = 0.03 + 0.1\rho_s^2$$

(4.22)

At saturation, the last term in eq. 4.20 becomes zero and

$$\lambda_s = A + B\phi$$

(4.23)

The constant $B$ can be evaluated from data, and is approximated by

$$B = 2.8 \phi_s \phi$$

(4.24)

where $\phi_s$ is the total volume fraction of solids.

For mineral soils, eq. 4.24 can also be written as

$$B = 1.06 \rho_s \phi$$

(4.25)
If the theory of deVries (1963) is used to find $\lambda_a$, eqs. 4.23 and 4.24 can be combined to give

$$A = \frac{(0.57 + 1.73\phi_q + 0.93\phi_m)(1 - 0.74\phi_q - 0.49\phi_m) - 2.8\phi_s(1 - \phi_s)}{1 - 0.74\phi_q - 0.49\phi_m} \quad (4.26)$$

where $\phi_q$ is the volume fraction of quartz and $\phi_m$ is the volume fraction of other minerals. The volume fraction of solids, $\phi_s$, is $\phi_q + \phi_m$. For many mineral soils, the quartz fraction can be taken as nil, and equation 4.26 can be approximated by

$$A = 0.65 - 0.78\rho_b + 0.60\rho_b^2 \quad (4.27)$$

The constant, $E$ can be assigned a value of 4. The constant $C$ determines the water content where thermal conductivity begins to increase rapidly, and is highly correlated with clay content. The correlation

$$C = 1 + 2.6 m_c^{1/4} \quad (4.28)$$

appears to fit data well where $m_c$ is the clay fraction.

The thermal conductivities calculated from eq. 4.20 using the constants from eqs. 4.21 - 4.28 are total conductivity, including both the sensible and latent heat components. The sensible heat conductivity is independent of temperature, but the latent component is temperature dependent. At high water content, and temperatures around 25°C, 10 to 15% of the conductivity may be due to latent heat transport. At low temperatures and low moisture levels, the latent heat component is negligible (Cass et al. 1984). The separation of these components will be considered in more detail later in conjunction with linked transport of heat and water. For the moment, it is enough to remember that the thermal conductivities calculated with eq. 4.20 can have a small temperature dependence.

4.6 NUMERICAL IMPLEMENTATION

An example program for simulating heat flow in soil is given as Program 4.1. For simplicity, the boundary layer conductance is assumed to be known. Statements to line 130 are for inputing data and setting up initial conditions and boundary conditions. Depth is input in meters, water content in m$^3$ m$^{-3}$, and temperature in °C. In line 160, $\eta$ (F in the program) is set to 0.6, so the solution is weighted slightly toward backward difference. If $F$ were set equal to 1, we would be using a backward difference, and if $F = 0$, the solution would be explicit, or forward difference. In line 240, the air temperature is simulated by a sine function. The heat storage terms are
' PROGRAM 4.1  BASIC PROGRAM FOR COMPUTING SOIL TEMPERATURE AND SOIL HEAT FLUX

I0 INPUT "NUMBER OF ELEMENTS";M
50 DIM W(M+1),T(M+1),TN(M+1),K(M+1),CP(M),A(M+1),B(M),C(M),D(M),Z(M+1)
60 TA=20:AM=15:BD=1.3:TB=20
70 K(0)=20 "BOUNDARY LAYER CONDUCTANCE IN W/(M+2 K)
80 INPUT "WATER CONTENT (M+3/M+3)";WV
90 FOR I=1 TO M
100 Z(I+1)=Z(I)+.005*1.5*(I-1)
110 T(I)=TB
120 NEXT
130 T(M+1)=TB:TN(M+1)=T(M+1):T(0)=TB
140 'TI IS TIME OF DAY;DT IS TIME STEP (SEC);DA IS DAY NUMBER
150 TI=0:DT=3600:DA=0
160 F=.6:G=1-F
170 MC=.12 'CLAY FRACTION
180 C1=.65-.78*BD+.6*BD*BD:C2=.12*BD*BD:BD=.12/SQR(MC):C4=.3*1.5*BD*BD
190 FOR I=1 TO M
200 K(I)=(C1+C2*WV-(C1-C4)*KEXP(-(C3*WV)+4))/((Z(I+1)-Z(I))
210 NEXT
220 TI=TI+DT/3600:IF TI>24 THEN TI=TI-24:DA=DA+1
230 TN(0)=TA+AM*SIN(.261799*(TI-6))
250 FOR I=1 TO M
260 C(I)=K(I)*F : A(I+1)=C(I)
270 B(I)=F*(K(I)+K(I-1)+CP(I)
280 D(I)=G*K(I-1)*T(I-1)+(CP(I)-G*(K(I)+K(I-1)))*T(I)+G*K(I)*T(I+1)
290 NEXT
300 D(I)=D(I)+K(I)*TN(I)*F
310 D(M)=D(M)+K(M)*F*TN(M+1)
320 FOR I=1 TO M-1
330 C(I)=C(I)/B(I)
340 D(I)=D(I)/B(I)
350 B(I+1)=B(I+1)-A(I+1)*C(I)
360 D(I+1)=D(I+1)-A(I+1)*D(I)
370 NEXT
380 TN(M)=D(M)/B(M)
390 FOR I=M-1 TO 1 STEP -1
400 TN(I)=D(I)+C(I)*TN(I+1)
410 NEXT
420 PRINT "DAY =";DA,"HOUR =";TI
430 PRINT "HEAT FLUX =";K(0)*G*(T(0)-T(I))+F*(TN(0)-TN(I)));"W/M^2"
440 PRINT "DEPTH","TEMPERATURE","K(I)"
450 FOR I=0 TO M+1
460 PRINT Z(I),TN(I),K(I)
470 T(I)=TN(I)
480 NEXT
490 IF DA<5 THEN GOTO 230
computed in line 200, and the element conductances in line 210. Line 180 computes the coefficients for eq. 4.20 for a typical low-quartz, mineral soil. Lines 320 to 410 are the Thomas Algorithm for setting up and solving the system of equations for the new temperatures, TN(I). In line 430, the heat flux at the surface is computed from the surface conductance and the average temperature difference over a time step. In line 460, the temperatures at the end of the time step are printed, and in line 470, the new temperatures are put into T(I) to form the initial conditions for the next time step. Line 490 causes the computer to loop back and start a new time step.

The first node (Z(1)) is at the soil surface (Z = 0). Since temperature changes rapidly near the surface and very little at depth, the best simulation will be obtained with short elements near the soil surface and longer ones deeper in the soil. The element lengths should go in a geometric progression. Ten to twelve nodes are probably sufficient for short term simulations (daily or weekly). Fifteen nodes would probably be sufficient for annual cycle simulation where a deeper grid is needed.

4.7 CYLINDRICAL HEAT FLOW: MEASUREMENT OF THERMAL CONDUCTIVITY

Program 4.1 can be modified for cylindrical heat flow and used to determine thermal conductivity of soil (Riha et al. 1980). The elements and node arrangement for solving the cylindrical heat flow problem are shown in Fig. 4.3.
Arguments similar to those for cylindrical oxygen diffusion are used to find the element conductances. Following the derivation of eq. 3.7,

\[ K(I) = \frac{2\pi \lambda}{\ln[R(I+1)/R(I)]} \quad (4.29) \]

Heat storage for node I will be in half the volume contained between the two adjacent nodes. Therefore

\[ CP(I) = 2\pi \rho C_p \left[ Z(I+1)^2 - Z(I-1)^2 \right]/2\Delta t. \quad (4.30) \]

The thermal conductivity measurement is made by heating or cooling an aluminum or glass rod, and at \( t = 0 \), thrusting the rod into the soil. The temperature of the rod is monitored as it cools or heats. The numerical solution for probe temperature, using an estimated thermal conductivity, is compared to the data, and model thermal conductivity is adjusted until the numerical solution agrees with the data.

The boundary conditions for this experiment are: no flow at the center of the cylinder, and constant temperature several centimeters from the probe surface. Since the thermal conductivity of the aluminum probe is much higher than that of the soil, we can assume that it remains isothermal. Node 1 can therefore be put at the probe surface, with \( K(0) = 0 \), and \( CP(1) \) equal to the sum of half the capacity of element 1 (soil) plus the entire capacity of element zero (aluminum). The probe used by Riha et al. (1980) was made from 6.35 mm diameter aluminum rod with a 0.7 mm diameter hole drilled axially for the thermocouple. The volumetric specific heat of aluminum is \( 2.43 \times 10^6 \) J m\(^{-3}\) K\(^{-1}\). The BASIC program for solving this heat flow problem (Program 4.2) shows appropriate element lengths and necessary input information.

A modification of this program can be used to determine thermal conductivity in another way. Parikh et al. (1979) suggested filling an aluminum tube with soil, placing it in a constant temperature water bath at \( t = 0 \), and monitoring its center temperature over time. They use an analytical solution to approximate the \( T \) behavior, but a numerical solution with a program similar to Program 4.2 is easier to use and gives better results because it does not require the approximations needed for the analytical solution.
PROGRAM 4.2 BASIC PROGRAM FOR COMPUTING TEMPERATURE OF A HEATED ALUMINUM ROD THRUST INTO SOIL AT TIME = 0

M=20
DIM W(M+1),T(M+1),TN(M+1),K(M+1),Z(M+1),A(M+1),B(M),G(M),D(M),Z(M+1)

INPUT "ESTIMATED THERMAL CONDUCTIVITY (W/(M K))";K
INPUT "SOIL BULK DENSITY (MG/M^3)";BD
INPUT "WATER CONTENT (M^3/M^3)";W
INPUT "SOIL TEMPERATURE (C)";TS
INPUT "INITIAL PROBE TEMPERATURE (C)";TP
INPUT "TIME STEP (S)";D
INPUT "LENGTH OF SIMULATION (S)";SL

Z(0)=0.00635:Z(1)=Z(0) 'PROBE RADIUS -M

FOR I=1 TO M
   Z(I+1)=Z(I)*1.1
   T(I)=TS
   NEXT

K(0)=0:F=.6:G=1-F:DT=D1/15
FOR I=1 TO M
   CP(I)=(2400000*BD/2.65+4180000*WV)*(Z(I+1)+2-Z(I-1)+2)/(2*DT)
   K(I)=2*K/LOG(Z(I+1)/Z(I))
   NEXT

CP(1)=CP(1)+2430000*Z(I+1)/DT 'ADD PROBE HEAT CAPACITY AT NODE 1
TT=TT+DT:DT=DT*2:IF DT>D1 THEN DT=D1
FOR I=1 TO M
   C(I)=K(I)*F : A(I+1)=C(I)
   B(I)=F*(K(I)+K(I-1))+CP(I)
   D(I)=G*K(I-1)*T(I-1)+(CP(I)-G*(K(I)+K(I-1)))*T(I)+G*K(I)*T(I+1)
   NEXT

D(M)=D(M)*K(M)*F*TN(M+1)
FOR I=1 TO M-1
   C(I)=C(I)/B(I)
   D(I)=D(I)/B(I)
   B(I+1)=B(I+1)-A(I+1)*C(I)
   B(I+1)=D(I+1)-A(I+1)*D(I)
   NEXT

TN(M)=D(M)/B(M)
FOR I = M-1 TO 1 STEP -1
   TN(I)=D(I)-C(I)*TN(I+1)
   NEXT

PRINT "TIME=";TT,"PROBE TEMP=";TN(1),"SOIL TEMP=";TN(M+1)
FOR I=1 TO M
   PRINT Z(I),TN(I),K(I)
   T(I)=TN(I)
   NEXT

IF TT<SL THEN GOTO 250
4.8 REFERENCES


4.9 PROBLEMS

4.1 Set up the numerical solution for heat flow (Program 4.1) with uniform thermal conductivity and a sine-function surface boundary condition, so that it should give results identical to the analytical solution (eq. 4.5) and then compare predictions from the numerical solution with those from the analytical solution to determine a) the error resulting from using finite depth increments, b) the error resulting from the use of finite time increments, and c) the effect of $\eta$ on error (compare time centered, forward difference and backward difference). Remember that the analytical solution requires a semi-infinite soil column, so use a column that is several damping depths long. Also remember that the initial conditions you choose for the numerical solution will have an effect for several cycles after you start the solution, so either allow plenty of time for these effects to damp out, or set up your initial conditions using the analytical solution.

4.2 Use program 4.1 to predict soil temperature as a function of time and depth. What effect would a surface residue mulch have on soil temperature? At what depth are temperature changes 180 degrees out of phase with the surface?

4.3 How should Program 4.1 be modified to account for changes in water content with depth? Make the changes and simulate temperature in a soil with a 10 cm deep, dry dust mulch.
Chapter 5

WATER POTENTIAL

Water potential plays a role in water flow theory similar to the role played by temperature in heat flow problems, or voltage in electrical circuit theory. Water flows in response to gradients in water potential. Darcy's law states that

\[ f_w = -k \frac{d\psi}{dx} \]

(5.1)

where \( f_w \) is the water flux density (kg m\(^{-2}\) s\(^{-1}\)), \( d\psi/dx \) is the water potential gradient that drives the flow, and \( k \) is the hydraulic conductivity. When water potential is uniform across a boundary, no water will flow, even though water content may be different on the two sides of the boundary.

The water potential is the potential energy per unit mass (or volume) of water in a system, compared to that of pure, free water. If potential energy per unit mass is used, the units of potential are Joules/kg. Potential energy per unit volume has units of Joules m\(^{-3}\), but this is dimensionally equivalent to Newtons m\(^{-2}\), or Pascal, which is a pressure unit. Since there are about 1000 kg of water in a m\(^3\), 1 J/kg = 1 kPa. The pressure unit, Bar, has been used for water potential. A bar is equal to 10\(^5\) Pa, so 1 bar = 100 J/kg or 100 kPa.

There are two advantages to using units of J/kg. The first is that these units are consistent with SI usage. The second is that the reference for mass basis water potential, the kilogram of water, does not change with temperature or pressure. The volume does change slightly with temperature and pressure.

The total potential is the sum of several component potentials:

\[ \psi = \psi_m + \psi_o + \psi_p + \psi_a + \psi_n + \psi_g \]

(5.2)

where the subscripts refer to matric (m), osmotic (o), hydrostatic pressure (p), pneumatic pressure (a), overburden pressure (n), and gravitational (g) potentials. Usually, only one or two of the component potentials needs to be considered in any given flow problem, but gradients in any of these potentials can result in water flow when conditions are right.

5.1 MATRIC POTENTIAL

The matric potential is one of the most important components of the water potential in soil and plant systems. It is defined as the amount of work, per unit mass of water, required to transport an infinitesimal quantity of soil
solution from the soil matrix to a reference pool of the same soil solution at
the same elevation, pressure and temperature. The reduction in potential
energy of water in porous materials is primarily the result of physical forces
which bind the water to the porous matrix. The water potential under a curved
air-water interface, such as might exist in a capillary tube or a soil pore,
is given by the capillary rise equation

\[ \psi_m = -2\sigma/r \rho_w \quad (5.3) \]

where \( r \) is the radius of curvature of the interface, \( \sigma \) is the surface tension
\( (7.27 \times 10^{-2} \text{ J m}^{-2} \text{ at } 20^\circ\text{C}) \), and \( \rho_w \) is the density of water. Equation 5.3
is often used to find the equivalent radius of the largest water-filled pore
in a soil at a given matric potential. For example, in a soil at \( \psi_m = -100 \text{ J/kg} \) we would expect pores with radii larger than
\( r = -2 \times 7.27 \times 10^{-2}/10^3 \times (-100) = 1.45 \mu\text{m} \) to be air filled.

At some water potential, perhaps in the range \( -10^4 < \psi_m < -10^3 \text{ J/kg} \),
the capillary analogy breaks down because most of the water is absorbed in
layers on particle surfaces rather than being held in pores between particles.

The matric component of water potential is important as a driving force
for flow in unsaturated soil and in the cell walls of root cortex and leaf
mesophyll tissue. Matric potential is always negative or zero.

5.2 OSMOTIC POTENTIAL

The osmotic potential is equivalent to the work required to transport
water reversibly and isothermally from a solution to a reference pool of pure
water at the same elevation. In practical terms, it is the energy one must
add to a solution to equilibrate the solution with pure water across a perfect
semipermeable membrane.

If the concentration of solute in a solution is known, the osmotic
potential can be calculated from

\[ \psi_o = -vc\chi R\theta \quad (5.4) \]

where \( v \) is the number of particles in solution per molecule of solute \( (v = 1 \)
for non-ionizing solutes; \( v = \) number of ions per molecule for ionizing
solute), \( c \) is the concentration (moles/kg), \( \chi \) is an osmotic coefficient, \( R \) is
the gas constant \( (8.3143 \text{ J mole}^{-1} \text{ K}^{-1}) \), and \( \theta \) is the kelvin temperature.
The osmotic coefficient is a function of solution concentration and solute
species. Osmotic coefficients for common solutes are given by Robinson and
Stokes (1965, p 483). If mixtures of solutes are present, the total osmotic
potential is the sum of the contributions from the components. In other
words, the interaction between species apparently is small.

When detailed data on the chemical composition of the soil solution are not available, the osmotic potential can still be estimated if the electrical conductivity is known (Richards, 1954). A rule of thumb for typical soils is

\[ \psi_{os} (J/kg) = -36 \times EC_s \]  

(5.5)

where \( \psi_{os} \) is the osmotic potential of the saturation extract, and \( EC_s \) is the electrical conductivity (dS/m) of the saturation extract. As soil dries, the solutes often remain, so, neglecting changes in \( \chi \) with \( c \), anion exclusion effects, and precipitation of sparingly soluble salts, we can write

\[ \psi_0 = \psi_{os} \theta_s / \theta \]  

(5.6)

where \( \theta_s \) is the saturation water content. These are only rough approximations but are adequate for many purposes if used with care.

The osmotic potential is an important component of water potential in plant cells, and affects water uptake by plants. Osmotic potential gradients in soil are usually unimportant as driving forces for flow because the salts move with the water. Osmotic potential is always negative or zero.

5.3 PRESSURE AND PNEUMATIC POTENTIAL

The pressure and pneumatic components of the water potential describe the effect, on water, of changing the hydrostatic or pneumatic pressure applied to the water. The relationship between potential and pressure is

\[ \psi_p \text{ or } \psi_a = P / \rho_w \]  

(5.7)

where \( P \) is pressure in Pa. Pressure can be either higher or lower than the reference pressure, so \( \psi_p \) and \( \psi_a \) can be either positive or negative. The pressure potential is an important component of the water potential below a water table, in plant cells, and in tensiometers which are used for measuring matric potential. The pneumatic component is used to describe the status of water under various laboratory conditions when pressure or suction is applied to equilibrate an external phase with soil or plant water. The suction plate, pressure plate, and pressure bomb are examples of equipment which use this principle.

5.4 OVERBURDEN POTENTIAL

The overburden potential is similar to the pressure potential, in that it is the increase in potential of water in a porous system which results from
the application of pressure to the water in the system. The difference is that, with the pressure potential, the pressure is applied directly to the water. This can only occur if the system is saturated. With the overburden potential, the pressure is applied to the water by the matrix. When mechanical pressure is applied to the matrix, some of the pressure is borne by the solid structure of the matrix itself, but part of it may be transferred to the water in the matrix. The overburden potential is a function of the pressure applied to the matrix and the fraction of the load that is transmitted to the water in the matrix. If the matrix has no resistance to deformation, then $\psi_0 = P/\alpha_w$. The overburden potential can be present in an unsaturated porous medium. It is mainly important in soil at depth, where the pressure of the overburden can be substantial. It is relatively unimportant in sand, but can be an appreciable fraction of the overburden pressure in wet clay.

5.5 GRAVITATIONAL POTENTIAL

The gravitational component of the water potential is fundamentally different to any of the other components since it is the result of "body forces" applied to the water as a consequence of the water being in a gravitational field. The gravitational potential is calculated from

$$\psi_g = -gz$$  \hspace{1cm} (5.8)

where $g$ is the gravitational acceleration ($9.8 \text{ m s}^{-2}$) and $z$ is depth from a reference level where $\psi_g$ is taken as zero. The reference level is usually taken as the soil surface, or the surface of a water table. In flow problems, we are interested in the gradient of the gravitational potential, which is $d\psi_g/dz = -g$, a constant.

5.6 WATER POTENTIAL--WATER CONTENT RELATIONS

Two components of the soil water potential depend on water content: the matric and the osmotic. In plant cells, a third potential, the turgor pressure, depends on water content. We have already shown how osmotic potential changes with water content when the solute content of the system stays constant (eq. 5.6). The relationship between matric potential and water content is called a soil moisture characteristic or moisture release curve. Figure 5.1 shows typical moisture release curves for sand, silt loam, and clay soils. For $\psi<\psi_e$, these curves are described by the function

$$\psi_m = \psi_e (\Theta/\Theta_s)^{-b}$$ \hspace{1cm} (5.9)
where $\psi_e$ is the air entry water potential (potential at which the largest water filled pores just drain), and $b$ is the slope of $\ln \psi$ vs $\ln \theta$. The values for $\psi_e$ and $b$ are usually found by plotting moisture release data on a log-log scale and fitting a straight line to the data. The slope and intercept of the best-fit line are used to find $\psi_e$ and $b$.

Fig. 5.1. Typical soil moisture characteristics for sand, silt loam, and clay soils. The inset shows the water potential close to saturation and the air entry potential.
5.7 PREDICTING MOISTURE CHARACTERISTICS FROM TEXTURE

A number of attempts have been made to predict moisture release functions from soil texture data (Hall et al. 1977; Gupta and Larsen, 1979; Bache et al. 1981). These attempts have not been completely successful. One usually finds that, even though the correlations fit the data with which they were developed quite well, they give relatively poor fits to data from other studies. In the examples just cited, the correlations differ markedly between studies.

There are several reasons for the failure of these correlations. The first is that pore size distribution, and not particle size distribution, determines moisture retention. The two are related but particle packing, shape, orientation, etc. are important as well. A second problem is that the moisture release data themselves may not be reliable. Most of the data used in the correlations are from pressure plates. Pressure plate equilibration is usually far from complete, even when outflow has apparently stopped, because of the low hydraulic conductivity of soil at low water potential. Finally, these correlations suffer from the failure of sand, silt, and clay fractions, by themselves, to provide a rational basis for correlation. The new textural analysis in section 2.4 of chapter 2 provides an improved basis for these correlations.

In spite of the difficulties encountered in producing moisture release functions from texture data, the benefits, especially for simulation models, of being able to produce one from the other justify additional effort in this area. The relationship we produce here will be based on eq. 5.9 and the ideas in Chapter 2.

We expect \( \psi_e \) to decrease (become more negative) as the mean pore diameter becomes smaller, and \( b \) to increase as the standard deviation of pore size increases (note that when \( b = 0 \), all of the water is held at a single potential, and when \( b \) approaches infinity, no change in water content occurs when \( \psi_m \) changes). We expect pore size and particle size to be correlated, so as geometric particle diameter \( (d_g) \) (eq. 2.16) increases, \( \psi_e \) should become less negative. As geometric standard deviation \( (\sigma_g) \) (eq. 2.16) increases, \( b \) should increase. By fitting eq. 5.9 to data by Hall et al. (1977) and Bache et al. (1981), we can deduce the following approximate relationships for soils at bulk density of 1.3 Mg m\(^{-3}\).

\[
\psi_{es} = -0.5 \ d_g^{-1/2}
\]  
(5.10)

\[
b = -2 \ \psi_{es} + 0.2 \ \sigma_g
\]  
(5.11)

where \( d_g \) is in mm (from Eq. 2.15 or Fig. 2.1) and \( \psi_{es} \) is in J/kg. The subscript \( es \) on the air entry potential is to indicate that it is for a
standard bulk density of 1.3 Mg m$^{-3}$. From Fig 2.1, we see that the expected range of $d_g$ is 0.003 to 0.7 mm, while the range of $c_g$ is 1 to 30. These values would give values of $J_{le}$ ranging from -9 J/kg to -0.6 J/kg and values of $b$ ranging from $b=24$ (at $d_g=0.003$ mm, $c_g=10$) to $b=2$ (at $d_g=0.7$ mm, $c_g=4$). More extreme values are possible, but not likely in typical soils.

5.8 EFFECT OF BULK DENSITY ON MOISTURE CHARACTERISTICS

In order to predict the effects of tillage or compaction on hydraulic properties, and to take account of density effects on moisture retention, we need to specify the effect of bulk density ($\rho_b$) on the parameters in eq. 5.9. The effect of $\rho_b$ on $\theta_s$ is already known from eq. 2.9. If this density dependence is substituted into eq. 5.9, without changing $J_{le}$ or $b$, the effect of bulk density on water content at a given potential is much larger than that found by Hall et al. (1977) or Gupta and Larsen (1979). It is in the correct direction however with increased bulk density decreasing water content at a given potential. An empirical correction which gives good agreement with the data of Hall et al (1977) is

$$
\psi_e = \psi_{es}(\rho_b/1.3)^{0.67b}
$$

(5.12)

where $\psi_{es}$ is the value from eq. 5.10, $b$ is from eq. 5.11, and $\rho_b$ is in Mg m$^{-3}$. A small correction could also be made to $b$. Both the Gupta and Larsen (1979) and the Hall et al. (1977) data show a decreasing effect of bulk density on moisture retention with decreasing potential. This would argue in favor of slightly increasing $b$ with bulk density, but the effect is small and the data are not reliable enough to warrant deriving such a correction now. We will therefore use eq. 5.11 for $b$. It is interesting to note that eq. 5.12 predicts an increase (less negative) in air entry potential when bulk density decreases in accordance with expectation.

5.9 MIXTURES OF MATERIALS

The moisture characteristics discussed so far are representative of well graded materials having a simple, unimodal pore size distribution function. More complex materials can be thought of as mixtures of materials with these simple characteristics. The moisture characteristic of a mixture of porous materials is

$$
\theta = \Sigma \theta_i \phi_i = \Sigma \phi_i a_i \psi^{-1/b_i}
$$

(5.13)

where $\phi_i$ is the volume fraction for component $i$, and $a_i$ and $b_i$ are constants for the moisture characteristic of component $i$. 
An example of an application of eq. 5.13 is its use to predict the effect of added straw on the moisture characteristic of soil-straw mixtures. Myrold et al. (1981) measured moisture characteristics of wheat straw, and found that they could be fit reasonably well by a power function. They then used eq. 5.13 to determine the effect of added straw on water potential at constant water content. They were able to show that even small additions of straw can cause substantial reductions in water potential.

5.10 SOIL MOISTURE HYSTERSIS

The relationship between water potential and water content is not unique. It depends on the wetting and drying history of the porous material. The curves in Fig. 5.1 represent the relationship one might obtain by drying saturated soil to the water content shown on the diagram. A different relationship would have been obtained if the soil had been wet from air dryness to the indicated water content. A still different relationship would have been obtained if the soil had been wet, say to -20 J/kg, then dried to -40 J/kg. When the soil wets from air dryness, or dries from saturation, the characteristics are called primary wetting or drying curves. The wetting curve always has a lower water content for a given potential than does the drying curve. The characteristics that result from drying a partially wet soil or wetting a partially dry soil are called scanning curves. They lie between the primary wetting and drying loops. An explicit analytical treatment of hysteresis has been worked out (Mualem and Miller, 1979), and hysteresis is sometimes included in water flow models (Gillham et al., 1979) but we will not attempt to include hysteresis in our models.

5.11 LIQUID- AND VAPOR-PHASE EQUILIBRIUM

When liquid water is in equilibrium with water in the vapor phase, the water potentials in the two phases are equal. The water potential in the vapor phase can be found by computing the work that would be required to create a unit volume of vapor (Campbell, 1977). The relationship so obtained between water potential and vapor pressure is

\[ \psi = R\theta/M_w \ln(p/p_o) \]  

(5.14)

where \( M_w \) is the molecular weight of water (0.018 kg/mole), \( p \) is vapor pressure (Pa), and \( p_o \) is the vapor pressure at saturation. The ratio, \( p/p_o \), is the relative humidity, \( h_r \). For humidities above about 0.95, eq. 5.14 can be approximated by the first two terms of the ln series. At \( \theta = 293 \text{ K (20°C)} \):

\[ \psi \approx 1.37 \times 10^5(h_r - 1) \]  

(5.15)
so a 1% reduction in relative humidity reduces water potential by 1370 J/kg. Obviously, humidities in moist soil (soil wetter than about -2000 J/kg) are always near 1.0.

The relationship between humidity and water potential is useful in describing vapor phase water in soils, and in providing a means for measuring water potential.

5.12 REFERENCES


5.13 PROBLEMS

5.1 Show that the vertical gradient of the total water potential below a water table is zero.

5.2 Make a table of air entry potentials and b values consisting of entries for representative members of each soil textural class. Use Fig. 2.1 or the program you developed in Problem 2.3 to get $d_g$ and $b_g$.
Chapter 6

HYDRAULIC CONDUCTIVITY AND WATER TRANSPORT EQUATIONS

In the last chapter, gradients in potential were shown to be the driving forces for water flow in porous materials. An analogy between water potential and temperature or voltage was used to illustrate the importance of water potential in the solution of water flow problems. Continuing the analogy, conductivity as well as temperature gradient must be known if a heat flux is to be computed. In water flow problems, both the water potential gradient and the hydraulic conductivity must be known to compute the water flux.

Even though potential and temperature play similar roles in these flow problems, potential is the more difficult to measure and understand. There are several component potentials in most systems, and the total driving force is some combination of these component potentials. Thermal conductivity and hydraulic conductivity also play similar roles in flow problems, but hydraulic conductivity is much more difficult to measure and characterize than thermal conductivity. The thermal conductivity of a material is generally assumed to depend only on the properties of the material. Any temperature dependence is usually small, and can be ignored in solutions to the heat flow equations. The hydraulic conductivity also depends on material properties, but often depends on the water potential as well. This adds complexity to the mathematics. The differential equations describing the behavior of the system become non-linear, and are more difficult to solve than the ones used previously for heat flow. However, one sometimes finds that the behavior of a system is easier to predict with potential-dependent conductivity than otherwise. In this chapter, the equations describing water transport will be presented, and ways of predicting hydraulic conductivity will be discussed.

6.1 FORCES ON WATER IN POROUS MATERIALS

Before considering the flow equation, it would be helpful to consider the forces that cause water to flow in soil and the forces that retard water flow. The units used to measure water potential are Joules per kilogram. A potential gradient therefore has units of Newtons per kilogram, or force per unit mass of water. A potential gradient can therefore be thought of as an actual force acting on the water in a porous system.

In steady flow, this force from the water potential gradient is balanced by a retarding force. Reynolds numbers for water flow in porous materials are less than $10^{-3}$, indicating that inertial forces are much smaller than viscous
forces. The retarding force on the water is therefore viscous drag. The energy in the flowing water is dissipated as heat from friction in the soil.

If we can assume that water in porous material behaves as a Newtonian fluid (viscosity independent of rate of shear) then the flux of water through a porous material can be shown to be directly proportional to the potential gradient (Baveye and Sposito, 1984). This relationship was experimentally derived by Darcy, and is known as Darcy's Law:

\[ f_w = -k \frac{d\psi}{dx} \]  \hspace{1cm} (6.1)

### 6.2 WATER FLOW IN SATURATED SOIL

When water flows in saturated soil, the driving force results from gradients in pressure, gravitational or overburden potentials. In this book, the potential which exists when the soil is saturated and the pore water pressure is negative is termed a matric potential. Thus, a matric potential can be a driving force in saturated soil. Matric potential is always negative or zero.

The hydraulic conductivity of saturated soil depends on the size and distribution of pores in the soil, and therefore on bulk density and soil texture. It is generally assumed to remain constant for a given material and location, though clogging of pores by clay migration can alter hydraulic conductivity markedly in saturated flow experiments.

If \( f_w \) and \( k \) are constant in eq. 6.1, then the variables can be separated and an integration performed to obtain

\[ f_w = -k_s \frac{A\psi}{Ax} \]  \hspace{1cm} (6.2)

Using eq.6.2 the flux density of water in saturated soil can be found if the saturated hydraulic conductivity and the potential difference across a soil column of length \( Ax \) are known. Alternatively, if the flux density of water, the pressure drop across a soil column and the length of the column are known, \( k_s \) can be determined.

### 6.3 MODELS FOR SATURATED HYDRAULIC CONDUCTIVITY

A number of equations have been derived for predicting saturated hydraulic conductivity from pore size distribution (Scheidegger, 1960). One begins with the Hagen-Poiseuille equation which describes the flux of water in a single capillary. Capillaries are interconnected in various ways to represent soil pores. A tortuosity correction is often applied to account for the increased path which must be covered by water moving through the porous material, and the equation is integrated over all pore sizes present in the
soil. The result of one such model is (Scheidegger, 1960)

\[ k_s = \phi w r^2 / v T^2 \]  \hspace{1cm} (6.3)

where \( \phi \) is the total porosity, \( T \) is a tortuosity factor, \( r \) is a "mean hydraulic radius" representative of the pore size distribution of the porous material, and \( v \) is the viscosity.

A different approach was used by Childs and Collis-George (1950) and Marshall (1958). Since this approach is useful for finding unsaturated as well as saturated conductivity, it will be examined in detail.

The Hagen-Poiseuille equation for flux density of a fluid in a tube of radius, \( r \) and length, \( Ax \) is

\[ f_w = (\rho_w r^2 / 8 v)(\Delta P / \Delta x) \]  \hspace{1cm} (6.4)

where \( v \) is viscosity (m²/s).

The hydraulic conductivity of the tube is \( r^2 / 8 v \). If the soil is seen as a large number of capillary tubes of varying sizes, then the flux density in soil is the flux density for each capillary size present in the soil multiplied by the area of that size capillary per unit cross section area of soil. Contributions from each pore class are summed to get the total flux. Since pores are not continuous, some provision must be made for the way pores can fit together. The Childs and Collis-George model assumes that only pores in a direct sequence contribute to flux, and that flux is always controlled by the smaller of two pores in a sequence.

If a soil column were broken at some arbitrary point, the exposed face could be examined to determine the area of pores having radii between \( r \) and \( r + dr \). This area can be expressed as

\[ dA/A = F(r) dr \]  \hspace{1cm} (6.5)

where \( F(r) \) is a pore size distribution function defined such that the total porosity of the soil is

\[ \phi = \int_0^{r_e} F(r) dr \]  \hspace{1cm} (6.6)

The limits of integration are zero and \( r_e \), the radius of the largest water-filled pore.

\( dA/A \) represents the probability of finding a pore of a given size on one soil face. The probability of finding a continuous pore from one face to the
other is the product of the probabilities of finding a given sized pore on either face. The contribution to conductivity for pores of radius \( r \) to \( r+dr \) is therefore

\[
(p_w r^2/8v)(dA/A)^2 = (p_w r^2/8v)F(r)dr F(r)dr.
\]

The hydraulic conductivity is the integral over all pore classes or

\[
k = \frac{p_w}{8v} \int_0^r \int_0^r r^2 F(r)dr F(r)dr
\]  

(6.7)

The pore size distribution function can be inferred from a moisture retention function if the pores are assumed to be cylindrical so that the capillary rise equation (eq 5.3) gives an estimate of the largest water-filled pore at any given matric potential. Combining eqs 5.3 and 5.9

\[
r = -(2\sigma/p_w \psi_e)(\theta/\theta_s)^b
\]  

(6.8)

Since the pores are assumed to be cylindrical, \( F(r)dr = d\theta \), the change in water content associated with draining all pores between radius \( r \) and \( r+dr \). Substituting for \( r^2 \) and \( F(r)dr \) in Eq. 6.7 and integrating gives

\[
k = \frac{\sigma^2 \theta_s^2}{2p_w \psi_e^2 (2b+1)(2b+2)} (\theta/\theta_s)^{2b+2}
\]  

(6.9)

The saturated conductivity is the value from eq. 6.9 when \( \theta = \theta_s \). Equation 6.9 says that the saturated hydraulic conductivity of a soil is determined by three soil properties: \( \theta_s \), \( \psi_e \), and \( b \). Of these, \( \psi_e \) is the most important. For soils with similar \( \theta_s \) and \( b \) values,

\[
k_s \psi_e^2 = \text{Constant}.
\]  

(6.10)

This important result is the basis for scaling in studies of variability in hydraulic properties of soils (Warrick et al., 1977; Russo and Bresler, 1980). It says that, at a given water content (again, assuming constant \( \theta_s \) and \( b \)) variation in \( \psi_m \) is directly related to variation in \( \psi_e \), and variation in \( k \) is inversely related to \( \psi_e^2 \). The scaling parameter used by Warrick et al. (1977) and Russo and Bresler (1980) is derived from a "characteristic microscopic length" for the soil (Miller, 1980). The characteristic length for a soil can be taken as the radius of the largest pores and is calculated
from the air entry potential using the capillary rise equation. It is apparent that for water flow and retention calculations \( \psi_e \) is an important soil parameter.

6.4 CALCULATING SATURATED CONDUCTIVITY FROM SOIL TEXTURE DATA

The relationships between moisture retention and soil texture in Chapter 5 and the result obtained in eq. 6.10 suggest that saturated conductivity might be related to soil texture. Engineers frequently use soil texture to estimate saturated conductivity for design purposes. Hydraulic Conductivities published by Israelsen and Hansen (1962) are given in Table 6.1 as examples.

Table 6.1. Typical saturated hydraulic conductivities for soils of various texture. Values are given in g s m\(^{-3}\). Multiply by 10\(^{-3}\) to get kg s m\(^{-3}\).

<table>
<thead>
<tr>
<th>Soil Texture</th>
<th>Silt fraction</th>
<th>Clay fraction</th>
<th>( k_s ) *</th>
<th>( k_s ) †</th>
<th>( k_s ) ‡</th>
</tr>
</thead>
<tbody>
<tr>
<td>sand</td>
<td>0.05</td>
<td>0.05</td>
<td>1.4(0.7-7)</td>
<td>1.3</td>
<td>2.6</td>
</tr>
<tr>
<td>loamy sand</td>
<td>0.10</td>
<td>0.07</td>
<td>1.0</td>
<td>1.9</td>
<td></td>
</tr>
<tr>
<td>sandy loam</td>
<td>0.25</td>
<td>0.10</td>
<td>0.7(0.4-2)</td>
<td>0.45</td>
<td>0.9</td>
</tr>
<tr>
<td>silt loam</td>
<td>0.65</td>
<td>0.15</td>
<td>0.07</td>
<td>0.14</td>
<td></td>
</tr>
<tr>
<td>loam</td>
<td>0.40</td>
<td>0.18</td>
<td>0.4(0.2-0.6)</td>
<td>0.17</td>
<td>0.29</td>
</tr>
<tr>
<td>sandy clay loam</td>
<td>0.13</td>
<td>0.27</td>
<td>0.36</td>
<td>0.42</td>
<td></td>
</tr>
<tr>
<td>silty clay loam</td>
<td>0.55</td>
<td>0.34</td>
<td>0.05</td>
<td>0.06</td>
<td></td>
</tr>
<tr>
<td>clay loam</td>
<td>0.35</td>
<td>0.34</td>
<td>0.2(0.1-0.4)</td>
<td>0.11</td>
<td>0.12</td>
</tr>
<tr>
<td>silty clay</td>
<td>0.47</td>
<td>0.47</td>
<td>0.07(0.01-0.1)</td>
<td>0.04</td>
<td>0.03</td>
</tr>
<tr>
<td>clay</td>
<td>0.20</td>
<td>0.60</td>
<td>0.1(0.04-0.3)</td>
<td>0.07</td>
<td>0.03</td>
</tr>
</tbody>
</table>

* From Israelsen and Hansen (1962). Numbers in parenthesis indicate range.
† Calculated using eq 6.11.
‡ Calculated using eq 6.12 with \( C = 4 \times 10^{-3} \) kg s m\(^{-3}\)

Bloemen (1980) related saturated hydraulic conductivity and air entry potential to properties of the particle size distribution function. Campbell and Campbell (1982) correlated the hydraulic conductivity data from Bloemen (1980) with silt plus clay content of the soil to obtain

\[
k_s = 2 \times 10^{-3} \exp[-4.26(m_s + m_c)]
\]  

(6.11)

where \( m_s \) and \( m_c \) are silt and clay mass fractions, and \( k_s \) is in kg s m\(^{-3}\). Saturated conductivity calculated using eq. 6.11 with representative values for silt and clay contents are also shown in Table 6.1.
While eq. 6.11 has a generally correct response to texture, the numbers in Table 6.1 suggest too great a sensitivity to the silt fraction. An equation which weighs clay more heavily than silt would give better results. It would also help to have an equation which correctly predicts changes in $k_s$ with bulk density. Combining eqs. 6.10, 5.10, 2.15, and 2.17, gives

$$k_s = C \exp(-6.9 m_c - 3.7 m_s) \quad (6.12)$$

with $C$, a constant, to be evaluated from data. Best fit to data from several sources appears to occur when $C = 4 \times 10^{-3} \text{ kg s m}^{-3}$, which corresponds to a value for the constant in eq. 6.10 of $1 \times 10^{-3} \text{ kg m s}^{-3}$. Values for $k_s$ calculated using eq. 6.12 are shown in the last column of Table 6.1. These are generally in good agreement with the other values, but do not show the exaggerated silt sensitivity of eq. 6.11.

Bulk density dependence of $k_s$ is introduced by substituting $\psi_e$ from eq. 5.12 into eq. 6.10 in place of $\psi_{es}$, which was used to obtain eq. 6.12. The resulting equation is

$$k_s = 4 \times 10^{-3} (1.3/\rho_p)^{1.3b} \exp(-6.9 m_c - 3.7 m_s) \quad (6.12a)$$

### 6.5 EFFECT OF SOIL STRUCTURE ON SATURATED HYDRAULIC CONDUCTIVITY

Implicit in all of the equations relating hydraulic conductivity to texture is an assumption that the solid matrix is more or less randomly dispersed in space. It should be obvious that equations like eq. 6.12 can never correctly predict the saturated hydraulic conductivity of a soil which contains large, interconnected cracks, worm holes, or root channels. These channels have large hydraulic radii, and, when full, conduct water much faster than a uniform soil.

McKeague et al. (1982) provide a scheme for estimating saturated hydraulic conductivity in the field, taking into account both soil texture and structure. There is general agreement between their values and those in Table 6.1, but their largest values are somewhat larger than the largest values in Table 6.1. Presumably these differences are due to structure.

### 6.6 TEMPERATURE DEPENDENCE OF HYDRAULIC CONDUCTIVITY

The effect of temperature on hydraulic conductivity can be determined directly from eq. 6.9. At least four terms have a temperature dependence: $\nu$, $\sigma$, $\rho_w$, and $\psi_e$. The temperature dependence of $\psi_e$ probably is similar to that of $\sigma$, and therefore cancels it, and the temperature dependence of $\rho_w$ is negligible compared to that of $\nu$. Therefore mainly due to the effect of temperature on $\nu$, which is given by (see
Chapter 3) \( \nu = \nu^0 \left( \Theta^0 / \Theta \right)^6 \), where \( \Theta \) is the kelvin temperature and the superscript \( ^0 \) indicates the reference value.

6.7 UNSATURATED HYDRAULIC CONDUCTIVITY

When the soil desaturates, the driving force for flow becomes the gradient in matric and gravitational potential. As the largest pores in the soil drain, the hydraulic conductivity is rapidly reduced. This leads to an apparent paradox where doubling the driving force for flow across a soil column by lowering the water potential on one end may actually decrease flow. This occurs because the hydraulic conductivity is reduced more than the driving force is increased.

Typical values of unsaturated hydraulic conductivity are shown as a function of water content in Fig. 6.1. Note that hydraulic conductivity ranges over many orders of magnitude between saturation and dryness. The dramatic reduction in unsaturated conductivity with water content results from the fact that, as water content is reduced, the largest pores empty first. According to the Hagen-Poiseuille law, small pores conduct water much less readily than large pores (eq. 6.4). In addition, the path for flow becomes much more tortuous as the soil desaturates. These factors have been successfully incorporated in models which give reasonable descriptions of unsaturated hydraulic conductivity as a function of water content (Brooks and Corey, 1966; Campbell, 1974).

![Fig. 6.1. Hydraulic conductivity as a function of water content for Botany sand and Guelph loam (from Campbell, 1974).](image-url)
Equation 6.9 is the result obtained by Campbell (1974), and can be rewritten as

\[ k = k_s (\theta/\theta_s)^m \]  

Equation 6.13 can be combined with eq. 5.9 to obtain

\[ k = k_s (\psi_e/\psi)^n \]  

where \( n = 2+3/b \).

Campbell (1974) suggested that a pore interaction term be included which makes \( m = 2b+3 \), rather than the \( 2b+2 \) shown in eq. 6.9. This result is identical to that of Brooks and Corey (1966) who used a derivation starting with eq. 6.3.

Equations 5.10 and 5.11 indicate that clays, because of their smaller mean particle diameter, have lower (more negative) air entry potentials and larger \( b \) values than coarse-textured soils. The hydraulic conductivity of a sand therefore decreases more rapidly with potential than does that of a clay (eq 6.14). In addition, the higher \( \psi_e \) causes \( k \) to start decreasing at a higher water potential in sand than in clay. Unsaturated hydraulic conductivity of fine-textured soils is therefore higher than that of coarse textured soils, even though coarse textured soils have much higher saturated conductivity. This explains the observation that water does not enter dry sand from wet, fine textured soil until the fine textured material is almost saturated.

6.8 WATER CONTENT AS A "DRIVING FORCE"

Water potential is difficult to measure, and measurements of water potential distributions in soil profiles are usually not made. On the other hand, water content is frequently measured, and data are much more readily available. It would therefore be useful to be able to describe water flow in soil in terms of water content gradients. Using the chain rule of calculus, eq. 6.1 can be rewritten as

\[ f_w = -k(\psi/d\theta)(d\theta/dx) \]  

The derivative, \( d\psi/d\theta \) is the reciprocal of the specific water capacity of the soil. The product, \( k \psi/d\theta \) is often combined and called a soil water diffusivity. Equation 6.15 therefore becomes

\[ f_w = -\rho_w D_w \theta/dx \]
where \( \rho_w \) is the density of water (kg m\(^{-3}\)) and is shown explicitly so that the diffusivity will have the familiar units of m\(^2\)/s.

Equation 6.16 appears to have made water content a "driving force" for water flow. It is important, however, to carefully examine the assumptions necessary for such a transformation. The most important assumption for this transformation is that \( \psi \) is a function of \( \theta \) (i.e. for each value of \( \theta \) there is only one possible value for \( \psi \)). We know that \( \psi_m \) and \( \psi_o \) are functions of \( \theta \), but other potentials are not. This transformation can therefore only apply when \( \psi_m \) or \( \psi_o \) is the driving force for flow. It will not work when pressure or gravitational components are present. Usually \( \psi_o \) is not important in moving water, so only situations where \( \psi_m \) alone is the driving force for flow will be considered. Also, the \( \psi(\theta) \) relationship is hysteretic, so the transformation would only apply when the soil is on a wetting or a drying cycle; it could not be applied for mixed wetting and drying. In addition, the \( \psi(\theta) \) relationship depends on the pore size distribution. This may vary with location within the soil. The transformation would therefore not be valid in describing water flow across boundaries from a material having one \( \psi(\theta) \) relationship to a material having a different \( \psi(\theta) \) curve. With these limitations, the transformation is not likely to be very useful in solving soil physics problems.

6.9 TRANSIENT EQUATIONS

So far only steady flow of water has been considered. There are few situations in the field when steady flow obtains. The more common situation, where water potential or content varies with both space and time, is conceptually and mathematically much more difficult.

Using arguments similar to those in Chapter 4 for the energy balance of a thin layer of soil, a water balance can be set up:

\[
\begin{align*}
  f_z - f_{z+\Delta z} &= \rho_w \Delta z \frac{d\theta}{dt} \\
  \Delta z &= \text{the volume per unit area of the soil layer. Equation 6.17 shows that the difference between the amount of water that flows into a layer and the amount that flows out equals the amount that is stored there. A source term could be added if needed. When the thickness of the soil element, \( \Delta z \), approaches zero, eq. 6.17 becomes}
\end{align*}
\]

\[
\rho_w \frac{d\theta}{dt} = -\Delta f_w/\Delta z .
\]
Substituting from eq. 6.1,

\[ \rho_w \partial \theta / \partial t = \partial (k \partial \psi / \partial z) / \partial z \]  \hspace{2cm} (6.19)

Before solutions to eq. 6.19 can be considered, either \( \psi \) or \( \theta \) must be eliminated. If the only component of \( \psi \) is \( \psi_m \), and if it can be assumed that \( \psi_m \) is uniquely related to \( \theta \), then, using the chain rule,

\[ \partial \theta / \partial t = \partial (D_w \partial \theta / \partial z) / \partial z \]  \hspace{2cm} (6.20)

or

\[ \rho_w C \partial \psi_m / \partial t = \partial (k \partial \psi_m / \partial z) / \partial z \]  \hspace{2cm} (6.21)

where \( C = \partial \theta / \partial \psi_m \), the specific water capacity.

When both \( \psi_m \) and \( \psi_g \) are important components of the water potential, \( \partial \psi / \partial z \) becomes \( \partial \psi_m / \partial z + \partial \psi_g / \partial z = \partial \psi_m / \partial z - g \). Equation 6.21 then becomes

\[ \rho_w C \partial \psi_m / \partial t = \partial (k \partial \psi_m / \partial z - k/g) / \partial z \]  \hspace{2cm} (6.22)

Solutions to eq. 6.22 describe water potential (or content) in soil under most of the conditions of interest in the field. An additional sink term, to account for root uptake and thermally induced vapor flow, would be added to the right side of the equation when needed. Much of the remainder of the book will be concerned with the solution of eq. 6.22.
6.10 REFERENCES


6.11 PROBLEMS

1. Plot "typical" hydraulic conductivity for sand, silt loam, and clay soil as a function of water potential using data from Table 6.1, and eq. 6.14. Use a log-log scale, and plot both saturated and unsaturated conductivity. Use the graphs to determine the water potential at which water would flow from silt loam into sand in a layered profile with infiltration.

2. Write a computer program in BASIC to compute saturated hydraulic conductivity from bulk density, silt fraction, and clay fraction (use eq. 6.12a). Use your program to investigate the effect of tillage on hydraulic conductivity (assuming that tillage changes the bulk density).
Chapter 7

VARIATION IN SOIL PROPERTIES

In each of the Chapters so far, physical properties of soil have been discussed. In several instances, relationships were derived between measured properties and other variables. Implicit in all of this is the assumption that a particular measurement or estimate of a property contains information about the value of that property, or a related property in the entire system represented by that sample. On the other hand, experience shows that measurements on several "identical" samples never produce identical results. A single sample or estimate is therefore unlikely to contain complete information about the value of that property for other possible samples.

How much information then is or can be contained in a given observation or set of observations? The theory of stochastic processes provides a means of properly describing systems with uncertainty or variation. A stochastic description of a property, can be used to determine the information content of data relating to that property.

In this chapter, appropriate statistical descriptions of soil physical properties will be given, and models will be extended to include uncertainty in input variables.

7.1 FREQUENCY DISTRIBUTIONS

In the language of stochastic process theory, a given soil property is represented as a continuous real random variable. The random variable represents, for example, all possible values of bulk density or thermal conductivity in a plot, field, or other specified area. A description of the random variable is required, based generally on observations of a small fraction of all possible realisations.

A first step in analysing variability in a set of observations of a physical property is to divide the range of the data into equal intervals, determine the number of observations falling within each interval, and plot numbers as a function of values of the variate, as is Figure 7.1.

The height of a bar represents the frequency of occurrence of values within the specified range, and the plot of all such bars represents a frequency distribution for that soil property.

Figure 7.1 is a useful, but bulky summary of our knowledge about the random variable, bulk density of Pima clay loam. To be useful, the properties of the random variable must be further summarized. Two obvious properties of the frequency distribution are its position and its spread.
Fig. 7.1. Frequency distribution for 180 bulk density observations on Pima clay loam (Warrick and Nielsen, 1980) and a normal distribution function with mean of 1.45 Mg m$^{-3}$ and standard deviation of 0.16 Mg m$^{-3}$.

Several measures of position are possible. The most useful is the arithmetic mean. It is calculated from

$$<x> = \frac{1}{n} \sum_{i=1}^{n} x_i$$  \hspace{1cm} (7.1)

where the $x_i$ are members of a set of n observations of the soil property x. The brackets indicate the mean or expected value. Other measures of position are the median and the mode. The median value is the central value - the value having half the observations smaller and half larger than it. The mode is the value of x at which the frequency distribution is maximum. For symmetrical distributions, such as in Fig. 7.1, the median, mean and mode coincide. For skew distributions, the median or mode may represent typical values better than the mean. Our discussion will cover only distributions that either are symmetrical, or can me made so by transformation. Properties of skew distributions will therefore not be discussed.

The spread, or dispersion about the mean can also be described in several ways. The most useful is called the variance, and is calculated from

$$s^2 = \frac{1}{n} \sum_{i=1}^{n} (x_i - <x>)^2$$  \hspace{1cm} (7.2)

The standard deviation is $s$, the square root of the variance, and represents the root mean square (rms) deviation of the observations from the mean.
The sample mean, $\bar{x}$, and variance $s^2$ can be used to estimate the mean, $\mu$, and the variance, $\sigma^2$ of the random variable. It can be shown (Webster, 1977) that best unbiased estimates of the population mean and variance are given by $\mu = \bar{x}$ and $\sigma^2 = s^2n/(n-1)$. The population variance is likely to be larger than the sample variance because deviations of sample values from $\mu$ are likely to be larger than the deviations from $\bar{x}$. It is generally more useful to know the mean and variance of the population rather than that of the sample.

The mean and variance of a sample are often combined to form a coefficient of variation. It is

$$CV = \frac{s}{\bar{x}}$$

and is often multiplied by 100 and expressed as a percent rather than a fraction. This is a convenient way of expressing variation relative to the mean value. It is easily misused, however, especially when the mean is with respect to an arbitrarily chosen zero - as is the case with temperature scales.

Warrick and Nielsen (1980) give a useful table of CV's for several soil properties. Table 7.1 shows averages of a few of their entries.

Table 7.1 Coefficients of variation for some soil properties.

<table>
<thead>
<tr>
<th>Property</th>
<th>Mean</th>
<th>Std. Dev.</th>
<th>CV-%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk Density (Mg m$^{-3}$)</td>
<td>1.4</td>
<td>0.098</td>
<td>7.0</td>
</tr>
<tr>
<td>Saturation water content (m$^3$ m$^{-3}$)</td>
<td>0.44</td>
<td>0.047</td>
<td>10.7</td>
</tr>
<tr>
<td>Saturated Conductivity (g s m$^{-3}$)</td>
<td>0.23</td>
<td>0.25</td>
<td>110</td>
</tr>
</tbody>
</table>

7.2 PROBABILITY DENSITY FUNCTIONS

The frequency distributions for many soil properties approximate the shape of an ideal frequency distribution known as the normal or Gauss distribution. For this distribution, the probability of occurrence of the value $x$ is given by

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]$$

Figure 7.1 compares a measured frequency distribution with eq 7.4, which represents the distribution one might obtain for a large number of samples.

Equation 7.4 gives the probability density at $x$. It is normalized so that $\int_{-\infty}^{\infty} p(x)dx = 1$. The area under any part of the probability density function (PDF) is equal to the probability of finding a value of the random variable, $x$, in that range. It is useful to keep a few of these probabilities in mind. The area between $\mu-\sigma$ and $\mu+\sigma$ is 0.68; the area from $\mu-2\sigma$ to $\mu+2\sigma$ is
0.95; from \( \mu - 3\sigma \) to \( \mu + 3\sigma \) is 0.997. Thus, if the random variable representing a given soil property has a normal probability density function, a mean, \( \mu \), and a variance, \( \sigma^2 \), 68% of the values will lie within ±1 standard deviation of the mean and 95% within two standard deviations. This provides useful information for determining how much a given sample or group of samples can tell us about the mean of the population, or how many samples are needed to reduce uncertainty to a given value. The relationship between uncertainty of an estimate of the mean and uncertainty in the individual observations is

\[
\sigma^2_{\bar{x}} = \frac{\sigma^2}{n}
\]

(7.5)

where \( n \) is the number of samples. This equation can be used to determine the number of samples needed to estimated mean bulk density to within ±0.1 Mg m\(^{-3}\) with 95% certainty. First set \( 2\sigma_{\bar{x}} = 0.1 \) Mg m\(^{-3}\) = \( 2\sigma/\sqrt{n} \). From Table 7.1, \( \sigma = 0.098 \) Mg m\(^{-3}\), so \( n = 4\sigma^2/(0.1)^2 = 3.81 \); four samples should therefore be sufficient.

### 7.3 Transformations

If the frequency distribution for a soil property follows a normal PDF, its position and dispersion are easily and conveniently described by the arithmetic mean and the variance. Probabilities of occurrence for various values of the property are easily found. Some soil properties do not follow the normal PDF, however. Figure 7.2a shows the frequency distribution of soil matric potential measured at a particular depth and time in Oxford clay.

The distribution is obviously not symmetric. This shape of the distribution is typical of those obtained not only for matric potential, but also for hydraulic conductivity, air entry potential, particle size, solute concentration, and several other properties. Rather than try to rederive ideal PDF's for these properties, it is more convenient to transform them so that the transformed variable becomes normally distributed.

The most useful of the transformations for soil physical properties is the log transform. Fig. 7.2b shows the transformed matric potential data. The frequency distribution of the transformed data is symmetric with a mean of

\[
<\ln x> = \frac{1}{n} \sum \ln x_i
\]

(7.6)

and variance

\[
\sigma^2 = \frac{1}{(n-1)} \sum (\ln x_i - <\ln x>)^2
\]

(7.7)
Fig. 7.2. Frequency distribution of soil matric potentials measured at 38 cm depth in Oxford clay (a), (Webster, 1977) and the frequency distribution of the log transformed data (b).

The mean calculated in eq. 7.6 is the geometric mean, and can also be calculated from

\[
g = \left( \prod_{i=1}^{n} x_i \right)^{1/n}
\]  

(7.8)

where \( \prod \) is the product operator: \( x_1 \cdot x_2 \cdot x_3 \cdot \ldots \cdot x_n \) (Webster, 1977). The geometric mean, \( g = \exp(<\ln x>) \), is preferable to the arithmetic mean for representing log normally distributed data. This can be seen by considering a hypothetical set of hydraulic conductivity values: \{0.1, 0.1, 0.1, 0.1, 10\} (the last value was for a core with a worm hole in it). The arithmetic mean is 2. The log or geometric mean is 0.25, a number much more representative of the data set. The log normal distribution was used in Chapter 2 to describe particle size distribution functions.

The reciprocal transform also deserves mention. For this, the mean is

\[
<l/x> = (1/n) \sum 1/x_i
\]

(7.9)

The reciprocal of \( l/x \) is known as the harmonic mean.

Stomatal resistances of plant leaves have a skew distribution, but their reciprocals (conductances) are normally distributed. One would therefore want to do reciprocal transforms on stomatal resistance data to compute means or perform statistical tests.
7.4 SPATIAL CORRELATION

All of the derivations so far have assumed that individual observations were independent and uncorrelated. This is likely to be a poor assumption for soils data since samples taken in close proximity to each other are generally more similar than more widely spaced samples. Data can be tested for spatial correlation using one of three related functions: the autocovariance function, \( c \), the autocorrelation function, \( r \), or the semivariogram function, \( \gamma \). All are calculated from sets of measured values of the soil property, \( x \), with measurements separated in space. Measurements in a grid pattern are best for computing these functions, since such data allow us to determine whether the functions are direction dependent.

The autocovariance, for separation (or lag) \( k \) is calculated from

\[
c_k = \frac{1}{n-k-1} \sum_{i=1}^{n-k} (x_i - \langle x \rangle)(x_{i+k} - \langle x \rangle)
\]

(7.10)

For lag 0 (\( k=0 \)), \( c_0 = \sigma^2 \). The autocovariance function is the set of values of \( c_k \) produced for all possible values of \( k \).

The autocorrelation is the ratio of the autocovariance at lag \( k \) to the total variance or autocovariance at lag zero:

\[
r_k = \frac{c_k}{c_0} = \frac{c_k}{\sigma^2}
\]

(7.11)

The autocorrelation is related to the correlation coefficient used in linear regression analysis. A linear regression of \( x_i \) on \( x_{i+k} \) would produce an estimate of a slope and intercept, and a correlation coefficient. The square of the correlation coefficient gives the fraction of the total variation in \( x_i \) that can be explained by variation in \( x_{i+k} \). The autocorrelation for lag \( k \) gives this same information. The set of values for all possible \( k \)'s produces the autocovariance function.

The semivariance is calculated from

\[
\gamma_k = \frac{0.5}{n-k-1} \sum_{i=1}^{n-k} (x_i - x_{i+k})^2
\]

(7.12)

For a stationary random process (one for which the means and variances of all possible samples are equal)

\[
\gamma_k = c_0 - c_k
\]

(7.13)
The semivariance is zero at zero lag, and with increasing lag, approaches \( \sigma^2 \). Some measure of the distance over which to expect significant correlation would be useful. Russo and Bresler (1981) used the term "integral scale" to describe such a measure. This is a term taken from the atmospheric turbulence literature (Lumley and Panofsky, 1964), and is defined as

\[ J = \left( \int_0^\infty r_k \, dk \right)^{\frac{1}{2}} \quad (7.14) \]

Russo and Bresler fit empirical equations to \( r_k \) data to find values for the integral scale. The integral scales they found typically were about half the distance required for \( r_k \) to go to zero or for \( \gamma_k \) to reach its maximum value. They found integral scales for saturated water content to be 40 - 80 meters, with the integral scale for conductivity being about half that.

Program 7.1 is a computer program which calculates the autocovariance, autocorrelation, and semivariance for a set of data. The data (given in statements 200 - 260 of the program) are taken from Warrick and Nielsen (1980) and represent water content of samples at -10 J/kg water potential. Samples are from a Pima clay loam, 50 cm depth, and spaced 20 cm apart. The functions, as calculated by the program are shown in Fig. 7.3.

Note that the autocorrelation value at the first lag is only about half that at zero lag. Such an effect can be the result of experimental error and is an artifact in this analysis. Most soil physical properties should give an autocorrelation value of 1 for short lag. The data of Russo and Bresler go smoothly to 1 at zero lag.

The next step is to ask what it means if data are correlated. Russo and Bresler (1982) provide answers to this question, but at a level beyond that of this book. Their results, and those of other similar studies can be summarized in more qualitative terms. Two questions might be considered. One would be how correlation affects our knowledge of adjacent, unsampled values, and the other would be how correlation affects our knowledge of characteristics of the population. For uncorrelated data, the best estimate of a value at an unsampled point is the population mean. Samples from any location are equally valuable in estimating the population mean, and an estimate of the uncertainty in the mean is given by eq. 7.5. For correlated data, a measurement taken near the location of an unsampled point should better represent the value at that point than does the mean. This is the basis of the mapping method known as Kriging (Burgress and Webster, 1980) where unknown values of a property are computed as weighted averages of sampled values with weights being proportional to correlations. On the other hand, two points separated by less than 2 integral scales provide less
PROGRAM 7.1 PROGRAM FOR COMPUTING CORRELATION, COVARIANCE, AND SEMIVARIANCE OF A SET OF DATA

N=100:Q=N/2

FOR I=1 TO N
READ X(I)

S=S+X(I)

XB=S/N

NEXT

PRINT "MEAN =";XB

FOR K=0 TO Q

C(K)=C(K)+(X(I)-XB)*(X(I+K)-XB)

G(K)=G(K)+(X(I)-X(I+K))^2

NEXT

C(K)=C(K)/(N-K-1)

G(K)=.5tG(K)/(N-K-1)

R(K)=C(K)/C(0)

PRINT K,C(K),R(K),G(K)

DATA 37.5,37.6,37.7,39,35,36,36.8,36.5,37.1,36.6,37.9,38.8,40,40.6,37.6,38.7
DATA 37.9,42.1,35.9,38,38.5,38.3,37.4,37.1,41.8,37.2,35.4,39.1,35.3,34.9
DATA 35.5,35,35.7,35.1,34.1,34,34.7,34.2,35.2,31.7,30.7,32.7,33.7,35.3,32.6
DATA 33.5,31.4,30.9,31.4,35.5,34.2,32.5,30.5,28.9,33,30.9,31.7,32,30.9,42.8
DATA 31,34.3,31.2,29.1,31.7,32.9,32.1,32.8,32.2,34.4,32.2,32.2,32.4,33.3
DATA 34.3,31.8,36.9,33.9,35.2,36.4,34.7,38.9,35,35.6,36.9,35.3,36.4,33.7
DATA 34.2,30.9,34.3,33.2,35.3,35.6,35.1,33.4,34,33.6,36.6

information about population properties than do samples separated by more than two integral scales. Efficient sampling for population properties therefore requires that sample locations be separated by several integral scales.

7.5 APPROACHES TO STOCHASTIC MODELING

The models presented in previous chapters have been deterministic - for a given set of input values, the output is completely determined. In this chapter, descriptions of variability for the input values have been developed. We will now show how variability in input parameters relates to variability in model output. The PDF and its properties have been used to describe the soil characteristics which are model inputs. The next step is to
Fig. 7.3. Correlogram and semivariogram functions for the bulk density data in Program 7.1. Data are from Warrick and Nielsen (1980).
make the model produce a PDF of output values. Once the output PDF is known, the mean, variance and other statistical moments of that property can be found.

In the last section data were transformed using log and reciprocal functions, and we noted that these transforms produced new PDF's. Other models can be thought of as transforms of the PDF as well. A model changes input variables into output variables and input PDF's into output PDF's. A deterministic model can therefore become a stochastic model by treating input parameters and variables as stochastic processes.

The simplest transforms, from a stochastic model point of view, are linear transformations. For these, the output PDF has the same shape as the input PDF's. If the inputs are Gaussian random processes, then the output PDF will be Gaussian. For a Gaussian process, the PDF is described by the mean and variance. If y is a function of variables a, b, and c:

\[ y = f(a,b,c) \]

then the expected value of y is obtained from

\[ \langle y \rangle = f(\langle a \rangle, \langle b \rangle, \langle c \rangle) \]  \hspace{1cm} (7.16)

If a, b, and c are uncorrelated, then (Young, 1962):

\[ \sigma_y^2 = \left( \frac{\partial y}{\partial a} \right)^2 \sigma_a^2 + \left( \frac{\partial y}{\partial b} \right)^2 \sigma_b^2 + \left( \frac{\partial y}{\partial c} \right)^2 \sigma_c^2 \]  \hspace{1cm} (7.17)

As an example, consider the error in air filled porosity ($\phi_g$) which would result from measurement error in bulk density ($\rho_b$) and water content ($w$). Combining eqs 2.10 and 2.13

\[ \phi_g = 1 - \rho_b \left( \frac{1}{\rho_s} - \frac{w}{\rho_w} \right) \]  \hspace{1cm} (7.18)

Assume the $\rho_s$ and $\rho_w$ are accurately known. The expected value for $\phi_g$ is the value obtained by calculation from eq. 7.18 using mean values of $\rho_b$ and $w$. If errors in $\rho_b$ and $w$ are uncorrelated, then

\[ \sigma_{\phi_g}^2 = \left( \frac{\rho_b}{\rho_w} \right)^2 \sigma_{\phi_g}^2 - \left( \frac{1}{\rho_s} - \frac{w}{\rho_w} \right)^2 \sigma_{\rho_b}^2 \]  \hspace{1cm} (7.19)

This equation is evaluated using mean values of $\rho_b$ and $w$.

One serious pitfall of this approach is the assumption that the errors are uncorrelated. It is likely that $w$ and $\rho_b$ are calculated from the same set of measurements. If, for example, the measured soil mass were too low,
that would decrease the calculated bulk density and increase the calculated water content.

Non-linear transforms, such as those for moisture characteristics or hydraulic conductivity functions often produce log-transformed PDF's. Water content has a Gaussian PDF. Water potential and hydraulic conductivity have log-normal distributions. Equations 7.16 and 7.17 can still be used to calculate means and variances, but these values are more difficult to interpret than for linear transforms.

If the mean and variance of a Gaussian process are known for an input variable of a non-linear transform, the PDF of the output can be generated using a technique called Monte Carlo simulation. For this technique, input variables are drawn from populations having the specified mean and variance. These are transformed using the desired transform, and, with repeated application, a frequency distribution of the output is obtained. A PDF is then fit to the output. Program 7.2 generates a frequency distribution of hydraulic conductivity values using eq. 6.13 with m = 15, k_s = 1, and ð = 0.5. The water content is assumed to have a mean of 0.20 and a standard deviation of 0.05. Note that the equation in line 80 generates random values of water content that are normally distributed with mean and variance as specified.

Any of the simulation models we have derived or will derive can be used as a transform in just the same way we have used the simple ones just presented. More computer time is required, but the procedure is the same as that just outlined.

Because of the heavy computing requirements and the difficulty of visualizing the effects of variability in several input variables at once, it is sometimes useful to use scaled variables (Miller, 1980). The most useful in spatial variability studies of water and salt movement have been based on eq. 6.10. If we assume that spatial variability in air entry potential can be represented by

\[ \psi_{ei} = \langle \psi_e \rangle / a_i \]  

(7.20)

then, from eq. 6.10

\[ k_{si} = a_i^2 \langle k_s \rangle \]  

(7.21)

The scaling factor, a, represents variation in both hydraulic conductivity and water potential. Warrick and Nielsen suggest that a is log-normally distributed. If the geometric mean is unity, confidence limits can
'PROGRAM 7.2 MONTE CARLO SIMULATION OF HYDRAULIC CONDUCTIVITY

DIM F(100)
N=1000
MEAN=.2: STD=.05
KS=1: WS=.5: M=15
FOR I=1 TO N
R=0
FOR J=1 TO 12
R=R+RND(1)
NEXT
W=MEAN+STD*(R-6)
X=KS*(W/WS)+M
S=S+X
S2=S2+X*X
IK=INT(100000!*X): IF IK>100 THEN IK=100
F(IK)=F(IK)+1
NEXT
PRINT"MEAN=";S/N," STD DEV=";SQR(S2/N-(S/N)+2)
PRINT
PRINT"FREQUENCIES FOR X FROM 0 TO 1E-3 IN STEPS OF 1E-5": PRINT
FOR J=0 TO 9
FOR I=0 TO 9
PRINT USING "lllllllll";F(10*J+I);
NEXT
PRINT
NEXT

be specified by knowing $\sigma_{\ln \alpha}$. The 68% confidence limits for $\alpha$ are $\bar{\alpha} - \sigma_{\ln \alpha}$ and $\bar{\alpha} + \sigma_{\ln \alpha}$. The 95% limits are twice and half these values. Warrick and Nielsen give a value for $\sigma_{\ln \alpha}$ of around 0.5, indicating that (eq. 7.20) only 68% of the hydraulic conductivities they measured would fall within a range of 0.25 and 4 times the geometric mean. This variation seems extreme.

A stochastic hydraulic model could be formed by using a deterministic model of the type to be used in Ch. 8, and a Monte Carlo simulation in which $\alpha$ values were generated from a log normal distribution having the appropriate mean and variance. This, however, would be extremely time consuming. A better approach would be to use $\alpha$ values representative of the mean, 68% confidence limits, and perhaps 95% confidence limits. This then defines a range for the output. Additional discussion of these methods is given by Bresler et al. (1982) and Warrick and Nelson (1980).
7.6 REFERENCES


7.7 PROBLEMS

1. Use Program 7.1 to produce correlograms and variograms for hypothetical data sets representing each of the following: a. Bulk density samples at close intervals across row-furrow sets of soil which has been deep-ripped with a chisel plow; b. Chemical composition samples at close intervals down a soil profile which has a sharp boundary between parent materials; c. Some soil property sampled within a complex where random sized patches of soil A are randomly dispersed throughout a large area of soil B. Indicate which of these data sets are stationary and which are not.

2. Use Program 7.2 to produce a frequency distribution of saturated conductivities, using eq. 6.10 if $\psi_e$ is normally distributed with a mean of -2 J/kg and $\sigma$ of 0.5 J/kg.
Chapter 8

INfiltration and Redistribution

Infiltration is the process by which liquid water enters soil. Through redistribution, water which entered the soil during infiltration redistributes itself after infiltration has stopped. Both infiltration and redistribution profoundly affect soil water balance. The soil water balance determines the availability of water and nutrients to plants, affects rates of microbial processes, erosion, and chemical weathering, and influences soil thermal and gas composition relations. Therefore an understanding of the processes of infiltration and redistribution is extremely important in the overall study of soils.

8.1 INFILTRATION

If water were applied to the surface of a uniform column of air-dry soil, and the rate of infiltration of water into the soil column were measured as a function of time, the infiltration rate would be shown to decrease with time, as is indicated in Fig. 8.1. The infiltration rate is high initially, but decreases with time to a constant value. If a similar experiment were done with a column of moist soil similar results would be obtained (Fig. 8.1), but the initial rate would be lower. If infiltration were into a horizontal, rather than a vertical column, once again similar results would be obtained, except that the infiltration rate would decrease toward zero, rather than the constant, non-zero value shown in Fig. 8.1.

Fig. 8.1. Infiltration rate for water in soil.
Fig. 8.2. Water content profiles at three times during infiltration.

If water content were measured at several times during infiltration, the water content profiles in the column would be similar to those in Figure 8.2. Two features of these profiles should be noted. First, there is a zone of almost constant water content extending from the soil surface to the apparent boundary between wet and dry soil. This zone is called the transmission zone. A visible wetting front or boundary between wet and dry soil exists at the lower end of the transmission zone. This sharp front is the result of the sharp decrease in hydraulic conductivity with water content that is a characteristic of unsaturated porous materials.

The observations in Figs. 8.1 and 8.2 are qualitatively consistent with predictions one might make from the Darcy equation:

Vertical flow: \( f_w = -k \frac{d\psi_m}{dz} + kg \)  \hspace{1cm} (8.1)

Horizontal flow: \( f_w = -k \frac{d\psi_m}{dx} \).

As water first infiltrates soil, \( d\psi_m/dz \) is large, so flux is large. As the length of the transmission zone increases, the absolute value of \( d\psi_m/dz \) decreases. When the transmission zone is very long, the matric potential gradient becomes negligible, so the flux becomes \( f_w = kg \). Since the transmission zone is near saturation, the \( k \) is probably near \( k_s \). For horizontal infiltration, \( f_w \) approaches zero as the matric potential gradient
approaches zero. The fact that infiltration rate is initially lower in moist soil is explained by the reduced matric potential gradient in moist soil.

8.2 ANALYTICAL SOLUTIONS TO THE FLOW EQUATION

A more quantitative analysis of infiltration is obtained by solving the differential equation which describes water potential in soil as a function of position and time (eq. 6.22). A number of solutions to the differential equation have been obtained. The one that is most frequently referred to is by Philip (1957). A simpler approach was taken much earlier, however, by Green and Ampt (1911). The latter solution gives the most important features of the infiltration process, so it will be examined in detail.

During horizontal infiltration, an observable wetting front or boundary moves through the soil. The water content (and therefore the water potential) at the wetting front is almost constant during infiltration, as long as the profile is uniform. If the distance from the soil-water boundary to the wetting front is \( x_f \), and the potentials at the boundary and wetting front are \( \psi_i \) and \( \psi_f \), respectively, then the infiltration rate (or flux at the boundary) is

\[
f_{\psi_1} = -k \frac{d\psi}{dx} = -k(\psi_f - \psi_i)/x_f
\]  

where \( k \) is the mean conductivity of the transmission zone.

The amount of water stored in the soil per unit time is the change in water content of the soil from its initial dry condition to the average water content of the transmission zone, multiplied by the rate of advance of the wetting front. To satisfy continuity, all of the water flowing in must be stored by advance of the wetting front so

\[
\bar{k}(\psi_f - \psi_i)/x_f = \rho_w \Delta \theta \frac{dx_f}{dt}.
\]  

Here \( \rho_w \) is the density of water, \( \Delta \theta = (\theta_i + \theta_f)/2 - \theta_o \); \( \theta_i \), \( \theta_f \), and \( \theta_o \) are the volumetric water contents at the inflow, wetting front, and unwetted soil and \( t \) is time. Separation of variables and integration gives the position of the wetting front as a function of time:

\[
x_f = \left[ 2 \bar{k}(\psi_1 - \psi_f)t/\rho_w \Delta \theta \right]^{1/2}.
\]

Equation 8.5 indicates that the distance to the wetting front is directly proportional to the square root of time.
The infiltration rate is obtained by combining eqs. 8.3 and 8.5 to obtain

\[ f_{w1} = \left[ \frac{\rho_w \Delta \theta K (\psi_i - \psi_f)}{2t} \right]^{\frac{1}{2}} \quad (8.6) \]

showing that the infiltration rate is directly proportional to \( \Delta \theta \frac{1}{2} \) and \( K \frac{1}{2} \), and inversely proportional to \( t \frac{1}{2} \).

Equation 8.6 can be integrated over time to find the cumulative infiltration. The result of integration is

\[ I = \left[ 2\rho_w \Delta \theta K t (\psi_i - \psi_f) \right]^{\frac{1}{2}} \quad (8.7) \]

indicating that the cumulative infiltration is proportional to \( t \frac{1}{2} \). All of these predictions agree with the qualitative observations in Figure 8.1.

The Green-Ampt equation can also be applied to vertical infiltration, but the result is somewhat less satisfying. The most important result is that, for long times, \( f_{w1} \) approaches a constant value; an observation made using eq. 8.1.

8.3 INFILTRATION INTO LAYERED SOILS

The analysis so far has been concerned only with infiltration into uniform soils. Such soils exist mainly in carefully prepared laboratory columns. In the field, processes of soil development, tillage, illuviation, etc. produce layering. When infiltrating water encounters a boundary between layers the infiltration rate generally decreases. An example of this is shown in Figure 8.3.

It is interesting that infiltration rate decreases for either sand or clay layers. The decrease with the clay layer is expected because water infiltrates clay less readily than coarser textured materials, so water slows down as it enters the clay, decreasing \( (\psi_i - \psi_f) \) and thus decreasing infiltration rate. The reason for the reduction in infiltration rate for a sand layer is more subtle. It was noted in Ch. 6 that the unsaturated conductivity of sand is much lower than the unsaturated conductivity for finer textured materials. The boundary must therefore be wet almost to saturation before the hydraulic conductivity of the sand increases sufficiently to start carrying the water away. This increase in water content at the boundary decreases \( \psi - \psi_f \), and decreases \( f_{w1} \). Note that the infiltration rate recovers after water enters the sand, but does not recover for the clay. Perched water tables are therefore common over clay layers, but are not possible over coarse textured materials.
Fig. 8.3. Effect of sand and clay layers on infiltration into Palouse silt loam (from Miller and Gardner, 1962).

8.4 NUMERICAL SIMULATION OF INFILTRATION

Many of the techniques used to simulate water movement in unsaturated soil are similar to those used for heat flow. The soil profile can be represented by a network of conductors and capacitors (Fig. 4.1), and the network problem can be solved to determine how water potential and water content change with time at each node in the network. The complicating factor is that, for the unsaturated flow problem, the hydraulic conductivity and water capacity are functions of the dependent variable (water content or potential). The relationships between water potential and capacity or conductivity are such that the differential equation for flow (eq. 6.22) is highly non-linear. The methods used to solve water flow problems are therefore more difficult than those used to solve heat flow problems. Methods which have been used to solve these non-linear equations are those which (a) use time steps and space increments small enough that $k$ and $C$ can be treated as constant for a time step, or (b) linearize the differential equation in space by a change of variable and use a Newton-Raphson procedure to solve the non-linear equations in time.

Method (a) has been used in most numerical simulations of soil water flow, but it requires very small time increments during infiltration and arbitrary assumptions about the element hydraulic conductivities. This
clearly is not the method one would use with a microcomputer. Method (b) requires only the lumped parameter assumption (that the continuum of soil and water can be adequately represented by a network of capacitors and resistors). Both methods will be discussed so that the reader can see the connection between previous gas flow and heat flow models, and the water flow models of this chapter, but programs will only be given for method (b).

8.5 NUMERICAL SOLUTION: LINEAR METHODS

The actual numerical procedure for method (a) is identical to the one used for heat flow in Chapter 4. The numbering of conductances, capacitances, depths, etc. is the same as that shown in Figure 4.1. The equation for water balance at a node is

$$\frac{C(\psi_{i+1} - \psi_{i})}{A_{t}} \left( z_{i+1} - z_{i} \right) = \frac{k_{i-1}(\psi_{i-1} - \psi_{i})}{z_{i} - z_{i-1}} + U_{i}$$  \hspace{1cm} (8.8)

where $C$ is the water capacitance, $k$ is the element hydraulic conductivity, and $\bar{\psi}$ is the node water potential. The overbar denotes a mean value over the time step and/or element length, and the superscript $j$ indicates the time. The water potentials are defined as with heat flow:

$$\bar{\psi}_{i} = \eta\psi_{i}^{j+1} + (1-\eta)\psi_{i}^{j}$$  \hspace{1cm} (8.9)

where $\eta$ is a number between 0 and 1.0. While any value in this range can be used, the nonlinearity of water flow problems makes $\eta=1$ the best choice in almost all cases. Hereafter, $\eta=1$ will always be used.

Ideally, $C$ and $k$ are appropriate mean values of the capacity and conductivity over a time step. The correct values, however, are not easily obtained since each depends partially on the unknown potential at the end of the time step. Two approaches are normally used to estimate $C$ and $k$ (Haverkamp et al., 1977). One is to use extremely small time steps so that $k_{i} = k_{j}^{i}$ and $C_{i} = C_{j}^{i}$. A second approach is to make two or more computations, the first based on values for $C$ and $k$ at time $j$, with subsequent estimates made using the average of the known potential at the beginning of the time step and the estimated potential at the end of the time step.

The source term in equation 8.8, $U_{i}$, combines all of the inputs and losses of water from the node that are not explicit in equation 8.8. These might include water extraction by roots, gravitational flux, and condensation or evaporation. In most infiltration problems, only the gravitational flux is
included so that

\[ U_i = g(K_{i-1} - K_i) \]  \hspace{1cm} (8.10)

When equation 8.8 is written for each node in a simulated soil profile, and solved for the unknown \( \psi_i^{+1} \)'s, the matrix of coefficients is tridiagonal (cf. equation 4.1). For four nodes, we can write

\[
\begin{bmatrix}
B(1) & C(1) & 0 & 0 \\
A(2) & B(2) & C(2) & 0 \\
0 & A(3) & B(3) & C(3) \\
0 & 0 & A(4) & B(4)
\end{bmatrix}
\begin{bmatrix}
PN(1) \\
PN(2) \\
PN(3) \\
PN(4)
\end{bmatrix}
= 
\begin{bmatrix}
D(1) \\
D(2) \\
D(3) \\
D(4)
\end{bmatrix}
\]  \hspace{1cm} (8.11)

where

\[ C(I) = A(I-1) = -\eta K(I), \]  \hspace{1cm} (8.12)

\[ B(I) = \eta[K(I) + K(I+1)] + CP(I), \]  \hspace{1cm} (8.13)

and

\[ D(I) = (1-\eta)K(I-1)P(I-1) + (CP(I)-(1-\eta)[K(I-1)+K(I)])P(I) + (1-\eta)K(I)P(I+1) + U(I). \]  \hspace{1cm} (8.14)

The potentials at the beginning and end of the time step are \( P(I) \) and \( PN(I) \). The conductance of each element is the element hydraulic conductivity divided by the element length:

\[ K(I) = \frac{E}{(z_{i+1} - z_i)} \]  \hspace{1cm} (8.15)

The element hydraulic conductivity is computed using the node water potentials and equation 6.14 or the node water contents and eq. 6.13. Initially these are computed using \( P(I) \), but, if iteration is used, subsequent estimates are made using an estimated average potential over the time step. Various schemes have been used for computing element hydraulic conductivity from the values at the nodes. These include arithmetic means, geometric means, and weighted arithmetic means. For infiltration, the most successful is a weighted mean with upstream weighting. Often the element conductivity is taken as the conductivity at the upstream node.
The storage term, $CP(I)$ is

$$CP(I) = \rho_w C_i(z_{i+1} - z_{i-1})/2\Delta t \quad (8.16)$$

where $\Delta t$ is the time step and $C_i$ is the hydraulic capacity, $d\theta/d\psi_m$ at the node. If we assume that (eq. 5.9)

$$\theta = \theta_s (\psi_e/\psi_m)^{1/b},$$

then

$$C = d\theta/d\psi_m = (1/b)\theta_s (\psi_e/\psi_m)^{1/b}/\psi_m = (1/b)\theta_s/\psi_m. \quad (8.17)$$

The initial estimate of $C_i$ is made using the water content and potential at the start of the time step. The capacity at the average water potential and content is used when iteration is desired.

### 8.6 BOUNDARY CONDITIONS

Either flux or potential boundary conditions can be specified at the top and bottom of the profile. At the bottom, the potential is usually set to a known value. If there is a water table, this can be zero. If not, it can be a measured potential that stays constant over an experimental run. At the top of the profile, the surface may be at saturation, in which case the potential is set to $\psi_e$. If water is applied at a rate below the infiltration capacity of the soil, the potential does not go to the air entry value, so a flux can be specified. This can be done by adding the flux to the source term at node 1. If potential boundary conditions are specified, these must be added to $D(1)$ and $D(M)$ as was done in eqs. 4.15 and 4.16.

### 8.7 INTEGRAL TRANSFORM METHODS

The methods just outlined have been extensively used to simulate soil water movement, but their success is based on the use of a powerful computer which can cope with short time steps and many solution nodes, and on arbitrarily chosen weighting factors to determine element hydraulic conductances. Some methods follow which are suitable for less powerful computers, and which avoid arbitrary choices for element conductance by linearizing the problem before putting it in difference form. Element conductances are therefore constant as they were in the heat flow calculation.

Gardner (1958) suggested using a "matric flux potential" (MFP) as a driving force for flow. The MFP is defined as
\[ \phi = \int_{-\infty}^{\psi} k \, d\psi \quad (8.18) \]

If the \( k(\psi) \) relationship given by eq. 6.14 is assumed, then for \( \psi \psi_e \).

\[ \phi = k \frac{\psi_m}{(1-n)} \quad (8.19) \]

Values for \( k \) and \( n \) are always positive, \( \psi_m \) is negative, \( n > 1 \), so \( \phi \) is always positive. At air entry, \( \psi_e = k \frac{\psi_m}{(1-n)} \), so \( \phi \) ranges from zero for dry soil to \( \psi_e \) for saturated soil. The use of \( \phi \) as the "driving force" in the flow equation, rather than \( \psi \) or \( \theta \), results in a linear equation for steady flow:

\[ f_w = -d\phi/dz \quad (8.20) \]

The variables here are easily separated for integration to obtain the difference equation

\[ f_i = -(\phi_{i+1} - \phi_i)/(z_{i+1} - z_i) \quad (8.21) \]

Combining eq. 8.20 with the continuity equation gives

\[ \rho C \frac{\partial \psi}{\partial t} = \frac{\partial^2 \phi}{\partial z^2} + gk \quad (8.22) \]

where \( C = d\theta/d\phi \).

Equation 8.19 can be combined with eq. 5.9 to find the relationship between MFP and water content:

\[ \phi = \phi_e (\theta/\theta_e)^{b+3} \quad (8.23) \]

Differentiating eq. 8.23 gives the capacity

\[ C = \theta/[(b+3)\phi] \quad (8.24) \]

Equation 8.22 can now be put into a difference form similar to eq. 8.8, but with \( \phi \) for the driving potential, unity for the conductivity, and \( C \) calculated from eq. 8.24.

The matric flux potential is a useful driving potential, since it results in constant conductances for the soil profile. It does have limitations, however. The most serious is that, like water content, it is not continuous across boundaries between materials having different properties. This is
evident from eq. 8.19. Note, however, that flux through an element is linearly related to the product, \( k\psi \) (eq. 8.19). We could therefore rewrite eq. 8.21 as

\[
f_i = -(k_{i+1}\psi_{i+1} - k_i\psi_i)/[(z_{i+1} - z_i)(1-n)]
\]  

This equation can be derived somewhat differently to make its meaning clearer. In the lumped-parameter models, steady flow within each element is assumed. For steady flow conditions, eq. 8.2 can be integrated analytically between any two nodes if eq. 6.14 is assumed to describe \( k(\psi) \). The result of the integration is eq. 8.21a.

We can also use eq. 8.21a to derive an analytically correct value for the element conductivity. It is

\[
k = (k_{i+1}\psi_{i+1} - k_i\psi_i)/[(\psi_{i+1} - \psi_i)(n-1)]
\]

This equation will not be used, but its derivation gives some insight into options available for solving infiltration and other water flow problems. We can either solve for the \( \phi_i \), using eq. 8.21 and the associated capacity and conductivity variables, or solve for the \( \psi_i \) using eq. 8.21a. For infiltration, numerical methods are most stable if MFP is used. Evaporation, plant water uptake, and redistribution work as well, or better using standard matric potential. We will develop numerical solutions using both potentials, but generally will use the latter throughout the remainder of the book.

The use of matric flux potential linearizes the steady flow equation and allows it to be integrated for each element, but the transient flow problem is still non-linear since \( C(\phi) \) and \( C(\psi) \) both vary with the dependent variable. The solution method must therefore be one which solves non-linear equations.

8.8 THE NEWTON-RAPHSON METHOD

The Newton-Raphson iterative method is often used to solve non-linear equations. The method can be illustrated using a non linear function of the variable \( x \), where the value or values of \( x \) for which \( f(x) = 0 \) are to be found.

The function and a solution (\( x = x^n \)) are illustrated in Fig. 8.4. The superscript indicates the iteration number. For some arbitrary value of \( x \), say \( x^0 \), \( f(x) \) will have some value, \( F^0 \), which usually will not be zero. The difference between \( x^0 \) and the true solution, \( x^n \), can be approximated as:

\[
\frac{\partial F}{\partial x}|_{x^0} (x^0 - x^1) = F^0
\]

where \( F = f(x) \) and the derivative is evaluated at \( x^0 \).
The improved estimate of the solution, $x^1$, is the only unknown in eq. 8.25, and it is easily found. This, then, becomes the next $x$ value at which to evaluate $F$ and $\partial F/\partial x$ to get $x^2$. The iteration goes on until $F$ is sufficiently small to assure that $x^n$ is a correct solution (assuming that the iteration does converge).

For simultaneous equations, the solution process is similar to that outlined for a single variable, but matrix algebra is used for the solution. $F$ and $x^{p+1} - x^p$ become vectors. The coefficient matrix is made up of the partial derivatives of each $F$ with respect to each $x$. This is the Jacobian matrix. The new set of $\Delta x$'s is found for each iteration by Gauss elimination on the Jacobian and back substitution, as has been done in the oxygen and heat flow programs. If $F = f(x_1, x_2, x_3)$, then values of $x_1, x_2, x_3$ for which $F = 0$ can be found by iteratively solving

$$
\begin{bmatrix}
\partial F_1/\partial x_1 & \partial F_1/\partial x_2 & \partial F_1/\partial x_3 \\
\partial F_2/\partial x_1 & \partial F_2/\partial x_2 & \partial F_2/\partial x_3 \\
\partial F_3/\partial x_1 & \partial F_3/\partial x_2 & \partial F_3/\partial x_3
\end{bmatrix}
\begin{bmatrix}
x_1^{p+1} - x_1^p \\
x_2^{p+1} - x_2^p \\
x_3^{p+1} - x_3^p
\end{bmatrix}
= 
\begin{bmatrix}
F_1 \\
F_2 \\
F_3
\end{bmatrix}
$$

(8.26)

The partials and $F$'s are evaluated at the $x^p$, and the equations solved for the $x^{p+1}$. These are then used to re-evaluate the $F$'s and partials and solved again. Convergence is determined by checking the $F$'s to see if they are sufficiently close to zero.

To apply this method to solution of the infiltration problem, the mass balance for node $i$ must first be written. The symbols are shown in Fig. 8.5. $P$'s represent matric potentials, $K$'s are conductances, $f$'s are matric induced fluxes, and $U$'s are gravity induced fluxes. The equations are written in terms of matric potentials, but could be written using MFP.
Fig. 8.5. Nodes, potentials and fluxes for the Newton-Raphson calculation.

The mass balance for node $i$ is

$$F_i = f_i - f_{i-1} + U_{i-1} - U_i + \rho_w(\theta_{i+1} - \theta_i)(z_{i+1} - z_{i-1})/2\Delta t \quad (8.27)$$

$f_i$, $U_i$, and $\theta_i$ all are non-linear functions of $\psi_i$. We need to find values for $\psi$ which will make $F_i = 0$ for $i = 1$ to $M$, the total number of nodes. It is important to note that the values for potential which force $F$ to zero at every node are those which assure mass balance at every node. The gravitational flux is $U_i = gk_i$, where $k_i$ is the conductivity at node $i$.

Using this with eq. 8.21a, we obtain

$$F = \frac{k_i\psi_i - k_{i-1}\psi_{i-1}}{(1-n)(z_i - z_{i-1})} - \frac{k_{i+1}\psi_{i+1} - k_i\psi_i}{(1-n)(z_{i+1} - z_i)} + g(k_{i-1} - k_i) + \frac{\rho_w(\theta_{i+1} - \theta_i)(z_{i+1} - z_{i-1})}{2\Delta t} \quad (8.28)$$

Here the $k$'s are hydraulic conductivities calculated from the corresponding node water potential at the most recent iteration. The solution is therefore backward difference.

To find the Jacobian, we take derivatives of $F_i$ with respect to each potential influencing it to obtain

$$\frac{\partial F_i}{\partial \psi_i} = k_i/(z_i - z_{i-1}) + k_{i+1}/(z_{i+1} - z_i) + \rho_w(z_{i+1} - z_{i-1})\theta_i/(2\psi_i\Delta t) - ngk_i/\psi_i \quad (8.29)$$

$$\frac{\partial F_i}{\partial \psi_{i-1}} = -k_{i-1}/(z_{i-1} - z_i) + ngk_{i-1}/\psi_{i-1} \quad (8.30)$$

$$\frac{\partial F_i}{\partial \psi_{i+1}} = -k_{i+1}/(z_{i+1} - z_i) \quad (8.31)$$

Using eqs. 8.28 - 8.31 to form a set of equations like 8.26 gives the set of equations which is solved to find new estimates of $\psi$ at the end of the time step.
Boundary conditions are easily applied in the Newton-Raphson solution scheme. For infiltration, the upper boundary will either have a constant flux or a constant potential. For the constant flux condition, the flux is added as a source to the $F$ equation at node 1. For constant potential, $\Psi_1^{i+1}$ is set at the start of the time step and assumed not to change during the time step. Since the Newton-Raphson method computes changes in $\Psi$ to bring $F$ to zero, if $F_1$ and $\delta F_1 / \delta \Psi_2$ are set to zero before the Gauss elimination, the value for $\Psi_1$ will stay constant from iteration to iteration. The lower boundary condition is usually a constant potential, and never becomes part of the solution.

8.9 NUMERICAL IMPLEMENTATION: MATRIC POTENTIAL WITH NEWTON-RAPHSON

Program 8.1 simulates infiltration using the Newton-Raphson method. Lines 10-190 set up conditions for the simulation. Line 150 sets up geometrically increasing node spacing. The boundary potential is set to $\Psi_e$ in line 200. The lower boundary condition is set to the initial water potential in line 180. In line 190, GR is the gravitational constant, and IM is the maximum overall mass balance error which is allowed. Line 210 is the time counter. Conductivities at each node are calculated in 220. The loop from 230 - 300 sets up the mass balance (line 280) and components of the Jacobian (lines 250 - 270). In line 310, the upper boundary condition is applied. Lines 320 to 420 are the Thomas Algorithm which was used in Chapters 3 and 4. Line 430 computes new water contents at the end of the time step. Line 440 checks convergence. Note that the convergence criterion is satisfied only if the sum of the absolute values of the node mass balances is less than IM. The program prints the value of SE each time step so you can see how fast convergence is occurring. SE represents the absolute mass balance error in kg m$^{-2}$s$^{-1}$. Once convergence is satisfied, results are printed, flux and change in profile water are calculated and printed, and water contents are updated.

The mass balance test, which is made by comparing the flux density of water moving into the profile with the flux calculated from change in profile water content, is an important part of any model. It is necessary to assure that water is not being created or destroyed by the model. Program 8.1 doesn't explicitly account for water loss from the bottom of the profile. When the M node is dry and gravitational flow from the bottom of the profile is small, "flux in" and "WC change" should be in almost perfect agreement. Note that the mass balance error is essentially zero until the wetting front approaches the bottom of the profile.
86
5 ' PROGRAM 8.1 INFILTRATION SIMULATION USING STANDARD MATRIC POTENTIAL
7 ' 10 INPUT "NUMBER OF ELEMENTS";M
20 FOR 1=1 TO M: A=1+A*I:NEXT
30 X=M+1: DIM A(X), B(X), C(X), F(X), P(X), Z(X), V(X), DP(X), W(X), WN(X), K(X), CP(X)
40 INPUT"INITIAL WATER CONTENT-M43/M43"; W
50 INPUT"SATURATED CONDUCTIVITY-KG S/M43"; KS
60 INPUT"AIR ENTRY POTENTIAL-J/KG"; PE: PE=-ABS(PE)
70 INPUT"SOIL B VALUE"; B
80 INPUT"SOIL BULK DENSITY-MG/M+3"; BD: WS=1-BD/2.6
90 INPUT"DEPTH TO LOWER BOUNDARY-M"; Z(M+1): DZ=Z(M+1)/A
100 INPUT"TIME STEP"; DT
110 B1=1/B: N=2+3/B: N1=1-N: WD=1000
120 Z(1)=0: Z(0)=0
130 FOR I=1 TO M
140 W(I)=W: P(I)=PE*(WS/W)+B: WN(I)=W
150 Z(I+1)=Z(I)+DZ*I*I
160 V(I)=WD*(Z(I+1)-Z(I-1))/2
170 NEXT
180 P(M+1)=P(M): W(1)=WS: WN(1)=WS: Z(0)=-1E+10: K(M+1)=KS*(PE/P(M+1))+N
190 GR=9.8: IM=.000001
200 P(1)=PE: P(0)=PE: K(0)=0
210 TI=TI+DT/60
220 SE=0: FOR I=1 TO M: K(I)=KS*(PE/P(I))+N: NEXT
230 FOR I=1 TO M
240 CP(I)=V(I)*WN(I)/(B*P(I)*DT)
250 A(I)=K(I-1)/((Z(I)-Z(I-1))+GR*N*K(I-1)/P(I-1))
260 C(I)=K(I-1)/((Z(I)-Z(I-1))
270 B(I)=K(I)/(Z(I-2)-Z(I-1))+K(I)/(Z(I-1)-Z(I))+CP(I)-GR*N*K(I)/P(I)
280 F(I)=((P(I)*K(I)-P(I-1)*K(I-1))/(Z(I)-Z(I-1))-(P(I+1)*K(I+1)-P(I)*K(I))
290 IF I>1 THEN SE=SE+ABS(F(I))
300 NEXT
310 F(1)=0: C(1)=0
320 FOR I=1 TO M-1
330 C(I)=C(I)/B(I)
340 F(I)=F(I)/B(I)
350 B(I+1)=B(I+1)-A(I+1)*C(I)
360 F(I+1)=F(I+1)-A(I+1)*F(I)
370 NEXT
380 DP(M)=F(M)/B(M): P(M)=P(M)-DP(M): IF P(M)>PE THEN P(M)=PE
390 FOR I=M-1 TO 1 STEP -1
400 DP(I)=F(I)-C(I)*DP(I-1): P(I)=P(I)-DP(I)
410 IF P(I)>PE THEN P(I)=(P(I)+DP(I)+PE)/2
420 NEXT
430 FOR I=1 TO M: WN(I)=WS*(PE/P(I))+B1:NEXT
440 PRINT SE: IF SE>IM THEN GOTO 220
450 PRINT
460 PRINT "TIME="; TI; "MIN"
470 PRINT "DEPTH (M)"; "WC (M43/M43)"; "MATRIC POT. (J/KG)"; "SW=0"
480 FOR I=1 TO M: SW=SW+V(I)*(WN(I)-W(I)): PRINT Z(I), WN(I), P(I), W(I)=WN(I): NEXT
490 IF P(I)>PE THEN P(I)=(P(I)+DP(I)+PE)/2
500 PRINT "FLUX IN = "; FL; " WC CHANGE = "; SW/DT
510 GOTO 210
8.10 NUMERICAL IMPLEMENTATION: MATRIC FLUX POTENTIAL WITH NEWTON-RAPHSON

Program 8.2 is similar to 8.1, but with matric flux potential as the dependent variable. Results obtained with this program are identical to those obtained with Program 8.1, but Pgm. 8.2 requires fewer iterations and is more stable at high water content. Note that, in line 410 of Pgm. 8.1, a special statement was required to prevent the water potential from becoming too large. No such statement is required in Pgm. 8.2, but, in line 410 there is a statement to prevent MFP from becoming too small.

We can see why these models behave as they do by combining eqs. 6.14 and 8.19 to obtain

\[ \phi = \frac{c}{\psi_m^{1+3/b}} \]  

(8.19a)

A typical value for \( b \) is 3, which would make \( \phi \) proportional to the inverse square of \( \psi_m \). Thus the transformation to MFP expands the wet range and compresses the dry range. This makes the MFP calculation easy in the wet range, but difficult for dry soil, while the opposite is true for matric potential.

8.11 TEST OF INFILTRATION MODELS

Ideally the infiltration models should be tested by comparison with analytical solutions of the differential equations, as was done with the heat flow equations. However, analytical solutions to water flow equations are much more difficult to obtain than those for heat. Solutions which are available generally use water content as the dependent variable, or approximate the moisture characteristic or hydraulic conductivity with functions which are not compatible with those used here. Simple tests must therefore be used which check to see that the results from the numerical procedures are consistent with experimental evidence and inferences made from theory.

General observations relating to infiltration were discussed at the beginning of this chapter. Figures 8.1 and 8.2, which were used to illustrate expected infiltration behavior, were generated using Program 8.2. These figures agree (qualitatively, at least) with experimentally observed infiltration data, indicating that the model is at least qualitatively correct.

A more demanding test would be to compare the result of simulations with eq. 8.7. Equation 8.7 predicts that cumulative horizontal infiltration will be proportional to \( t^{1/3} \). Even though the derivation of eq. 8.7 involved some major simplifications, the time dependence it predicts is identical to that predicted by less restrictive derivations (cf Hillel, 1980) and is a
5 ' PROGRAM 8.2 INFILTRATION WITH MATRIC FLUX POTENTIAL
7
10 INPUT "NUMBER OF ELEMENTS"; M
20 FOR I=1 TO M:A=A+I*I:NEXT
30 X=M+1: DIM A(X), B(X), C(X), P(X), Z(X), V(X), DP(X), W(X), WN(X), K(X), CP(X)
40 INPUT "INITIAL WATER CONTENT-M+3/M+3"; W
50 INPUT "SATURATED CONDUCTIVITY-KG S/M+3"; KS
60 INPUT "AIR ENTRY POTENTIAL-J/KG"; AE: AE = -ABS(AE)
70 INPUT "SOIL B VALUE"; B
80 INPUT "SOIL BULK DENSITY-MG/M43"; BD: WS = 1 - BD/2.6
90 INPUT "DEPTH TO LOWER BOUNDARY-M"; Z(M+1): DZ = Z(M+1)/A
100 INPUT "TIME STEP"; DT
110 B1 = B+3: B2 = 1/B1: B3 = (2*B+3)/(B+3)
120 PE = KS*AE/(1-3/B): WD = 1000
130 Z(1) = 0: Z(O) = 0
140 FOR I=1 TO M
160 FOR I=1 TO M
170 Z(I+1) = Z(I) + DZ*I*I
180 V(I) = WD*(Z(I+1) - Z(I-1))/Z
190 P(M+1) = P(M): W(1) = WS: WN(1) = WS: Z(0) = -1E+10: K(M+1) = KS*(P(M+1)/PE) + B
200 GR = 9.8: IM = .000001
210 TI = TI + DT/60
220 SE = 0
230 FOR I=1 TO M
240 K(I) = KS*(P(I)/PE)*B3
250 CP(I) = V(I)^4*WS/(B1*P(I)*DT)
260 A(I) = 1/(Z(I) - Z(I-1)) - GR*B3*K(I-1)/P(I-1)
270 C1(I) = 1/(Z(I+1) - Z(I))
280 B(I) = 1/(Z(I) - Z(I-1))^2 + 1/(Z(I) - Z(I-1)) + CP(I) + GR*B3*K(I)/P(I)
290 F(I) = (P(I) - P(I-1))/(Z(I) - Z(I-1) - (P(I+1) - P(I))/(Z(I) - Z(I-1))
300 IF I>1 THEN SE = SE + ABS(F(I))
310 NEXT
320 F(1) = 0: C(1) = 0
330 FOR I=1 TO M-1
340 C(I) = C(I)/B(I)
350 F(I) = F(I)/B(I)
360 B(I+1) = B(I+1) - A(I+1)*C(I)
370 F(I+1) = F(I+1) - A(I+1)*F(I)
380 NEXT
390 DP(M) = F(M)/B(M): P(M) = P(M) - DP(M): IF P(M) < 0 THEN P(M) = .000001
400 FOR I=M TO 1 STEP -1
410 DP(I) = F(I) - C(I)*DP(I+1): P(I) = P(I) - DP(I): IF P(I) < 0 THEN P(I) = .000001
420 NEXT
430 FOR I=1 TO M: WN(I) = WS*(P(I)/PE) + B: NEXT
440 PRINT SE;: IF SE > IM THEN GOTO 220
450 PRINT "TIME=": TI; "MIN"
460 PRINT "DEPTH","WC M+3/M+3","MATRIC FLUX POT."; SW = 0
470 FOR I=1 TO M: SW = SW + V(I)*(WN(I) - W(I)): PRINT Z(I), WN(I), P(I): W(I) = WN(I): NEXT
480 IF M = P(1)-F(2))/(Z(2)-Z(1)) + GR*K(I)
490 PRINT "FLUX IN = ""FL""; WC CHANGE = ""; SW/DT
500 GOTO 210
characteristic of any system which is described by a parabolic differential equation.

Figure 8.6b shows cumulative infiltration as a function of $t^{1/2}$ for two choices of node spacing. Time steps were started at 1 s and doubled each following step. Note that the infiltration predicted by the model with

Fig. 8.6. Simulated infiltration into a horizontal soil column with $b=3$, $v_e= -2$ J/kg, $k_s=0.001$ kg s m$^{-3}$, column length = 50 cm. Geometric node spacing (as used in Program 8.2) or fixed spacing, as indicated, was used. Infiltration rate is shown in a, and cumulative infiltration in b.
geometrically increasing node spacing increases linearly with $t^{\frac{1}{2}}$ and extrapolates to zero, as expected. The infiltration with 5 cm node spacing also increases linearly (after the first few minutes) but does not extrapolate to zero. The reason for this is apparent from Fig. 8.6a, which shows infiltration rate. The infiltration rate stays constant until the first few nodes wet, then decreases linearly with $t^{-\frac{1}{2}}$, as expected. The effect of having a large capacity in the first few nodes is to delay this wetting, and therefore delay infiltration, as shown in Fig. 8.6a. The reader is encouraged to investigate the numerical approximations in more detail in Problem 8.1.

8.12 REDISTRIBUTION - ANALYTICAL ASPECTS

If, after infiltration has occurred over some period of time, the addition of water to the soil is stopped, the water that is in wetter parts of the soil will redistribute to drier locations. Figure 8.7 shows a typical redistribution process. Note that the water content in the top 10 cm zone which was initially wetted changes little with depth, and that the change in water content with time in that initially wetted zone decreases over time.

![Graph showing redistribution process](image)

**Fig. 8.7.** Redistribution of soil water following infiltration. Soil parameters are the same as Fig. 8.6.

The latter point is easier to see if the water content in the initially wetted zone is plotted as a function of time, as in Figure 8.8. Note that the rate of water loss initially is high, but decreases with time. It does not
however, go to zero. Information such as that presented in Figure 8.8 is used to determine the field capacity of a soil. When the rate of internal drainage decreases to a value which is considered negligible in comparison with water inputs or losses, the soil is said to be at field capacity. The definition of field capacity depends on the amount of internal drainage considered negligible, since the drainage rate never goes completely to zero. Soil is normally considered to be at field capacity within a few days following irrigation or a heavy rain.

Gardner (1970) suggested a simple analysis which can be used to find field capacity if the hydraulic conductivity of the profile is known, or the profile hydraulic conductivity if the rate of drainage of the wetted part of the profile is known. Start with the water flow equation:

\[ \rho_w \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ \frac{\partial \psi_m}{\partial t} \frac{\partial \psi_m}{\partial z} \right] . \]  

(8.32)

From figure 8.7, note that in the wetted zone \( d\psi_m/dz \) is near zero, implying that \( d\psi_m/dz \) is also near zero. Note also that \( d\theta/dt \) does not change with depth since the wetted zone drains almost uniformly. Using these two facts, equation 8.32 can be rewritten as

\[ \rho_w (d\theta/dt) dz = -g dk. \]  

(8.33)
Integration over the depth of wetting gives

\[ L \frac{d\theta}{dt} = -gk/\rho_w. \]  

(8.34)

The rate of change of profile water content is \( L \frac{d\theta}{dt} \). If drainage rate is considered to be negligible when it is less than some value, \( \varepsilon \), then field capacity is the water content or potential when (using eq. 6.13)

\[ k = k_s (\theta/\theta_s)^m = \rho_w \varepsilon / g \]  

(8.35)

or

\[ \theta_{fc} = \theta_s (\rho_w \varepsilon / g k_s)^{1/m} \]  

(8.36)

Field capacity, then, depends only on the arbitrary choice of a negligible drainage rate and the hydraulic properties of the profile. In other words, it is a dynamic property of the profile and has nothing to do with binding of water by soil, as is sometimes supposed.

The time dependence of the drainage rate (as shown in Fig. 8.8) can be found by integrating eq. 8.34 to obtain

\[ \theta = \left[ \theta_i^{1-m} - (m-1) \frac{k_s g \theta_t}{\rho_s \rho_w L} \right]^{1/1-m} \]  

(8.37)

where \( \theta_i \) is the initial water content of the wetted zone.

In layered soils, redistribution is not as simple as this. The increased resistance to flow across a boundary between layers may increase field capacity substantially. Clothier et al. (1977) give a simple analysis for a soil underlain by a coarse-textured layer.

8.13 NUMERICAL SIMULATION OF REDISTRIBUTION

Numerical models for redistribution involve only a change in boundary condition in the infiltration models. If line 310 in Program 8.1 and the IF statement from line 290 are removed, there will be no influx of water and redistribution of the water will be simulated.

8.14 SIMULATION OF INFILTRATION AND REDISTRIBUTION IN LAYERED SOILS

Program 8.1 was prepared for uniform profiles. If the profile is layered, the soil hydraulic properties \((k_s, \psi_e, b)\) would become arrays. Since these properties are defined at each node, the transition from one soil material to another would occur within an element. To minimize errors from this, the length of the element that separates the layers should be small.
compared to adjoining elements. Since changes may occur rapidly near these boundaries, it may also be advisable to decrease the spacing of several elements around the boundary. The models as they are written will not simulate saturated flow, so water potential at any point in the soil profile should not be allowed to go above the air entry potential.

8.15 INFILTRATION AND REDISTRIBUTION IN TWO DIMENSIONS

Many problems in infiltration and redistribution cannot be solved using one-dimensional models. Irrigation using furrows or trickle sources obviously must be described in terms of two or three dimensional flow. Analysis of a number of the methods used to measure hydraulic properties, such as infiltrometers, also requires consideration of two or three dimensional flow fields. Multidimensional flow will not be treated in detail here, though an example program which simulates two dimensional flow in a rectangular grid will follow. Readers with an interest in multidimensional flow should be able to extend this example to cover more difficult flow problems. The development of this two-dimensional flow model will be similar to that of Redinger et al. (1984). The soil is divided into a 2-D grid, as shown in Fig. 8.8. The numbering system for element conductances and nodes is also shown. Horizontal conductances are labeled $K_x$, and vertical, $K_z$. Potentials and water contents define the driving forces and storages at each node throughout the grid. The grid is assumed horizontal, so that gravitational potential influences only the vertical flow component.

Fig. 8.9. Flow network for two-dimensional infiltration-redistribution showing node and conductance numbering.
Program 8.3 is a BASIC code for simulating two dimensional infiltration and redistribution. It uses matric flux potential, as in Program 8.2. Starting with line 20, note that conductances, potentials, and old and new water contents are now double subscripted variables. In lines 90 and 100, node positions for the x and z directions are read in. This program is meant to simulate infiltration into a slot or irrigation furrow placed at node (1,1). We assume that the nodes at and under the furrow (at x=1) lie on a symmetry plane, and that another irrigation furrow lies at 2X(M), so that X(M+1) is another symmetry plane. We assume that flux is zero across symmetry planes.

The double loop at lines 110-170 sets initial water contents, potentials, element volumes, and conductances. The element conductances are similar to those in Prog. 8.2, except that now they are multiplied by the widths or depths of the flow path. The conductances at the top and left side of the column are automatically zero, since BASIC automatically initializes all variables to zero when a program is run. Statement 160 sets conductances on the right to zero. Statement 180 sets the bottom boundary condition as a constant potential condition.

In line 190, the variable, IR, is an irrigation flag. When IR ≠ 1, irrigation has stopped and redistribution occurs. In line 200 the irrigation boundary condition is set. When irrigation is applied, the slot size is half the distance to each node surrounding the wetted node. The slot is therefore 5 cm x 5 cm.

The solution is similar to Prog. 8.2. Line 240 computes the gravitational sinks for each node. Line 250 eliminates the irrigated node from the calculation when water is being applied. Lines 270 and 260 are the mass balance and its derivative with respect to node I,J. New node potentials are computed in line 290.

The solution method used here is still Newton-Raphson, but only the diagonal of the Jacobian matrix is used to calculate the new water potentials. As justification for this simplified scheme, note that the full Jacobian for a two dimensional problem has at least 5 diagonals, rather than the three previously used in one dimensional problems. Two of the diagonals are immediately adjacent to the main diagonal, just as they are in the one dimensional problem. These are the conductances right above and below the solution node. The other two diagonals are offset in the matrix by as many places as there are vertical nodes in the grid, because they represent the conductances to the left and right of the node. Even though such a matrix is sparse, and therefore easier to reduce than a full MX x MZ matrix, the reduction of the matrix is still time-consuming on a small computer. For most 2-D flow problems, most of the information needed to determine the new
I PROGRAM 8.3 TWO-DIMENSIONAL WATER FLOW SIMULATION WITH MFP

MZ=6:MX=5:B=MZ+l:C=MX+l

DIM W(B,C),WN(B,C),P(B,C),Z(B),KZ(B,C),U(B,C),V(B,C),KX(B,C),X(C)

INPUT"INITIAL WATER CONTENT - Mf3/Mf3";W

INPUT"SATURATED CONDUCTIVITY - KG S Mf-3";Ks

INPUT"AIR ENTRY POTENTIAL - J/KG";AE:AE=-ABS(AE)

INPUT"TIME STEP - S";DT

INPUT"SOIL B VALUE";B

B3=1/(B3=(2+S+3)/(B+3)):PE=KS*AE/(-1-3/B):WD=1000:WS=.5

FOR I=0 TO MZ+l:READ Z(I):NEXT:DATA 0,0,.1,.2,.3,.5,.8,1.5

FOR J=0 TO MX+l:READ X(J):NEXT:DATA 0,0,.1,.2,.3,.5,.5

FOR J=1 TO MX


KZ(I,J)=X(I+1)-X(I-1))/(2*X(I+1)-X(I))

IF J<MX THEN KX(I,J)=(Z(I+1)-Z(I-1))/(2*X(I+1)-X(I)) ELSE KX(I,J)=0

NEXT:NEXT

FOR J=1 TO MX:P(MZ+l,J)=P(MZ,J):NEXT

GR=9.8:IM=.000001:IR=1

TI=TI+DT/3600:IF IR=1 THEN P(1,1)=PE:W(1,1)=WS:WN(1,1)=WS

SE=0

FOR J=1 TO MX

FOR I=1 TO MZ

U(I,J)=((X(I+1)-X(I-1))/2)*GR*Ks*(P(I,J)/PE)+B

IF I=1 AND J=1 AND IR=1 THEN GOTO 310

DF=KZ(I-1,J)*KZ(I,J)*KKX(I,J)+V(I,J)*WN(I,J)/(B1*P(I,J)*DT)

+U(I,J)*B3/P(I,J)

P=KKZ(I-1,J)*P(I,J)-P(I-1,J)+KX(I,J)*P(I,J-1)+KX(I,J-1)*P(I,J-1)+KX(I,J-1)*P(I,J-1)+KX(I,J-1)*P(I,J-1)+WN(I,J)

-W(I,J)*V(I,J)/DT+U(I,J)-U(I-1,J)

SE=SE+ABS(F)

DP=F/DF:P(I,J)=P(I,J)-DP

WN(I,J)=WS*P(I,J)/PE+B2

NEXT:NEXT

IF SE>1M THEN PRINT SE:;GOTO 210

PRINT:PRINT "TIME = ";TI;" HRS"

FL=KZ(I,1)*P(I,1)-P(2,1)+KKX(1,1)*P(1,1)-P(1,2)+U(I,1)

SF=SF+FL*DT:SW=0

FOR I=1 TO MZ:FOR J=1 TO MX

SW=SW+V(I,J)*WN(I,J)-W(I,J))

NEXT:NEXT

PRINT:PRINT "WC CHANGE = ";SW/DT;"FLUX IN = ";FL;"CUM INFILT = ";SF

GOTO 200
potentials is contained in the diagonal of the Jacobian. When the cost in computing time of iterating a few more times with only the diagonal Jacobian is compared with that of inverting the full Jacobian, the method used in Program 8.3 is almost always substantially faster. The simple method is slower when elements with very small conductance are adjacent to elements with very large conductance. This should be avoided if the method in Program 8.3 is used.

A few additional observations on Program 8.3 may be useful. The flux, calculated in line 340, has units of kg per meter of slot, but the simulation assumed a symmetry plane at and below the slot. The total infiltration for the full problem (both right and left halves) is twice the value given by FL. When IR is set to zero, FL will not go immediately to zero in the present program because water continues to come from storage at node (1,1). A simple modification could be made to eliminate this flow, if desired.

A number of simple modifications to Program 8.3 can be made to allow other types of simulation. For example, uneven surface topography could be simulated by a stair-step pattern, with conductances to nodes above the soil surface set to zero. Non-uniform infiltration could be simulated by applying different fluxes to different nodes across the soil surface. Radially symmetric, three dimensional infiltration (such as from a single trickle emitter) could be simulated by calculating radial conductances as was done in Chapter 3, and adjusting volumes and flow cross-sections appropriately.
REFERENCES


PROBLEMS

8.1 Modify Program 8.2 to have uniform node spacing and no gravitational flux (horizontal column GR=0). Then simulate infiltration into the column, trying different node spacings, initial water contents, and time steps. Plot cumulative infiltration as a function of $t^2$ and discuss results.

8.2 Modify Program 8.1 to simulate a constant flux density at the surface (rain or sprinkler irrigation) at a value well below $g_k$. This is done by deleting line 310, rewriting line 290 without the IF statement, and adding at 285 IF $I=1$ THEN $P(1)=F(1)-FLUX$. Remember that FLUX is in kg m$^{-2}$ s$^{-1}$. Compare profiles which result from comparable total infiltration amounts, but varying input rates.

8.3 Use Program 8.2 to compare vertical downward infiltration (GR=9.8), vertical upward infiltration (GR=-9.8), and horizontal infiltration (GR=0). Plot cumulative infiltration as a function of $t^4$ and discuss the results.

8.4 Make a program that simulates 2 hours of infiltration and then several days of redistribution. Plot water content of the initially wetted soil as a function of time following infiltration. Compare results with Fig. 8.8 and eq. 8.36.

8.5 Modify Program 8.1 to simulate the water potential distribution of a soil sample in a pressure plate apparatus.
Chapter 9

EVAPORATION

As water is being redistributed in the soil, it is also evaporating from the soil surface. The amount of water that evaporates depends on soil properties and environmental conditions. Under some conditions most of the precipitation received at a soil surface may be lost by evaporation. Even when the soil is covered by vegetation, evaporation is probably at least 10% of evapotranspiration. These observations indicate that evaporation at the soil surface is always an important component of the water budget. In dryland farming and desert soils, evaporation can be the largest loss component in the water budget.

9.1 GENERAL CONCEPTS

If the surface of a soil column were wet, and water loss were measured as a function of time, the evaporation rate would stay nearly constant for some time, and then suddenly decrease, as is shown in Fig. 9.1. Three stages of drying are often identified. During the first stage, the evaporation rate is relatively constant. The soil surface is wet, and the evaporation rate is determined entirely by the vapor concentration difference between the surface and the air, and the boundary layer resistance of the air above the soil surface. When the soil dries sufficiently that water cannot be supplied to the surface fast enough to meet the evaporative demand, the soil surface dries and the evaporation rate is reduced. This reduction is caused by the increased

![Fig. 9.1. Evaporation rate for a bare soil surface.](image-url)
diffusion resistance of the dry soil which is between the wet soil and the atmosphere. As the depth of the dry layer increases, the evaporation rate decreases. A third stage of drying is often identified when the rate of decrease of evaporation with time becomes small. The point at which this starts is arbitrary, however, and there is some question as to whether a third stage of drying needs to be (or can be) defined.

Following first stage drying, evaporation can be analyzed either as a vapor diffusion problem or as a liquid flow problem. The depth of the dry layer which forms is determined by the rate at which liquid water can be supplied to the drying front. If liquid water supply is too slow, the dry layer deepens, causing an increase in vapor diffusion resistance. This reduces evaporation rate until supply and demand are brought back into balance.

Because of these self-adjusting features of the system, some aspects of the evaporation process are relatively easy to analyze. A complete analysis, however, must take into account both liquid and vapor flow, and must consider effects of temperature gradients on water movement. Isothermal vapor flow will be considered first, and then thermally induced flow will be included.

9.2 SIMULTANEOUS TRANSPORT OF LIQUID AND VAPOR IN ISOTHERMAL SOIL

The flux density of vapor is described by Fick's law:

\[ f_v = -D_v \frac{dc_v}{dz} \]  \hspace{1cm} (9.1)

where \( D_v \) is the vapor diffusivity in soil (\( m^2 s^{-1} \)) and \( c_v \) is the soil vapor concentration (\( g m^{-3} \)). The diffusivity in soil is computed from eqs. 3.8 and 3.10. We will assume \( \varepsilon = 0.66 \phi_g \). The vapor concentration can be written as

\[ c_v = h_r c_v^* \]  \hspace{1cm} (9.2)

where \( h_r \) is the relative humidity and \( c_v^* \) is the saturation vapor concentration at soil temperature. If the soil is isothermal, then \( \frac{dc_v}{dz} = c_v^* \frac{dh_r}{dz} \). The relative humidity, in turn, is a function of soil water potential (eq. 5.14):

\[ h_r = \exp(\frac{M_w \psi}{R \theta}) \]  \hspace{1cm} (9.3)

where \( M_w \) is the mass of a mole of water, \( R \) is the gass constant (\( 8.3143 \) J mole\(^{-1} \) K\(^{-1} \)), and \( \theta \) is Kelvin temperature. Using the chain rule:

\[ \frac{dh_r}{dz} = \left( \frac{dh_r}{d\psi} \right) \left( \frac{d\psi}{dz} \right) \]  \hspace{1cm} (9.4)
Using eq. 9.3,

\[ \frac{dh_r}{d\psi} = \frac{h_r M_w}{R \theta} \]  

(9.5)

Using 9.5, 9.4, 9.2, and 9.1,

\[ f_v = -k_v \frac{d\psi}{dz} \]  

(9.6)

where the combination of terms

\[ k_v = D_vc_v \frac{h_r M_w}{R \theta} \]  

(9.7)

is a vapor conductivity which can be added to the liquid conductivity to calculate the total water flux (liquid + vapor).

The vapor conductivities for sand, loam, and clay soils, calculated using eq. 9.7, are compared with liquid conductivities in Fig. 9.2. The initial increase in \( k_v \) with decreased potential results from the increase in \( D_v \) as pores empty and \( \theta \) increases. The subsequent decrease is from the decrease in \( h_r \) with water potential. It is interesting to note that vapor transport

![Graph](image)

**Fig. 9.2.** Comparison of liquid (dashed lines) and vapor (solid lines) conductivities for typical sand, silt loam, and clay soils. Note that the water potential scale is logarithmic.
is negligible compared to liquid transport, until soils become quite dry. This is particularly true for clay soil. Equation 9.7 indicates that $k_v$ has about the same temperature dependence as $c_v$, which is around 5% per degree at 20°C.

The total flux in a soil is the sum of the liquid and vapor fluxes, and both are functions of the matric potential gradient. Osmotic potential gradients are somewhat more difficult to treat, however since they are as effective as matric potential gradients in driving vapor flow, but have little effect on liquid flow. This fact must be taken into account if one is modeling vapor transport in soils which have high salt concentrations. The effect of the gravitational potential gradient on vapor flow is negligibly small.

9.3 NON-ISOTHERMAL VAPOR FLOW

A more general analysis of evaporation must include effects of thermal gradients on water transport. As the temperature of soil water is increased, the pressure of both the liquid and gas phases increases. Water will therefore tend to move from warm soil to cold soil. Liquid-phase transport is described using

$$f_l = -k \frac{d\psi}{dz} = -k(\frac{d\psi}{dT})(dT/dz) \tag{9.8}$$

Equation 9.1 is used for vapor flow in a temperature gradient, but now both $h_r$ and $c^*_v$ can vary with distance:

$$f_v = f_{v\theta} + f_{vT} = -D_v c^*_v \frac{dh_r}{dz} - D_v h_r \frac{dc^*_v}{dz} \tag{9.9}$$

The $f_{v\theta}$ term is eq. 9.6. The $f_{vT}$ term can be written as

$$f_{vT} = -D_v h_r s \frac{dT}{dz} \tag{9.10}$$

where $s = \frac{dc^*_v}{dT}$ is the slope of the saturation vapor concentration function.

The observed transport of water vapor in a temperature gradient generally exceeds that predicted by eq. 9.10, often by a factor of 5-10 or more (Cass et al. 1984). Equation 9.10 is therefore multiplied by a dimensionless enhancement factor, $\eta$, to give the correct vapor flux. The function, $\eta$, has the same form as eq. 4.20. The constants for eq. 4.20 are: $A = 9.5$, $B = 6$, $D = 1$, and $E = 4$ (Cass et al. 1984). The variable, $C$ is a function of clay content, and is given by eq. 4.28. The enhancement factor has a value between
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10 and 12 at high water content and becomes unity as water content approaches zero.

9.4 EFFECT OF WATER VAPOR FLOW ON THE HEAT FLOW EQUATIONS

Two corrections can be made to the heat flow equations in Ch. 4 to make them compatible with the vapor flow equations just derived. First, the thermally induced latent heat flow can now be explicitly calculated. Since the latent heat flux is the latent heat of vaporization, \( L \), times the vapor flux, the apparent thermal conductivity becomes the conductivity for sensible heat plus \( L \) times the vapor conductivity

\[
\lambda_a = \lambda + D_v h_v s n L
\]  

(9.11)

This conductivity is the apparent soil thermal conductivity used in Ch. 4 for heat flow calculations.

The second correction accounts for the latent heat which is transported by water potential gradients. The vapor flux is given by eq. 9.6, so a source term is added to the heat flow equation which is the latent heat of vaporization multiplied by the divergence in vapor flux. This term is negligibly small except possibly at the soil surface.

9.5 COMPARISON OF THERMALLY INDUCED LIQUID AND VAPOR FLOW

The flux of water from thermally induced liquid flow is given by eq. 9.8. Thermally induced vapor flow is computed using eq. 9.10. It is useful to compare the fluxes in these two phases to determine when each might be important. The thermal liquid conductivity, \( k \frac{d\psi}{dT} \), was computed by Philip and deVries (1957) assuming that only the surface tension of the water changed with temperature:

\[
\frac{d\psi_m}{dT} = (d\psi_m/d\sigma)(d\sigma/dT)
\]  

(9.12)

where \( \sigma \) is the surface tension. From eq. 5.3,

\[
\frac{d\psi_m}{d\sigma} = \frac{\psi_m}{\sigma}.
\]  

(9.13)

The temperature dependence of water potential is therefore predicted to be around \( 2 \times 10^{-3} \frac{\psi_m}{T} \) at 20°C. Taylor and Stewart (1960) found \( \frac{d\psi_m}{dT} \) to be about 10 times this large for a silt loam soil. If the temperature dependence found by Taylor and Stewart (1960) is assumed, then typical thermal liquid conductivities for a silt loam soil would be \( 3 \times 10^{-7} \) kg s\(^{-1}\) m\(^{-1}\) K\(^{-1}\) at \( \psi = -10 \) J/kg, \( 5 \times 10^{-8} \) kg s\(^{-1}\) m\(^{-1}\) K\(^{-1}\) at -20 J/kg, and \( 6 \times 10^{-10} \) kg s\(^{-1}\) m\(^{-1}\) K\(^{-1}\) at 0°
at \( \psi = -100 \) J/kg. Thermal vapor conductivity is around \( 4 \times 10^{-8} \) kg s\(^{-1}\) m\(^{-1}\) K\(^{-1}\), or about the same as the liquid value at -20 J/kg. Thermally induced liquid flow would therefore be important only in wet soil. At saturation, a temperature gradient of 1 K/m apparently could produce a flux of \( 2 \times 10^{-5} \) kg m\(^{-2}\) s\(^{-1}\), about 0.5% of the saturated hydraulic conductivity. Observed fluxes in temperature gradients are not this large. Thermally induced liquid flow is therefore usually not large enough to require consideration, while thermally induced vapor flow may be important in drying soil.

9.6 MODELING EVAPORATION

Incorporation of the ideas discussed so far in this chapter into the numerical models for water flow is not difficult, but a complete model which includes linked transport of liquid, vapor and heat is quite long and may be slower and more complicated than would be necessary for most applications. It is therefore useful to consider the information needed from the model before deciding how far to go in incorporating vapor flow. The simplest option, and one which is often used in modeling soil water flow, is to neglect vapor flow except at the soil surface. The evaporation during second- and third-stage drying is then controlled by the humidity at the evaporating surface and liquid flux in the soil. If we assume that the potential evaporation rate is known, then the actual evaporation rate at any time is

\[
E = \frac{E_p(h_s - h_a)}{(1 - h_s)} \quad (9.14)
\]

where \( E_p \) is the potential evaporation rate, \( h_s \) is the humidity at the soil surface (eq. 9.3) and \( h_a \) is the atmospheric humidity. The value given for \( E_p \) is only important during first stage drying (when \( E = E_p \)). The value chosen for \( h_a \) is relatively unimportant, since after first stage \( E \) is determined by liquid flow to the surface and not by the values chosen for eq. 9.14.

This approach can give quite reasonable estimates of evaporation rate during the first stages of drying when most of the water is lost. It should therefore be adequate for many water budget models. However, it will not correctly predict the water content or water potential profile in the soil and will also fail to give correct estimates of evaporation rate during third stage drying. The profile obtained when vapor flux in the soil is ignored is shown in Fig. 9.3, along with a profile with vapor flux included. The profile with vapor flux shows a definite drying front, as is observed with drying soil, while the other does not. If it is necessary to predict moisture profiles, vapor flux must be included in the model.
For the isothermal condition, vapor fluxes in each element can be computed from

$$f_{vi} = D_v c_v (h_{i+1} - h_i)/(z_{i+1} - z_i) \quad (9.15)$$

Program 9.1 is a modification of program 8.1 to allow for vapor flow within the profile and evaporation at the soil surface. Some of the changes need explanation. Equation 9.6 implies that the vapor and liquid conductivities should be added to give the total conductivity. This is not feasible in Program 8.1 because liquid fluxes are expressed as differences in $k \psi$ over elements. However, using the Newton-Raphson procedure, vapor fluxes can be explicitly calculated and added directly to the mass balance equation (line 320). The derivative of the vapor flux must also be added to the diagonal elements of the Jacobian (line 310) to assure quick convergence to the correct potentials. The fluxes and derivatives within the soil are calculated in line 270, and the soil surface values are calculated in line 240. For isothermal soil, the fluxes are given by eq. 9.15. The humidity at each node is therefore needed for the calculation. This is calculated initially in line 150, and subsequently in line 460.

In line 190 a large positive number is substituted for the lower boundary depth after the node volume is calculated. The effect of this is to prevent
PROGRAM 9.1 SIMULATION OF EVAPORATION FROM A BARE-SURFACE SOIL

INPUT "NUMBER OF ELEMENTS"; M
FOR I=1 TO M: A=ATI'*I: NEXT
X=M+1: DIM A(X), B(X), C(X), P(X), Z(X), V(X), W(X), WN(X), K(X), CP(X), H(X), JV(X), DJ(X)

INPUT "INITIAL WATER POTENTIAL -J/KG"; P: P=-ABS(P)
INPUT "SATURATED CONDUCTIVITY -KG/SM43"; KS
INPUT "SOIL B VALUE"; B
INPUT "SOIL BULK DENSITY -MG/SM43"; BD: WS=1-BD/2.6
B1=1/B: N=2+3/B: N1=1-N: WD=1000: DT=3600
Z(1)=0: Z(0)=0: MW=.018: T=293: R=8.310001
FOR I=1 TO M
P(I)=P
Z(I+1)=Z(I)+DZ*I*I
V(I)=WD*(Z(I+1)-Z(I-1))/2
NEXT
P(M+1)=P(M): H(M+1)=H(M): Z(0)=-1E+20: Z(M+1)=1E+20: K(M+1)=KS*(PE/P(M+1)): N
GR=9.8: IM=.000001: DV=.000024: VP=.017
P(0)=P(1): K(0)=0: HA=.5
TI=TI+DT/3600
SE=0: FOR I=1 TO M: K(I)=KS*(PE/P(I)): NEXT
JV(0)=EP*(H(1)-HA)/(1-HA): DJ(0)=EP*MW*H(1)/(R*T)
260
270
280
290
300
310
320
330
340
350
360
370
380
390
400
410
420
430
440
450
460
470
480
490
500
510
520
530
540

40 INPUT "SOIL B VALUE"; B
40 INPUT "INITIAL WATER POTENTIAL -J/KG"; P; P=-ABS(P)
40 INPUT "SATURATED CONDUCTIVITY -KG/SM43"; KS
40 INPUT "SOIL B VALUE"; B
40 INPUT "SOIL BULK DENSITY -MG/SM43"; BD: WS=1-BD/2.6
40 PRINT "DEPTH TO LOWER BOUNDARY -M"; Z(M+1): DZ=Z(M+1)/A
40 B1=1/B: N=2+3/B: N1=1-N: WD=1000: DT=3600
40 Z(1)=0: Z(0)=0: MW=.018: T=293: R=8.310001
40 FOR I=1 TO M
40 P(I)=P
40 Z(I+1)=Z(I)+DZ*I*I
40 V(I)=WD*(Z(I+1)-Z(I-1))/2
40 NEXT
40 P(M+1)=P(M): H(M+1)=H(M): Z(0)=-1E+20: Z(M+1)=1E+20: K(M+1)=KS*(PE/P(M+1)): N
40 GR=9.8: IM=.000001: DV=.000024: VP=.017
40 P(0)=P(1): K(0)=0: HA=.5
40 TI=TI+DT/3600
40 SE=0: FOR I=1 TO M: K(I)=KS*(PE/P(I)): NEXT
40 JV(0)=EP*(H(1)-HA)/(1-HA): DJ(0)=EP*MW*H(1)/(R*T)
40 K(I)=K(I-1)/(Z(I+1)-Z(I-1))/2
40 P(I)=P(I)*K(I)/Z(I)/Z(I-1)/Z(I+1)/Z(I)
40 B(I)=B(I)/(Z(I)-Z(I-1))/Z(I)/Z(I+1)/Z(I-1)
40 F(I)=(P(I)*Z(I)-P(I-1)*K(I-1))/Z(I)-Z(I-1)
40 C(I)=C(I)/B(I)
40 P(I)=P(I)/B(I)
40 P(I)=P(I)+A(I)*C(I)
40 P(I)=P(I)+A(I)*C(I)
40 NEXT
40 DP(M)=F(M)/B(M): P(M)=P(M)-DP(M): IF P(M)>PE THEN P(M)=PE
40 FOR I=1 TO 1 STEP -1
40 DP(I)=F(I)-C(I)*DP(I+1): P(I)=P(I)-DP(I)
40 IF P(I)>PE THEN P(I)=(P(I)+DP(I)+DP(I))/2
40 NEXT
40 FOR I=1 TO M: W(I)=WS*(PE/P(I)): H(I)=EXP(MW*P(I)/(R*T))
40 NEXT
40 PRINT SE;: IF SE>IM THEN GOTO 230
40 EP=EP*(H(1)-HA)/(1-HA)
40 NEXT
40 FOR I=1 TO M-1
40 C(I)=C(I)/B(I)
40 P(I)=P(I)/B(I)
40 B(I+1)=B(I+1)-A(I+1)*C(I)
40 P(I)=P(I)+A(I+1)*C(I)
40 NEXT
40 DP(M)=F(M)/B(M): P(M)=P(M)-DP(M): IF P(M)>PE THEN P(M)=PE
40 FOR I=1 TO 1 STEP -1
40 DP(I)=F(I)-C(I)*DP(I+1): P(I)=P(I)-DP(I)
40 IF P(I)>PE THEN P(I)=(P(I)+DP(I)+DP(I))/2
40 NEXT
40 FOR I=1 TO M: W(I)=WS*(PE/P(I))+B1*H(I)=EXP(MW*P(I)/(R*T)): NEXT
40 PRINT SE;: IF SE>IM THEN GOTO 230
40 H(1)=H(M)
40 PRINT PRINT "TIME"; TI; "HRS"
40 PRINT "DEPTH (M)", "WC (M43/M43)", "MATRIC POT. (J/KG)", "SW=0"
40 FOR I=1 TO M: SW=SW+V(I)*(WN(I)-W(I)): PRINT Z(I), WN(I), P(I), W(I)=WN(I): NEXT
40 FL=EP*(H(1)-HA)/(1-HA)
40 PRINT "EVAP. RATE = "FL; " WC CHANGE = "SW/DT; " E/EP = "FL/EP
40 GOTO 220
upward flux from the bottom of the soil profile during evaporation. The profile can still drain through gravitational flux. This is not a realistic boundary condition for most field simulations, but it allows comparison of evaporation rates and drying profiles for varying soil textures without the complicating effects of upward flow. When simulating actual field situations, two-way flux across the bottom boundary would usually be required.

If vapor flux in the soil is ignored, lines 260, 270, and the humidity calculations (except one at the soil surface), could be deleted from the program. This would decrease execution time slightly, but probably not enough to compensate for the loss in accuracy of the model. Figure 9.1 is an example of the output of Program 9.1, and Fig. 9.3 compares predictions of the model with and without soil vapor flow.

9.7 MODELING LINKED TRANSPORT

The extension of Program 9.1 to include linked transport is fairly straightforward. It requires that the heat flow model from Program 4.1 be incorporated into Program 9.1. Though the combined model will not be given here, such models are required for detailed predictions of water distribution and fluxes in a drying soil over a diurnal cycle or for predictions of heat loss from buried powerlines and heating cables. Hammel et al. (1981) used a linked-transport model to predict seedzone moisture under summer-fallow conditions. They found that simulated seedzone moisture was higher when linked transport was assumed. Adequate seedzone moisture is often critical for the establishment of fall wheat in summer-fallow. Some farmers wait to plant until cool nights obtain, claiming that cool nights draw the moisture toward the surface sufficiently to allow germination. Simulations using linked-transport models confirm that upward moisture migration does occur under these conditions. Details of the linked transport model can be found in Hammel et al. (1981).
9.8 REFERENCES


9.9 PROBLEMS

9.1 Simulate first and second-stage evaporation with varying potential evaporation rates and soil texture. Plot the results. What effect does each of these have on the length of first stage evaporation?

9.2 Plot cumulative evaporation for varying potential evaporation rates. What effect does rate have on cumulative evaporation?

9.3 Compare moisture profiles for simulations with and without vapor flow in soil.
Chapter 10

SOLUTE TRANSPORT IN SOILS

The ability to predict the rate of movement of solutes in soils and the effect of the soil on this rate would be useful for many purposes. Knowing the rate of loss of various solutes carried in water moving out of the soil would assist in forming more accurate nutrient budgets and increase the understanding of nutrient cycling. Also, there is interest in knowing the amount and concentration of fertilizer nutrient below the root zone in order to design management schemes that minimize fertilizer losses and keep concentration of certain solutes, such as nitrate, within acceptable water quality standards. In addition, understanding the movement of pesticides and other toxic compounds, heavy metals, viruses, and radioactive materials, once they have been applied to soils, is essential to predicting their impact on the environment. A knowledge of transport in soils is also employed to reclaim salt-affected soils and to devise management practices for irrigated crop land to prevent excessive salt accumulation in soil. Finally, an understanding of solute transport to roots would allow better prediction of the effect of soil on plant nutrition.

Equations describing the movement of a solute through a porous medium such as soil have been derived and investigated by many researchers (Nielsen and Biggar, 1961; Bresler, 1973; Selim et al., 1977). These equations use both analytical and numerical techniques to describe non-interacting as well as interacting solute transport. A particularly good summary of the work is given by Bresler et al. (1982). These equations will be developed in the following sections beginning with the simple case of a non-interacting solute. Following this, some consideration will be given to situations where solutes interact with the soil.

10.1 MASS FLOW

Chemical species dissolved in water are transported with the water. This type of transport is termed the mass flow of solutes. The change in concentration with time, at a given point in the soil, of a solute moving by steady mass flow, can be described by the equation:

$$\rho_b \frac{\partial S}{\partial t} = f_w \frac{\partial c}{\partial z}$$  \hspace{1cm} (10.1)

where \( c \) is solute concentration in the soil solution (kg/kg), \( S \) is solute present per unit mass of soil, \( f_w \) is water flux density (kg m\(^{-2}\)s\(^{-1}\)), \( z \) is soil depth (m), \( \rho_b \) is bulk density (kg m\(^{-3}\)), and \( t \) is time (s).
A very simple model of solute transport is obtained by assuming that flow through all the soil pores is of uniform velocity. In this case, the flux of a solute into and out of a soil can be described by eq 10.1 if the initial solute concentration and water flux density in the soil are known. A typical method used to compare calculated solute flow to actual solute flow is to establish a saturated column of soil in the laboratory where water flow is initiated in the column at a rate, $f_w$. A slug of solute then is introduced at the top of the column and the amount of water moving through the column, as well as the solute concentration in the water at the bottom of the column, is measured. If the solute moved only through mass flow, and the flow of all the water in all pores were uniform, then the breakthrough curve of the solute would appear as in Figure 10.1a. This is termed piston flow.

![Diagram](image)

**Fig. 10.1.** Convection (a) without and (b) with dispersion. Initial concentration of the solute is low. At time 0, solute with concentration $c_0$ is introduced at the top of the column. $c/c_0$ is the ratio of outflow to inflow concentration.
The amount of time required for the solute to appear in the outflow is equal to the amount of time taken to replace all the water in the soil (one pore volume) with the introduced water. This depends on \( f_w \), the water flux density in the soil column. Increasing or decreasing the hydraulic conductivity would increase or decrease the time taken for the solute to appear, but would not change the shape of the breakthrough curve.

It is, of course, not realistic to assume that all the water in all the pores is moving at the same speed. If we accept that the Hagen-Poiseuille equation, developed to describe the flux of water in cylindrical tubes, can at least qualitatively describe the influence of viscosity on water flow in non-uniform soil channels, then we can assume that water flux density will be directly proportional to the square of the pore radius (eq. 6.4). In other words, water, along with the solutes dissolved in it, will move fastest through the largest pores. Solute flowing in channels of average pore size would break through after one pore volume. Solute in larger channels would break through sooner than the average, and water in small pores would come through well behind the average. The result would be a breakthrough curve like Fig. 10.1b. Furthermore, these curves cannot be expected to be linearly correlated with the pore size; the variations around the "average" hydraulic conductivity will not have a Gaussian distribution (Van de Pol et al., 1977).

Solute transport due to mass flow, therefore, might be more precisely described by the equation

\[
p_b \frac{\partial S}{\partial t} = (\partial c/\partial z) f_w \]

where \( f_w = -k_i \partial \psi/\partial z \), \( k_i \) is a function of both pore size and the number of pores in a pore size class, and \( f_w \) is the water flux density per pore.

Laminar flow through a porous medium further complicates the mass flow of solutes because flow within a single pore is not uniform (i.e. there is a gradient in velocity within the pore). According to Newton's law of viscosity, this gradient in velocity will be proportional to the shear force in the flowing liquid, divided by the viscosity. The water flux density at any one point in the pore is therefore a function of distance from the center of the pore

\[
f_w = \rho_w (a^2 - r^2)/4v (\Delta P/\Delta x) \]

where \( a \) is the radius of the pore, \( r \) is the radial distance from the center of the pore and \( v \) is viscosity. In other words, solutes dissolved in water near the side of the pore will flow more slowly than those in the middle of the pore.
In summary, two major problems involved with predicting the mass flow of solutes in soil are 1) determining the effect of differing water velocities in different sized pores, and 2) determining the effect of differing water velocities within a single pore. One solution to these problems has been to place the dispersing effect that different pore sizes has on solute flow in the diffusion rather than the mass flow portion of the solute transport equation.

10.2 DIFFUSION AND HYDRODYNAMIC DISPERSION

Solutes move in response to concentration gradients, as well as moving with water in response to hydraulic potential gradients. The equation for such movement is called the Fick diffusion equation, and can be written as

\[ \frac{\partial c}{\partial t} = D \left( \frac{\partial^2 c}{\partial z^2} \right) \]

where \( D \) is a diffusion coefficient \((m^2s^{-1})\) which can include both molecular diffusion and hydrodynamic dispersion.

In order to predict the change in concentration of a solute with time due to diffusion, eq 10.4 indicates that both the concentration gradient of the solute and the diffusion coefficient must be known. When there are no sources or sinks for the solute in the soil, then in order to predict \( c \) as a function of depth and time, we need only to know the initial concentration of the solute in the soil and the amount of solute being introduced at the surface of the soil as a function of time. The cases involving active sources and sinks are more complex and will be dealt with later in the chapter.

Diffusion coefficients for various solutes in free water are available in handbooks. However, to predict the diffusion of an ion in soil we must use a diffusion coefficient that accounts for both the tortuosity in a porous medium such as soil and the cross-sectional area of water available for diffusion (which is a function of the water content of the soil).

Several equations have been proposed for calculating the molecular diffusion of an ion in soil. One commonly used equation was proposed by Bresler (1973):

\[ D_m = D_o \ e^{b\theta} \]  

(10.5)

where \( D_o \) is the diffusion coefficient of the ion in water \((m^2 \text{s}^{-1})\) and \( a \) and \( b \) are soil-dependent constants. Papendick and Campbell (1980) later proposed the equation

\[ D_m = D_o \ e^{3\theta} \]  

(10.6)
where \( a \) is a constant (around 2.8) to account for tortuosity. Equations 10.5 and 10.6 give similar results except in dry soil where eq. 10.6 appears to give more realistic values. Diffusivity is predicted to decrease rapidly with decreasing water content by both equations.

As mentioned earlier, the fact that the convective transport of a solute cannot be accurately described by an average water flux density has led to the inclusion in the diffusion coefficient of a term for hydrodynamic dispersion. Bresler (1973) suggests that the diffusion coefficient for eq. 10.4 be calculated from

\[
D = D_m + \kappa f_w / \theta 
\]

where \( \kappa \) is a soil dependent constant. The dispersion effect, \( (\kappa f_w / \theta) \) is a function of \( f_w \) and at most flow rates is more important than real diffusion (Nye and Tinker, 1977; Olsen and Kemper, 1968). Figure 10.2 compares the two components in eq. 10.7 for varying water flux.

10.3 SOLUTE-SOIL INTERACTION

In eqs 10.1 and 10.4, the flux of solute is determined by the concentration in solution, \( c \), while the storage at any point in the soil is shown by changes in the variable, \( S \). Before the transport equation can be solved, the relationship between \( c \) and \( S \) must be specified. This relationship may be extremely complex. In addition to the solute in solution, that present in a solid phase, or in complexed and exchangable forms must be included.

Fig. 10.2. Comparison of molecular diffusion and hydrodynamic dispersion as a function of flow velocity (after Olsen and Kemper, 1968)
The presence of each of these can depend on the concentrations of other solutes as well as the exchange characteristics of the soil. Equilibrium chemistry models are available for determining the concentrations of a suite of ions and complexes in soil, and such models have been used in conjunction with water flow models to predict transport and precipitation of salts in calcareous and gypsiferous soils (Robbins et al., 1980). Often the absorbed and solution-phase solute concentrations can be related by a Langmuir equation:

\[ N = \frac{kQc}{(1+kc)} \]  \hspace{1cm} (10.8)

where \( k \) and \( Q \) are constants for a given soil and solute. These constants depend on the CEC of the soil and concentrations of other ions in the soil solution. Values for \( k \) and \( Q \) would normally be found from experiments or the more complete equilibrium chemistry models mentioned previously. Values from Smith (1979) for ammonium, phosphorus, and potassium are given in Table 10.1.

<table>
<thead>
<tr>
<th>Solute</th>
<th>( k ) (kg water/kg salt)</th>
<th>( Q ) (kg salt/kg soil)</th>
<th>( kQ ) (kg water/kg soil)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phosphorus</td>
<td>( 3 \times 10^5 )</td>
<td>( 2 \times 10^{-4} )</td>
<td>60</td>
</tr>
<tr>
<td>Potassium</td>
<td>( 8 \times 10^2 )</td>
<td>( 8 \times 10^{-3} )</td>
<td>6.4</td>
</tr>
<tr>
<td>Ammonium</td>
<td>( 2 \times 10^3 )</td>
<td>( 3 \times 10^{-3} )</td>
<td>5.6</td>
</tr>
</tbody>
</table>

The total amount of solute in the soil is the sum of the adsorbed phase and the solution phase, and is given by

\[ S = N + wc \]  \hspace{1cm} (10.9)

where \( w \) is the mass-basis water content (kg/kg).

Solute concentrations in soil often are sufficiently low that the denominator of eq. 10.8 is near unity. For these conditions, eq. 10.9 becomes

\[ S = (kQ + wc) \]  \hspace{1cm} (10.10)

Equation 10.10 allows the comparison of quantities of adsorbed and solution-phase solutes. For the soil represented by the values in Table 10.1, at a water content of 0.2, the adsorbed phase contains 300 times as much phosphorus, 32 times as much potassium, and 28 times as much ammonium as the solution phase. Changes in soil pH and CEC will influence these values, but these numbers give some idea of amounts of these nutrients in the soil.
solution compared to total soil amounts. For non-interacting solutes such as Cl\textsuperscript{-}, NO\textsubscript{3}\textsuperscript{-}, or SO\textsubscript{4}\textsuperscript{2-}, eq. 10.10 still can be used, but k is set to zero.

10.4 SOURCES AND SINKS OF SOLUTES

In addition to dissolution-precipitation reactions, which are treated by equilibrium chemistry models, biological sources and sinks of solutes must be considered. Nitrification consumes ammonium and produces nitrite and nitrate. Ammonium is a product of decomposition. Microbes and roots take up nutrients from the soil solution. Detailed models of these processes are given by Smith (1979) and Nye and Tinker (1977).

10.5 NUMERICAL SOLUTIONS TO SOLUTE TRANSPORT PROBLEMS

Solving the convection-dispersion solute transport equations requires methods similar to those used previously for other transport problems. The first step is to write the mass balance for a solute at node i:

\[
F_i = \frac{\rho_i (s_i^{j+1} - s_i^j) \Delta z_i}{\Delta t} - f_{i-1} (\delta_{i-1} - \varepsilon_{i-1} - \zeta_{i-1}) + f_i (\delta_i - \varepsilon_i - \zeta_i) + A_i \\
- \frac{\nu D_i (\zeta_i - \zeta_{i-1})}{z_i - z_{i-1}} + \frac{\nu D_i (\zeta_{i+1} - \zeta_i)}{z_{i+1} - z_i} + A_i
\]

Here f represents the water flux and A the sink. The concentrations are mean values over the time step calculated from

\[
\bar{c} = \eta c_i^{j+1} + (1-\eta) c_i^j
\]

the \(\delta's\) and \(\varepsilon's\) are defined such that

\[
\delta = 1, \varepsilon = 0 \text{ for } f > 0 \\
\delta = 0, \varepsilon = 1 \text{ for } f < 0 \\
\delta = \varepsilon = 0 \text{ for } f = 0
\]

Finally, \(\Delta z = (z_{i+1} - z_{i-1})/2\).

Concentrations, as functions of time and depth, are found by solving the water flow equations for the f's. Mass balance equations like 10.11 are written for each node in the soil, and these are solved for the solute concentrations, using the Newton-Raphson method. Solutions are found for each of the solute species of interest.
10.6 STEADY FLOW SOLUTIONS

It is useful to consider simple solute transport models in order to determine their characteristics and investigate special problems which arise in convection models. We will consider solute transport with a steady downward flux of water. Sources and sinks, as well as diffusion and dispersion, will be excluded from consideration. With these simplifications, eq. 10.11 becomes

\[ \rho_b (s_i^{j+1} - s_i^j) \Delta z / \Delta t = f_w (c_{i-1} - c_i) \] (10.13)

Now, if \( \eta = 0 \) and solute concentrations are low enough for eq. 10.10 to be valid, eq. 10.13 can be rearranged to give

\[ c_i^{j+1} = c_i^j + f_w \Delta t (c_{i-1}^j - c_i^j) / [\rho_b (kQ + w) \Delta z] \] (10.14)

Consider first a non-interacting solute, where \( k = 0 \). The combination of terms

\[ v^*_w = f_w \Delta t / \rho_b \Delta z \] (10.15)

is a dimensionless water velocity equal to the fraction of the pore volume associated with one node that is swept out by the moving water in one time step. If \( v^*_w = 1 \), then, from eq. 10.14,

\[ c_i^{j+1} = c_i^{j-1} \] (10.16)

The solute concentration at node \( i \) is just the concentration at node \( i-1 \) at the previous time step. Transport with \( v^*_w = 1 \) would simulate piston flow, with a sharp boundary between the inflowing and antecedent concentrations.

Values for \( v^*_w > 1 \) are not allowed, but values of \( v^*_w < 1 \) produce an interesting result. Physically, if less than one pore volume moves during a time step, the solute front does not reach the next node by the end of the time step. However, numerically, according to eq. 10.14, any concentration difference between nodes results in a "numerical dispersion" which smears the solute front in a way similar to physical diffusion and dispersion. van Genuchten and Wierenga (1974) show that the numerical dispersion resulting from the forward difference approximation used in eq. 10.14 is equivalent to the physical dispersion that would occur with a dispersion coefficient of

\[ D_n = v_o (\Delta z - v_o \Delta t) / 2 \] (10.17)
where \( v_o \) is the pore water velocity, given by

\[
v_o = \frac{f_w}{D_{ww}}.
\]  

(10.18)

This provides the justification for omitting dispersion in eq. 10.13. If values for \( \Delta z \) and \( \Delta t \) are correctly chosen, numerical dispersion can substitute for physical dispersion. At low velocity, when \( v_o \Delta t << \Delta z \), numerical dispersion even has the same dependence on \( f_w \) that is assumed in eq. 10.7; but at larger velocities or time steps, \( D_n \) decreases with increasing velocity. The more complete transport equation (eq. 10.11) can be corrected for numerical dispersion by subtracting \( D_n \) from \( D \). It seems more appropriate, however, to leave out the physical dispersion terms and use numerical dispersion to substitute, since the models are simpler and more easily solved. If the desired dispersion coefficient is known, the appropriate time step is selected by rearranging eq. 10.17 to give

\[
\Delta t = \frac{\rho_w (\Delta z - 2D_{pw}c/f_w)}{f_w}.
\]  

(10.19)

10.7 NUMERICAL SOLUTION OF THE STEADY FLOW EQUATIONS

Numerical simulation of steady solute transport, where \( S \) is linearly related to \( c \), is simple and fast, since no implicit equations are involved. Equation 10.14 is used at each node to calculate the concentration at the new time from the new concentration at the upstream node and the old concentration at the solution node. Changes in amount are accounted for automatically through eq. 10.10. A simple BASIC program is shown as Program 10.1. The program, though simple, will allow experimentation with many aspects of the solute transport problem. Flow is steady, but may be saturated or unsaturated, depending on the choice of water content. If saturated flow is desired, any number equal to or larger than the saturation water content may be entered and the program will set water content and hydraulic conductivity to the saturation values. The water flux is assumed to result only from a gradient in the gravitational potential. The flux density is computed in line 130.

The solute interaction value, \( kQ \), is entered in line 70. For a non-interacting solute such as chloride or nitrate, \( kQ = 0 \). Values for some interacting solutes are given in Table 10.1.

Various choices of boundary and initial conditions are offered in lines 90-110. Dimensionless concentrations are used for convenience, though actual concentrations would work as well. As long as the relationship between amount and concentration is linear (eq. 10.10), the actual numbers used for the
PROGRAM 10.3 SIMULATION OF SOLUTE TRANSPORT WITH NUMERICAL DISPERSION

10 INPUT "HYDRAULIC CONDUCTIVITY-KG/S/M+3";KS
20 INPUT "SOIL B VALUE";B
30 INPUT "BULK DENSITY-MG/M+3";BD
40 INPUT "WATER CONTENT-KG/KG";W: IF W*BD>1-BD/2.65 THEN W=(1-BD/2.65)/BD
50 INPUT "TIME STEP-S";DT
60 INPUT "NODE SPACING-M";DZ
70 INPUT "SOLUTE INTERACTION KG-KG/KG";KQ
80 INPUT "NUMBER OF NODES";N: DIM C(N+1),CN(N+1)
90 INPUT "PULSE LENGTH-HRS";PL
100 INPUT "DIMENSIONLESS ANTECEDENT CONCENTRATION-C/CO";C
110 INPUT "DIMENSIONLESS INFLOW CONCENTRATION-C/CO";C(1):CN(1)=C(1)
120 FOR I=2 TO N+1:C(I)=C(N+1):NEXT
130 JW=9.8*KS*(W*BD/((1-BD/2.65)^2*(2*B+3))
140 V=JW*DT/(DZ*BD*1000*(KQ+W)):IF V>1 THEN DT=DT/2:GOTO140
150 TI=TI+DT/3600:IF TI>=PL THEN F1=1 ELSE F1=2
160 FOR I=F1 TO N+1
170 CN(I)=C(I)+V*(C(I-1)-C(I))
180 NEXT
190 PRINT "TIME=";TI;"HRS JW=";JW;"KG/M\[2/S V*=";V
200 PRINT "TOTAL OUTFLOW =";JW*TI*3600;" MM ";
210 PRINT "OUTFLOW CONCENTRATION =";CN(N+1):PRINT "DEPTH","CONCENTRATION"
220 FOR I=1 TO N+1:PRINT (I-1)*DZ, CN(I);C(I)=CN(I):NEXT
230 PRINT:PRINT
240 GOTO 150

Solute transport calculation do not influence the result. This would not be the case for a non-linear adsorption relation, of course.

By setting the inflow concentration in line 110, two things are accomplished. First, the initial concentration and amount at the top of the profile are established. Second, if PL>0 in line 90, the concentration in line 110 becomes a constant concentration boundary condition at the soil surface for the duration of the time set in PL. Large values of PL simulate a complete flushing of the soil by the new solution. Smaller values simulate a pulse. The rate of redistribution of a broadcast fertilizer application, for example, could be simulated by setting PL to zero, with an inflow concentration of 1. The fertilizer would then be removed from node 1 and transported to the lower nodes.

In line 140, V* is calculated and checked to assure that it is less than or equal to unity, so that solutions to the flow equation are stable. If
If $v > 1$, $DT$ is reduced and a new value of $v^*$ is calculated. If it were desirable to match a given dispersion coefficient, eq. 10.19 could be used in place of line 140. In line 150, the time counter is incremented and the boundary condition determined. If $T > PL$, then pure water is assumed to be flowing in. Otherwise, the inflow concentration is set to the value provided in line 110. Obviously either salt loading or unloading of a column can be simulated by proper choices of inputs in lines 100 and 110. Program output gives total water efflux and salt concentration in the outflow.

Figure 10.4 compares output from this model with an analytical solution to the transport equation given by van Genuchten and Wierenga (1974). Numerical dispersion has been set to just substitute for physical dispersion. A line showing the effects of combined physical and numerical dispersion is also shown.

Fig. 10.3. Comparison of numerical and analytical solutions to the solute transport equation. The analytical solution (solid line) and the numerical solution with diffusion and numerical dispersion (dashed line) are from van Genuchten and Wierenga (1974). The numerical solution with numerical dispersion substituting for physical dispersion (o) was calculated from Program 10.1 with $t=3240$ s, $x=3$ cm, $k_s=2.362 \times 10^{-4}$ kg s $^{-3}$, $p_h=1.325$ kg $m^{-3}$, $w=0.377$ kg/kg, $PL=18$ hrs, total simulation time = 36 hrs.
10.8 EFFECT OF SALT ON WATER FLOW

The discussions in Chapter 5 indicated that a gradient in osmotic potential can provide a driving force for water flow under some conditions. Osmotic potential gradients are usually present whenever there are solutes in the soil solution. It is therefore important to know whether these gradients significantly influence water flow.

Solute which are completely free to move within the soil cannot provide a driving force for water flow. On the other hand, solutes which cannot move can give rise to osmotic potential gradients which are as effective as matric or gravitational potential gradients in causing water to move. The steady water flow equation is usually written as

\[ f_w = -k(\psi_m/dz + \psi_g/dz + \sigma_s d\psi_o/dz) \]  

(10.20)

where \( k \) is the hydraulic conductivity and \( \sigma_s \) is a reflection coefficient. The reflection coefficient is a measure of the effectiveness of osmotic potential gradients in driving water flow. A vapor gap gives \( \sigma_s=1 \), for low vapor pressure solutes. Plant membranes generally have \( \sigma_s=1 \). Soil, however, generally has \( \sigma_s \) values close to zero. Letey et al. (1969) reported values around 0.03 at water potentials of -25 to -100 J/kg. It would appear that water flow resulting from osmotic potential gradients generally need not be considered.

10.9 NUMERICAL SOLUTIONS WITH TRANSIENT FLOW

For a complete simulation of water and solute movement in the field, the equations from this chapter are combined with the water flow programs from Chapters 8 and 9. Simulation of root uptake of water and nutrients would also be required in addition to subroutines for microbial uptake, release, and transformation of solutes. Ideally, eqs. 10.11 and 10.20 would be used with corrections for numerical dispersion. Results from such a model are described by Bresler et al. (1982). They found field variability to be so large that solute effects on water flow and precise dispersion corrections are negligible by comparison. They suggest using the simple convection equations with numerical dispersion. These results would suggest using only the first three terms on the right hand side of eq. 10.11 in the solute transport subroutine of the flow model. The time-step of the solute transport model could be made independent of the time step in the water model, using only average fluxes from the water model, so that any desired dispersion coefficient could be simulated.
10.10 APPLICATION TO NUTRIENT TRANSPORT

A simulation such as that in Program 10.1 can be useful in understanding nutrient-soil interaction. Nutrients are often classified as either "mobile" or "immobile". These generalizations are useful for determining where samples should be taken to determine fertilizer requirements and how fertilizer should be applied for best availability, but they can be misleading. It should be obvious from the discussion earlier in this chapter that all nutrients are mobile. The question is not whether or not they move, but rather, how fast they move. These simulations, together with appropriate constants for the nutrients and soils of interest, should give a better understanding of rates of nutrient redistribution in soil.
10.11 REFERENCES


10.12 PROBLEMS

1. Use Program 10.1 to determine the distribution of NO$_3^-$, K$^+$, NH$_4^+$, and phosphorus in a fallow soil after a broadcast application of these nutrients. Assume 200 mm or more of infiltration.

2. Modify Program 10.1 to allow specification of a dispersion coefficient, and then rerun the experiment shown in Fig. 10.3 for various dispersion coefficients.
Chapter 11

TRANSPERSION AND PLANT-WATER RELATIONS

Now that models have been developed for water and solute transport in soil, consideration can be given to the interaction between the physical environment described by such models and biological systems that are influenced by that environment. A very important concern which fits into this category is that of water transport and water potentials in the soil-plant-atmosphere-continuum (SPAC). Water flows from soil to roots, through xylem, through mesophyll cells and cell walls, and finally evaporates into substomatal cavities. It then diffuses out of the stomates, through the leaf and canopy layers, and is mixed with the bulk atmosphere. Water potential is highest in the soil, and decreases along the transpiration path. This potential gradient provides the driving force for water transport from the soil to the atmosphere. Water potentials, water fluxes, and resistances to flow in the SPAC will be considered in this chapter.

11.1 GENERAL FEATURES OF WATER FLOW IN THE SPAC

Figure 11.1 shows a simple analog of the SPAC and indicates where the most important resistances and potentials are located. Evaporation from the

Fig. 11.1. Analog of the SPAC showing potentials and resistances.
leaf is shown as a current source since the plant water potential has no direct effect on the flux (humidity in substomatal cavities is always near 1.0). Since van den Honert (1948) it has been popular to use analogs such as Fig. 11.1 to describe the potentials in the SPAC in the form

$$E = \frac{\psi_{XL} - \psi_L}{R_L} = \frac{\psi_{XR} - \psi_{XL}}{R_X} = \frac{\psi_r - \psi_{XR}}{R_r} = \frac{\psi_s - \psi_r}{R_s} \tag{11.1}$$

where $E$ is transpiration rate (kg m$^{-2}$ s$^{-1}$), $R$ is resistance (m$^4$ kg$^{-1}$ s$^{-1}$) and $\psi$ is water potential (J/kg). The equation, in this form, is similar to the steady state oxygen diffusion problem considered in Chapter 3. All of the potentials can be predicted if the flux and the soil water potential are known. Before actually doing that, however, some simple predictions from eq. 11.1 will be considered.

If an overall resistance is defined as the series combination of all resistances in Figure 11.1, then

$$E = \frac{\psi_s - \psi_L}{R}. \tag{11.2}$$

This equation can be rearranged to predict leaf water potential:

$$\psi_L = \psi_s - ER. \tag{11.3}$$

Equation 11.3 predicts that leaf water potential will be below soil water potential by an amount determined by transpiration rate and resistance to transport. When soil moisture is not limiting, $E$ is independent of $\psi_L$, and $R$ is about constant, so $\psi_L$ just varies with $E$. Figure 11.2 shows a simulation of leaf water potential as it responds to fluctuations in $E$. Until soil water becomes limiting, this response apparently is passive and has little, if any, direct effect on photosynthesis of leaves.

Turgor in leaves is $\psi_p = \psi - \psi_o$, and therefore fluctuates with $E$. Decreased turgor does slow cell expansion, and therefore may indirectly affect plant photosynthesis over time by reducing the photosynthetic area. Reduced turgor apparently does not affect photosynthesis of leaves that are already in place until stomatal closure begins.

It seems reasonable to assume that water stress responses in plants depend on some integrated value of the turgor pressure, since the turgor pressure combines factors of soil water supply, atmospheric demand, and plant osmotic potential. This has not yet been proven, however. It also seems apparent that a plant's response to water stress is such that some turgor is maintained. The response to short-term stress is to close stomates, reducing $E$ so that $\psi_L$ is increased. The response to prolonged stress, for many
species, is to reduce leaf area index so that the leaves that remain are operating at maximum efficiency.

With these ideas in mind, each of the resistances in the transpiration stream will be considered, and the relationship between transpiration rate and leaf water potential will be determined.
11.2 RESISTANCES TO WATER FLOW WITHIN THE PLANT

From Chapter 6 we know that soil conductance is high when soil is wet. Measurements of water potentials and fluxes for transpiring plants growing in moist soil can therefore be used to find plant resistances. Measurements typically show that xylem resistance is negligible compared to other resistances, though notable examples to the contrary are found in diseased plants and spring-sown cereals (Passioura, 1972). The major resistances within the plant are at the endodermis, where water enters the root stele, and in the leaf, perhaps at the bundle sheath. Water may flow in cell walls and xylem vessels through most of the transpiration stream, but must cross membranes at the endodermis and perhaps at the bundle sheath. For typical plants growing in moist soil, the potential drop across the endodermis is 60 to 70% of the total. Thirty to forty percent of the potential drop is at the leaf. This may be demonstrated by stopping transpiration on a leaf by covering it with aluminum foil and a polyethylene bag and measuring its water potential after allowing a few hours for equilibration. The water potential of the covered leaf is equal to the water potential of the xylem. If the soil resistance and water potential are negligible, then the ratio of xylem water potential to water potential of a freely transpiring leaf is equal to the ratio of root resistance to total resistance (eq. 11.1).

Rough estimates of plant resistance can be made by considering typical potentials and transpiration rates. In a potato crop, for example, after canopy closure, typical leaf water potentials are around -1200 J/kg when transpiration rate is $2.4 \times 10^{-4}$ kg m$^{-2}$ s$^{-1}$, so a typical total resistance would be around $5 \times 10^6$ m$^4$ s$^{-1}$ kg$^{-1}$ and the leaf resistance would be $2 \times 10^6$ m$^4$ s$^{-1}$ kg$^{-1}$. The root resistance is the difference, or $3 \times 10^6$ m$^4$ s$^{-1}$ kg$^{-1}$. The xylem resistance is perhaps a factor of 10 smaller than these in a healthy plant.

For modeling purposes, it is often useful to have an estimate of the resistance per unit length of root. This can be used with estimates of root density to find the resistance to water uptake for any soil layer. Data which provide rooting density estimates, transpiration measurements, and water potentials are difficult to find, but some values are given by Bristow et al. (1984) for sunflower. They found values of resistance per unit length of root of $2.5 \times 10^{10}$ m$^3$ kg$^{-1}$ s$^{-1}$. To check this against the calculation just made for potato, a rooting depth of 0.3 m and a root density of $3 \times 10^4$ m$^{-2}$ (meters of root per cubic meter of soil) might be assumed. The resistance per meter of root divided by the length of root per square meter of ground area gives the root resistance. For potato this calculation gives $R_r = 2.8 \times 10^6$ m$^4$ s$^{-1}$ kg$^{-1}$, which is close to the estimate given above.
11.3 EFFECT OF ENVIRONMENT ON PLANT RESISTANCE

It is difficult to find quantitative information on the relationship between resistances to water flow and environmental variables for plants growing in field conditions. Several qualitative observations are possible, however. Since water crosses living cells at the endodermis, anything that affects cell metabolism affects resistance. Decreases in temperature, decreases in oxygen supply, and decreases in root water potential all decrease root permeability, and therefore increase resistance to flow across the endodermis.

11.4 DETAILED CONSIDERATION OF SOIL AND ROOT RESISTANCES

The resistances encountered by water as it flows from the bulk soil to the root xylem are highly variable in both space and time. These resistances are the ones most susceptible to alteration by management practices, so a knowledge of their response to environment is important if the soil is managed for maximum crop production.

An electrical analog of the root-soil system similar to that suggested by Hillel (1980) is shown in Figure 11.3. At each level in the soil, a soil and a root resistance are in series. Axial resistances within the root are

![Electrical analog of the soil-root system](image)

Fig. 11.3. Electrical analog of the soil-root system showing water potential with depth in the soil and soil and root resistances to water uptake.
also shown, though for computations these are assumed to be negligible compared to soil and root resistances. An interfacial resistance for coarse-textured soil (Bristow et al. 1984) can be added to the soil resistance to simulate water uptake in sandy soils.

The resistance to water uptake in any soil layer, \( i \), is inversely proportional to the length of root in that layer. Therefore, for the root resistance in layer \( i \):

\[
R_{ri} = \frac{\rho_r}{L_i \Delta z}
\]  

(11.4)

where \( \rho_r \) is the resistance per unit length of root, \( L_i \) is the density of the root system in layer \( i \), and \( \Delta z \) is the depth of the layer. Gerwitz and Page (1974) describe root density as a function of depth using the equation

\[
L_i = L_0 \exp(-az_i)
\]  

(11.5)

where \( L_i \) is the root density \((m^{-2})\) (length of root per unit volume of soil) at depth \( i \), \( L_0 \) is the rooting density at the surface, and \( a \) is the reciprocal of the depth at which \( L_i \) is 63% of \( L_0 \). Integrating eq. 11.5 between any two depths in the soil, we obtain an expression for the average root density in layer \( i \):

\[
L_i = L_0 \left[ \exp(az_{i-1}) - \exp(az_{i+1}) \right] / (z_{i+1} - z_{i-1})
\]  

(11.6)

Some typical root distributions are given by Robertson et al. (1980).

The resistance of the soil for water flow to roots is determined by soil hydraulic conductivity, root density, and water uptake rate (Gardner, 1960; Cowan, 1965). An equation for this resistance is obtained by considering uptake of water from soil by a cylindrical root. If the rate of water uptake by a root is \( q \) (kg/s) then

\[
q/A = -k \frac{d\psi_m}{dr}
\]  

(11.7)

where \( k \) is unsaturated hydraulic conductivity, and \( r \) is the radial distance from the center of the root. If we assume steady flow, then \( q \) is constant with \( r \). The area is \( A = 2\pi r l \), where \( l \) is the length of root. Substituting eq. 6.14 into 11.7, and integrating from the root surface, \( r_1 \) to a distance, \( r_2 \) which represents the mean distance between roots, gives

\[
\frac{(q/2\pi l)\ln(r_2/r_1)}{1-n} = \frac{(k_2\psi_2 - k_1\psi_1)}{(1-n)}
\]  

(11.8)
The water uptake per unit length of root can be related to the root density, soil depth, and water extraction rate by

\[ \frac{q}{L} = \frac{E_i}{L_i \Delta z_i} \quad (11.9) \]

where \( E_i \) is the uptake rate from soil layer \( i \), \( L_i \) is the rooting density, and \( \Delta z_i \) is the thickness of the soil layer. The mean distance between roots is (Gardner, 1960)

\[ r_2 = (\pi L_i)^{-\frac{1}{2}} \quad (11.10) \]

Making these substitutions and solving for \( E_i \),

\[ E_i = \frac{(k_{ri} \psi_{ri} - k_{si} \psi_{si})}{B_i} \quad (11.11) \]

where

\[ B_i = (1-n) \ln(\pi r_i^2 L_i)/(4 \pi L_i \Delta z_i) \quad (11.12) \]

It is interesting to note that eq. 11.11 predicts a maximum rate at which water can be taken up by the plant. If \( \psi_{ri} \) were \(-\infty\), \( k_{ri} \) would approach zero, and \( E_i \) would equal \( k_{si} \psi_{si}/B_i \), which is constant for a given soil water potential.

The soil resistance to water uptake is

\[ R_{si} = \frac{(\psi_{si} - \psi_{ri})}{E_i} \quad (11.13) \]

so, using eq. 11.11

\[ R_{si} = \frac{B_i(\psi_{si} - \psi_{ri})/(k_{ri} \psi_{ri} - k_{si} \psi_{si})}{(11.14)} \]

Using these equations for soil and root resistance, and returning to Fig. 11.3, the analysis of water uptake can be continued. The transpiration rate must be the sum of the rates of water extraction for each of the soil layers:

\[ E = \sum E_i \]

so

\[ E = \sum (\psi_{si} - \psi_{ri})/(R_{si} + R_{ri}). \quad (11.15) \]

If it can be assumed that the axial resistances are small compared to other resistances, then eq. 11.15 can be solved for \( \psi_{ri} \).
\[ \psi_{XR} = \{ -E + \Sigma \left[ \psi_{S_i}/(R_{S_i} + R_{r_i}) \right]/\Sigma \left[ 1/(R_{S_i} + R_{r_i}) \right] \} \]  

(11.16)

The leaf water potential is given by (assuming negligible xylem resistance)

\[ \psi_L = \psi_{XR} - E R_L \]  

(11.17)

so, using eq. 11.16

\[ \psi_L = \frac{\Sigma \left[ \psi_{S_i}/(R_{S_i} + R_{r_i}) \right]}{\Sigma \left[ 1/(R_{S_i} + R_{r_i}) \right]} - \frac{E}{\Sigma \left[ 1/(R_{S_i} + R_{r_i}) \right]} - ER_L \]  

(11.18)

The first term on the right in eq. 11.18 can be considered a weighted mean soil water potential, \( \bar{\psi}_S \). This can be seen by noting that, when \( E = 0 \), \( \psi_L \) equals \( \bar{\psi}_S \). The last term is the transpiration rate multiplied by the sum of two resistances, \( R_L \), and a weighted mean root-soil resistance, \( R_{sr} \).

### 11.5 Numerical Implementation

The equations we have developed can now be put together in a computer program which will simulate water uptake and loss by plants. Program 11.1 provides such a simulation. The program through line 600 is similar to Program 9.1. The subroutine at line 1000 computes potential evapotranspiration and partitions it between potential evaporation and potential transpiration by simply assigning 10% to evaporation and the rest to transpiration. More sophisticated subroutines for this will be given in Chapter 12. The subroutine at line 2000 computes soil resistance, actual transpiration rate, leaf water potential, and water uptake from each layer. Water uptake (\( E(I) \)) for each layer becomes a sink term for the mass balance equation in line 340.

The soil resistance is a non-linear function of the water potential at the root surface (eq. 11.14), which, in turn, depends in a complex way on the rate of uptake of water from each soil layer, and rate of water loss from the plant. An iterative method which finds the correct soil resistances, water uptake rates, and water potentials is possible, but difficult and slow to run on the computer. Since soil resistance is seldom large enough to contribute significantly to the overall resistance, an approximate soil resistance is used. This is calculated in line 2030 for each layer by assuming that the conductivity is constant in the rhizosphere. In line 2060 the weighted mean soil water potential and weighted mean resistance are calculated. Lines 2070-2110 calculate actual transpiration rate from potential transpiration rate and water uptake rate. The equations are based on the assumption that transpiration rate is inversely related to stomatal resistance, and that
' PROGRAM 11.1 SIMULATION OF EVAPOTRANSPIRATION AND PLANT WATER POTENTIAL

M=12: X=M+1
DIM A(X), B(X), C(X), F(X), P(X), Z(X), V(X), DP(X), W(X), WN(X), K(X), CP(X), H(X), DV(X), JV(X), DJ(X)

INPUT"INITIAL WATER POTENTIAL - J/KG"; P: P=-ABS(P)
INPUT"SATURATED CONDUCTIVITY - KG/M^43"; KS
B1=1/B: N=2+3/B: N1=1-N: WD=1000: DT=3600
Z(0)=0: Z(1)=B: Z(2)=0.01: Z(3)=.075: Mw=.018: T=293: R=8.3143
B1=1/B: N=2+3/B: N1=1-N: WD=1000: DT=3600
Z(0)=0: Z(1)=B: Z(2)=0.01: Z(3)=.075: Mw=.018: T=293: R=8.3143
FOR I=1 TO M
P(I)=P
W(X)=WS*(PE/P(I)))+B: WN(I)=W(I): H(I)=EXP(MW*P(I)/(R*T))
K(I)=KS*(PE/P(I))4N
IF I>2 THEN Z(I)=Z(I)+DZ
NEXT
P(M+1)=P(M): H(M+1)=H(M): Z(0)=-E+10: K(M+1)=KS*(PE/P(M+1))4N
GOSUB 1500
GR=.8: IM=.000001: DV=.0000024: VP=.017
P(0)=P(1): K(0)=0: HA=.5: Z(M+1)=1E+20
TI=TI+DT/3600: IF TI>24 THEN TI=TI-24: DA=DA+1
GOSUB 1000: GOSUB 2000
SE=0: FOR I=1 TO M: K(I)=KS*(PE/P(I))4N: NEXT
JV(0)=EP*(H(1)-HA)/(1-HA): DJ(0)=EP*MW*H(1)/(R*T*(1-HA))
For I=1 TO M
KV=.66*DV*VP*(WS-(WN(I)+WN(I+1))/2)/(Z(I+1)-Z(I))
JV(I)=KV*(H(I+1)-H(I))/Z(I+1)-Z(I)+K(I)/(Z(I+1)-Z(I))
CP(I)=-V(I)*WN(I)/B(I)*DT
C(I)=C(I)/B(I)
F(I)=C(I)*F(I)
F(I+1)=C(I)*F(I)
NEXT
DP(M)=F(M)/B(M): P(M)=P(M)-DP(M): IF P(M)>PE THEN P(M)=PE
FOR I=M-1 TO 1 STEP -1
DP(I)=F(I)-C(I)*DP(I+1): P(I)=P(I)-DP(I)
IF P(I)>PE THEN P(I)=(P(I)+DP(I)+PE)/2
NEXT
FOR I=1 TO M: WN(I)=WS*(PE/P(I)))+B: H(I)=EXP(MW*P(I)/(R*T)): NEXT
PRINT SE; IF SE>IM THEN GOTO 250
131

500 H(M+1)=H(M)
510 PRINT:PRINT "DAY=";DA;"TIME=";TI;"HRS"
520 PRINT "DEPTH (M), WC (M4/M4), MP (J/KG), R- SOIL/(R- SOIL+R- ROOT)";SW=0
530 FOR I=1 TO M:SW=SW+V(I)*(WN(I)-W(I)):W(I)=WN(I)
540 PRINT Z(I),WN(I),P(I),RS(I)/(RS(I)+RR(I));NEXT
550 FI=EP*(H(1)-HA)/(1-HA)
560 PRINT "EVAP RATE =";FL;" TSP RATE = ";TR;" WC CHANGE = ";SW/DT
570 PRINT "DRAIN RATE = ";GR*K(M);" PS LEAF =";PL
580 GOTO 230
590 END
600 '1000 EVAPOTRANSPIRATION SUBROUTINE
1010 E=2.3*ET*(.05+(SIN(.0175*7.5*T1)))/86400
1020 E2=1.1*E:TP=E-EF
1030 'RAIN OR IRRIG. CAN BE ADDED BY SETTING E(0) TO - THE DESIRED FLUX DENSITY
1040 RETURN
1050 '1500 SUBROUTINE TO INITIALIZE ROOT WATER UPTAKE VARIABLES
1510 ' M AND Z(I) MUST BE KNOWN BEFORE CALLING THIS SUBROUTINE
1520 DIM RR(M),L(M),E(M),RS(M),PR(M),BZ(M)
1530 RW=2.5E10:PC=-1500:RL=20000001:PI=3.14159:SP=10:RI=.001
1540 FOR I=1 TO M:READ L(I);L(I)=10000*L(I):NEXT
1550 DATA 0,4,4,1.9,0.8,0.8,0.4,0.4,0.2,0.1,1,1
1560 FOR I=1 TO M
1570 IF L(I)>0 THEN RR(I)=2*RW/(L(I)*(Z(I+1)-Z(I-1))):
1580 ELSE RR(I)=1E+20:BZ(I)=0
1590 NEXT
1600 '2000 PLANT WATER UPTAKE SUBROUTINE
2010 PB=0:RB=0
2020 FOR I=1 TO M
2030 RS(I)=BZ(I)/K(I)
2040 PB=PB+P(I)/(RR(I)+RS(I)):RB=RB+1/(RS(I)+RR(I))
2050 NEXT
2060 PB=PB/RB:RB=1/RB
2070 IF PL>PB THEN PL=PB-TP*(RL+RB)
2080 XP=(FL/PC)+SP
2090 SL=TP*(RL+RB)*SP*XP/(PL*(1+XP)*(1+XP))-1
2100 P=PB-PL-TP*(RL+RB)/(1+XP):PRINT "DPL=";F;
2110 PL=PL-XP:SL:IF ABS(F)>10 THEN GOTO 2080
2120 TR=TP/(1+XP)
2130 FOR I=1 TO M
2140 E(I)=(P(I)-PL-RL*TR)/(RR(I)+RS(I))
2150 NEXT
2160 RETURN
stomatal resistance varies with leaf water potential according to eq. 12.28. An improved equation will be derived in Chap. 12 using the Penman-Monteith equation. This section of code searches for a stomatal resistance and a leaf water potential which balance supply and demand. Since stomatal resistance is a non-linear function of leaf water potential, iteration must be used. In this case, a Newton-Raphson procedure is used. The loop at line 2130 calculates the water uptake at each node. Time steps are short enough that changes in soil water potential during the time step are assumed not to influence uptake during a time step. Output from this program is shown in Fig. 11.2.

This model can be used to give insight into several aspects of soil-plant water relations. The following observations can be made:

1. When soil water potential is uniform, water is taken from the layers of soil with the highest rooting densities.

2. As soil dries and water is taken from layers with fewer roots, the mean soil potential, \( \bar{\psi}_s \), decreases, even though some roots are still in moist soil. This reduction in soil water potential decreases plant water potential, closes stomates, and decreases transpiration and production.

3. When rooting density varies in a root system, soil hydraulic resistance appears to be relatively unimportant in all cases.

4. It should be possible to specify a value of the weighted mean soil water potential at which irrigation should occur for maximum production.
11.6 REFERENCES


11.7 PROBLEMS

11.1. Use the SPAM model (Prog. 11.1) to find soil water distributions when T/T_p = 0.9 and T/T_p = 0.5 for a typical transpiration rate and root distribution. What causes the reduction in transpiration rate? How important is soil resistance?

11.2. Compare water extraction rates, water extraction patterns, and fraction of available soil water used at three potential transpiration rates. What effect does transpiration rate have on available water? Available soil water is that water held between field capacity and permanent wilting water content to the depth of root penetration.
Chapter 12

ATMOSPHERIC BOUNDARY CONDITIONS

All of the models developed so far have required specification of a surface boundary condition. In the case of evaporation, soil heat flow, and plant water uptake, this boundary condition took the form of a specified potential or flux. In the case of evaporation and transpiration a maximum flux was specified, which could be reduced by the soil or crop depending on water supply. In each case information for determining the boundary condition was assumed to be available.

In working with the models, it was apparent that the actual values chosen for the atmospheric boundary conditions had a profound effect on the model behavior, and that meaningful modeling results depend as heavily on using the correct boundary conditions as on the correct behavior of the model itself. With this in mind, it is the objective of this chapter to develop the equations for heat and vapor exchange at crop and soil surfaces and show how these are used with the models derived in earlier chapters. The subject will not be developed in detail here, however, and the reader is referred to Campbell (1977) for a more complete treatment.

12.1 RADIATION BALANCE AT THE EXCHANGE SURFACE

The energy which heats crop and soil surfaces and evaporates water from them comes from the sun. A secondary source of energy is long-wave radiation from the atmosphere. The first step in deriving equations describing the upper boundary is to specify the amount of energy that is available from these two sources. The term $R_{abs}$ is the radiation absorbed at the soil surface and is calculated from

$$R_{abs} = a_s S_t + \varepsilon_a 0.64$$

(12.1)

where $a_s$ is short-wave absorptivity ($1$-albedo), $S_t$ is global short wave on a horizontal surface, $\Theta_a$ is the air temperature (in kelvins), and $\varepsilon_a$ is the atmospheric emissivity. For clear skies, $\varepsilon_a$ can be calculated from the vapor concentration of the air (Brutsaert, 1975):

$$\varepsilon_a = 0.58 c_{va}^{1/7}$$

(12.2)

where $c_{va}$ is the vapor concentration of the air ($g$ m$^{-3}$). The atmospheric vapor concentration is normally an input variable, but it can also be approximated as the saturation vapor concentration at minimum temperature.
When skies are cloudy, the atmospheric emissivity becomes (Unsworth and Monteith, 1975)

$$\varepsilon_{ac} = (1 - 0.84c_1)\varepsilon_a + 0.84c_1$$  \hspace{1cm} (12.3)$$

where \(c_1\) is the fractional cloud cover. A simple relationship exists between \(c_1\) and the atmospheric transmission coefficient for solar radiation, \(T_t\) (ratio of potential to measured daily global solar radiation). It is

$$c_1 = 2.33 - 3.33T_t$$  \hspace{1cm} (12.4)$$

which is, of course, only valid for values of \(c_1\) between 0 and 1. IF statements must be included in the computer program to set \(c_1\) to zero if it is less than zero, and to unity if it is greater than 1. Normally the daily global solar radiation is a measured input variable, but in cases where it is not available, it can be calculated from maximum and minimum temperature data (Bristow and Campbell, 1984). The potential radiation is calculated from

$$Q_o = 117.5(h_s \sin \phi \sin \delta + \cos \phi \cos \delta \sin h_s)/\pi$$  \hspace{1cm} (12.5)$$

with \(\cos h_s = -\tan \phi/\tan \delta\). The latitude is \(\phi\), and the solar declination, \(\delta\) is calculated from the day of the year, \(J\), using:

$$\sin \delta = 0.3985 \sin[4.869 + 0.172J + 0.03345 \sin(6.224 + 0.0172J)]$$  \hspace{1cm} (12.6)$$

Units of potential solar radiation in eq. 12.5 are MJ.

The short wave absorptivity in eq. 12.1, \(a_s\), depends on the nature of the surface and, for soil, the water content. For crops, \(a_s\) varies from 0.75 to 0.85 (Monteith, 1975). For bare soil surfaces which are dry, \(a_s\) is often around 0.7, and increases linearly with water content of the surface layer to around 0.88 at field capacity (Idso et al., 1975).

The models developed in earlier chapters used 1-hour time steps in order to provide adequate resolution of short-term processes. Input data generally have, at best, one day resolution. Some means of generating hourly values from daily input is therefore needed. The values in eq. 12.1 which require interpolation are \(S_t\) and \(\theta_a\). The surface absorptivity can be calculated using data from the soil moisture model, and the atmospheric vapor concentration can usually be assumed to be constant over a day.

Air temperature data are usually in the form of daily maximum and minimum temperature. No entirely satisfactory interpolation scheme exists for converting these to hourly temperatures, but a reasonable approximation is to
assume a sinusoidal interpolation function between the min and the max, or between the max and the min. The max is assumed to occur at 1500 hours, and the min at 300 hrs.

Hourly solar radiation values are calculated using the daily atmospheric transmission, $T_t$, calculated from the ratio of measured daily global radiation and eq. 12.5. The atmospheric transmission coefficient is multiplied by the radiation received on a horizontal surface outside the earth's atmosphere at any time of day to give hourly ground level irradiance. Thus

$$S_t = 1360 \ T_t \ \sin \ e \ .$$

(12.7)

$S_t$ is in W m$^{-2}$ and $e$ is the solar elevation angle, given by

$$\sin e = \sin \phi \ \sin \delta + \cos \phi \ \cos \delta \ \cos 0.2618(t - t_o) .$$

(12.8)

Angles in these equations are assumed to be in radians. In eq. 12.8, $t$ is hour of the day, and $t_o$ is the time of solar noon.

The other component of the radiation balance at the surface is the long-wave radiation emitted from the surface. This is proportional to the fourth power of the surface temperature. Because surface temperature is generally not known, it is convenient to write the surface emittance as the sum of two components. One component is proportional to the difference between surface and air temperature, and can therefore be combined with the convective heat transfer term. The other term is proportional to the fourth power of the air temperature, and is therefore known. The binomial expansion gives

$$\Theta_s^4 = (\Theta_a + \Delta \Theta)^4 = \Theta_a^4 + 4 \Theta_a^3 \Delta \Theta ,$$

where only the first two terms of the expansion are retained, the others being negligible for $\Delta \Theta \ll \Theta$. The $4 \Theta_a^3 \Delta \Theta$ term can now be subtracted from $R_{abs}$ to give an approximation of the energy absorbed at the surface. This is often termed the net isothermal radiation (Monteith, 1975). The term, $4 \Theta_a^3 \Delta \Theta$, which multiplies the temperature difference between surface and air, can be thought of as a radiative conductance:

$$K_r = 4 \Theta_a^3 \ .$$

(12.9)

This is added to the boundary layer conductance, which will be considered in the next section, to form a combined conductance for heat transfer in the atmospheric boundary layer. The equations developed to this point are summarized in Program 12.1.
1 ' PROGRAM 12.1 PROGRAM SEGMENT FOR INPUT OF DAILY DATA AND CONVERSION TO
2 ' HOURLY VALUES. M1(24) MUST BE DIMENSIONED IN THE MAIN PROGRAM.
3 ' NORMALLY THE INPUT WOULD BE FROM A DISK FILE, AND STATEMENT
4 ' 3040 WOULD INDICATE A BUFFER NUMBER.
5 '
6 ' 3000 ' SUBROUTINE FOR DAILY INPUTS AND CONVERSIONS. INPUT IS ASSUMED TO BE
3010 ' DAY NUMBER, DAILY MAXIMUM AND MINIMUM TEMPERATURE (IN DEG. C), DAILY
3020 ' PRECIPITATION (MM), AVERAGE DAILY WIND (M/S), AND TOTAL DAILY SOLAR
3030 ' RADIATION (MJ).
3040 INPUT JD,TX,TY,PR,W,DS
3050 PSR=0
3060 SD=.3985*SIN(4.869+.0172*JD+.03345*SIN(6.224+.0172*JD))
3070 CD=SQR(1-SD*SD)
3080 FOR I=1 TO 24
3090 M1(I)=SD*SIN(LA)+CD*COS(LA)*COS(.2618*(I-12))
3100 IF M1(I)>0 THEN PSR=PSR+1360*M1(I)
3110 NEXT
3120 PSR=PSR*.0036 ' CONVERTS W-HR/M^2 TO MJ/M^2
3130 PR=DS/PSR
3140 CL=2.33-3.33*FR
3150 IF CL<0 THEN CL=0
3160 IF CL>1 THEN CL=1
3170 CVA=EXP(31.3716-6014.79/(TY+273)-7.924953-(TY+273)/7.924953)
3180 RETURN
3200 ' SUBROUTINE TO GIVE HOURLY TEMPERATURE, RADIATION ETC. FROM DAILY VALUES
3210 IF INT(TI+.1)=3 THEN TH=TX
3220 IF INT(TI+.1)=15 THEN TL=TY
3230 TA=.5*(TH+TL+(TH-TL)*COS(.2618*(TI-15)))
3240 IF M1(TI)>0 THEN SR=FR*1360*M1(TI) ELSE SR=0
3250 EA=(1-.84*CL)*1.556*RHOVA+(1/7)+.84*CL
3260 RNI=.75*SR+5.67E-08*(EA-.96)*(TA+273)^4
3270 IF PR=0 THEN INF=0:GOTO 3300 ' INF IS INFILTRATION RATE (KG/(M^2 S))
3280 IF PR<10 THEN INF=PR/3600:PR=0:GOTO 3300
3290 PR=PR-10:INF=.0027778
3300 RETURN
12.2 BOUNDARY LAYER CONDUCTANCE FOR HEAT AND WATER VAPOR

The models in Chapters 9 and 11 used boundary layer conductances \([K(0)]\) which were assumed to be known. Equations for computing these conductances will now be developed.

Heat and water vapor are transported by eddies in the turbulent atmosphere above the crop. Boundary layer conductance would therefore be expected to vary depending on the wind speed and level of turbulence above the crop. The level of turbulence, in turn, is determined by the roughness of the surface, the distance from the surface, and the thermal stratification of the boundary layer. An equation which combines these terms in the appropriate way to give boundary layer conductance is (Campbell, 1977):

\[
K_h = kC_hu^*\left\{\ln\left[\frac{(z - d + z_h)}{z_h}\right] + \Psi_h\right\}.
\]  

(12.10)

Here, \(C_h\) is the volumetric specific heat of air (1200 J m\(^{-3}\) K\(^{-1}\) at 20°C and sea level), \(u^*\) is the friction velocity, \(k\) is von Karman’s constant (which is generally assumed to be 0.4), \(z\) is the height above the surface at which temperature is measured, \(d\) is the zero plane displacement for the surface, \(z_h\) is a surface roughness parameter for heat, and \(\Psi_h\) is a stability correction factor for heat. The friction velocity is defined as

\[
u^* = ku\left\{\ln\left[\frac{(z - d + z_m)}{z_m}\right] + \Psi_m\right\}
\]

(12.11)

where \(z_m\) and \(\Psi_m\) are the roughness factor and stability correction for momentum, and \(u\) is the mean wind speed measured at height \(z\).

The zero plane displacement and roughness parameters depend on the height, density, and shape of surface roughness elements. For typical crop surfaces, the following empirical correlations have been obtained:

\[
d = 0.77 \; h
\]

(12.12)

\[
z_m = 0.13 \; h
\]

(12.13)

\[
z_h = 0.2 \; z_m
\]

(12.14)

where \(h\) is the height of the roughness elements (height of the crop).

The stability correction parameters, \(\Psi_h\) and \(\Psi_m\), correct the boundary layer conductance for the effects of buoyancy in the atmosphere. When the air near the surface is hotter than the air above, the atmosphere becomes unstable, and mixing at a given wind speed is greater than than would occur in a neutral atmosphere. If the air near the surface is colder than the air.
above, the atmosphere is stable, and mixing is suppressed. A stability parameter, \( \zeta \), has been defined which is an index of the relative importance of thermal and mechanical turbulence in boundary layer transport. It is calculated from:

\[
\zeta = -\kappa gH/(C_h \theta u^2) .
\] (12.14)

Here, \( g \) is the gravitational constant (9.8 m s\(^{-2}\)), \( H \) is the sensible heat flux in the boundary layer, and \( \theta \) is the kelvin temperature.

The stability correction factors, \( \psi_h \) and \( \psi_m \) are functions of \( \zeta \). Businger (1975) suggests the following relationships. For stable conditions, when surface temperature is lower than air temperature, \( H \) is negative, and \( \zeta \) is positive, \( \psi_m \) and \( \psi_h \) are given by:

\[
\psi_m = \psi_h = 4.7 \zeta .
\] (12.15)

For unstable conditions, when surface temperature is higher than air temperature, \( H \) is positive, and \( \zeta \) is negative,

\[
\psi_h = -2 \ln\{[1 + (1 - 16\zeta^2)]/2\} ,
\] (12.16)

and

\[
\psi_m = 0.6 \psi_h .
\] (12.17)

The heat flux density in eq. 12.14 is the product of the boundary layer conductance and the difference between surface and air temperatures. Since the boundary layer conductance is a function of the heat flux density, an iterative method must be used to find the boundary layer conductance. Program 12.2 gives a BASIC subroutine for finding the boundary layer conductance using a simple iterative scheme. For sensible heat flow calculations, where net isothermal radiation is used, the radiative resistance from eq. 12.9 should be added to the value obtained from Prog. 12.2. The conductance for water vapor is the same as that for sensible heat, so Prog. 12.2 can be used to find the boundary layer resistance for water vapor as well.

Boundary layer conductances were used in Ch. 4 for soil heat flow models, in Ch. 9 for soil evaporation models, and in Ch. 11 for evapotranspiration models. Of these, the evapotranspiration model is the most complex since it involves exchange of heat and vapor from sources which are distributed throughout the plant canopy. A detailed plant canopy model is beyond the scope of this book. Interested readers should consult Norman and
PROGRAM 12.2. PROGRAM SEGMENT FOR CALCULATING BOUNDARY LAYER CONDUCTANCE

I PM=0 : PH=0 : VK=0.4 : CH=1200

FOR I=1 TO 3

USTAR=W*VK/(LN((Z-D+ZM)/ZM)+PM)

KH=CH*W*USTAR/(LN((Z-D+ZH)/ZH)+PH)

SP=-VK*Z*GR*KH*(TN[1]-TA)/(C*(TA+273)*FV+3)

IF SP>0 THEN PH=4.7*SP:PM=PH
ELSE PH=-Z*LN((1+SQR(1-16*SP))/2):PM=0.6*PH

NEXT

K[0]=KH

RETURN

Campbell (1983) for more information on such models. Simple approximations for calculating evapotranspiration from crops will be discussed later in this chapter. For these, a boundary layer conductance calculated assuming \( \frac{\gamma_m}{\gamma_h} = 0 \) is adequate.

In Ch. evaporation from the soil surface was modeled as an isothermal process. Stability corrections are not likely to be important in that model. During first-stage drying, evaporation prevents the surface from becoming hot, so stability corrections are small. Once the surface dries and becomes hot, boundary layer resistance is relatively unimportant in determining evaporation rate, anyway. Here, as with evapotranspiration, Prog. 12.2 would be used without iteration and without calculating stability parameters.

The use of stability corrections is important in Prog. 4.1. A dry soil surface reaches temperatures well above air temperature during the day, and can be well below air temperature on a clear night. Thermal stratification on a clear night can be strong enough to reduce sensible heat exchange between the soil surface and the air to almost nothing. If stability corrections are not made, soil temperature profiles predicted by the Prog. 4.1 can have large errors. In using Prog. 12.2 with Prog. 4.1, it is important to iterate the entire soil heat flow calculation at least once, since surface temperature depends on heat flux to the atmosphere, but heat flux to the atmosphere is determined, in part, by the surface temperature.

12.3 EVAPOTRANSPIRATION AND THE PENMAN-MONTEITH EQUATION

The transpiration rate for a crop can be computed from

\[
E = \frac{(c_{VS} - c_{VA})}{(r_{VC} + r_{VA})}
\]  
(12.18)
where $c_{vs}$ and $c_{va}$ are vapor concentrations at the evaporating surface and in the air above the crop, respectively, and $r_{vc}$ and $r_{va}$ are resistances to vapor diffusion for the canopy and atmospheric boundary layer. The canopy resistance, $r_{vc}$ is an equivalent resistance for all of the leaves in the canopy. If the total area of leaves in the canopy is assumed to consist of $n$ groups of leaves, each having area index, $F_i$, and stomatal diffusion resistance, $r_{vsi}$, then the canopy resistance can be calculated from

$$1/r_{vc} = \Sigma F_i/r_{vsi}$$  \hspace{1cm} (12.19)

where the sum is taken over the $n$ groups of leaves. If all of the leaves have the same diffusion resistance, then $r_{vc} = r_{vs}/F$, where $F$ is the total leaf area index of the canopy. The boundary layer resistance $r_{va}$, is $C_h/K_h$, where $K_h$ is the boundary layer conductance from eq. 12.10.

The concentration of vapor at the evaporating surface is generally assumed to be the saturation concentration at canopy temperature, since the humidity of the substomatal cavities is always near unity. The surface concentration can therefore be calculated from canopy temperature using

$$c'_v = \frac{\exp(31.3716 - 6014.79/\theta - 0.00792495\theta)}{\theta}.$$  \hspace{1cm} (12.20)

where the ' on the $c$ indicates saturation, $\theta$ is the canopy temperature in kelvins, and $c'_v$ is in g m$^{-3}$.

The difficulty with eq. 12.18 is that canopy temperature must be known to predict transpiration rate. Transpiration rate, however, influences canopy temperature. One option would be to ignore differences in canopy and air temperature, and calculate evaporation rate using air temperature in eq. 12.20. This option can be evaluated by rewriting eq. 12.18 as

$$E = (c'_v - c'_a)/(r_v) + (c'_{va} - c_{va})/r_v.$$  \hspace{1cm} (12.21)

The second term on the right is the isothermal evaporation rate, or the evaporation one would predict by assuming that canopy temperature and air temperature are the same. The vapor concentration difference in the first term on the right of eq. 12.21 can be approximated as $s(T_s - T_a)$, where $s$ is the slope of the saturation vapor concentration function at $T_a$ (or preferably at the average of $T_s$ and $T_a$). Values for $s$ can be calculated from

$$s = c'_v(L/M_w/\theta - 1)/\theta$$  \hspace{1cm} (12.22)

where $L$ is the latent heat of vaporization (2450 J/g at 20°C), $M_w$ is the
molecular mass of water (0.018 kg/mole), and R is the gas constant (8.3143 J mol\(^{-1}\) K\(^{-1}\)).

The error which results from the isothermal approximation can be assessed by taking the ratio of the first to the second terms on the right hand side of eq. 12.21:

\[
W = \frac{s(T_s - T_a)}{(c'_va - c_va)}
\]  

(12.23)

Order of magnitude estimates of W can be obtained by taking \(c_va\) as 10 g m\(^{-3}\) and \(T_a\) as 20°C. Then \(s=1\) g m\(^{-3}\), \(c'_va=17.3\) g m\(^{-3}\), and \(W\) is 0.13 per degree temperature difference between canopy and air. If vapor density stays constant, but temperature increases, then \(W\) decreases. It is 0.08 at 30°C and 0.06 at 40°C.

Tall crops which are rapidly transpiring maintain surface temperatures which are generally within a few degrees of air temperature. For these conditions, the isothermal approximation may be adequate. In most cases, however, it appears that the temperature difference between crop and air must be accounted for.

Penman combined eq. 12.21 with the energy budget equation to obtain the well-known Penman formula for predicting potential evapotranspiration. A form of the equation more similar to the equation we will derive was obtained by Monteith (1964) and is known as the Penman-Monteith formula.

The energy balance for the crop surface can be written as

\[
R_{ni} - G - LE - K_{hr}(T_s - T_a) = 0
\]

(12.24)

where \(R_{ni}\) is the isothermal net radiation discussed earlier, \(G\) is the ground heat flux density (calculated from equations in Ch. 4), and \(K_{hr}\) is the sum of boundary layer and radiative conductance (eqs. 12.9 and 12.10). Storage of heat in the canopy and energy used for photosynthesis have been ignored. Equations 12.21 and 12.24 can now be combined to give the Penman-Monteith equation:

\[
E = \frac{s}{s + \gamma^*} \frac{R_{ni} - G}{L} + \frac{\gamma^*}{s + \gamma^*} \frac{c'_va - c_va}{r_v + r_{va}}
\]

(12.25)

The apparent psychrometer constant, \(\gamma^*\) is calculated from

\[
\gamma^* = r_v K_{hr}/L ,
\]

(12.26)

where \(r_v = r_v + r_{va}\).
Equation 12.25 can be used to calculate evapotranspiration when $R_{\text{abs}}$, air temperature, vapor concentration, and resistances are known. It is difficult to know canopy resistance, however, since it depends on leaf water potential, and therefore on transpiration rate. It is useful to calculate a potential transpiration rate using eq. 12.25 with a minimum canopy resistance. This potential transpiration rate can then be adjusted, through iteration, to find the correct actual transpiration for any given leaf water potential. This procedure was followed in Prog. 11.1.

In eq. 12.25, only $\gamma^*$ and $r_{\text{VC}}$ change when stomates close. If $E_p$ is defined as the potential transpiration rate when stomatal resistance is minimum, and the ratio $E/E_p$ is taken using eq. 12.25, one obtains

$$E = E_p(s + \gamma^*)/(s + \gamma^*)$$

(12.27)

where $\gamma^*_{p}$ represents the value from eq. 12.26 when crop resistance is minimum. Using eq. 12.27 and a relationship between canopy resistance and leaf water potential, it is then possible to correctly calculate actual transpiration rate for any canopy water status and potential transpiration rate.

In most species, leaf water potential has little effect on stomatal resistance until some critical value of potential is approached. At potentials below the critical value, stomatal resistance increases rapidly. An empirical equaiton which fits this behavior, well is

$$r_{\text{VS}} = r^0_{\text{VS}}[1 + (\psi_L/\psi^c)^n] .$$

(12.28)

Here, $r^0_{\text{VS}}$ represents the stomatal resistance with no water stress, $\psi^c$ is the critical leaf water potential (water potential at which stomatal resistance reaches twice its minimum value) and $n$ is an empirical constant which determines how steeply resistance increases with decreasing potential. Tongyai (1977) found values of $n$ around 3 for Ponderosa pine seedlings, but data from Cline and Campbell (1976) show much higher values for broad-leaf species, with some values as high as 20.

Combining eqs. 12.28, 12.26, and 12.27, then

$$E = E_p[s + K_{\text{HR}}(r_{\text{VA}} + r^0_{\text{VC}})/L]/{s + K_{\text{HR}}[r_{\text{VA}} + r^0_{\text{VC}}(1+\psi^0_p/\psi^c)]/L} .$$

(12.29)

In eq. 12.29, the canopy resistance is assumed to have the same water potential dependence as leaf stomatal resistance.

In the limit as boundary layer resistance becomes negligibly small, eq. 12.29 becomes $E = E_p/[1+(\psi_L/\psi^c)^n]$, which was used with eq. 11.18 to find leaf water potential in lines 2180 to 2210 in Prog. 11.1. Equations 12.29 and
11.18 can be solved simultaneously using the Newton Raphson procedure from Prog. 11.1. Values for \( s, K_{hr}, r_{va} \), and \( r_{vc} \), must be supplied to the subroutine. The derivation of the equations to replace those in lines 2090, 2100, and 2120 of Prog. 11.1 is straightforward, and is left as an exercise.

12.4 PARTITIONING OF EVAPOTRANSPIRATION

In program 11.1, potential evapotranspiration was arbitrarily partitioned into 10% evaporation and 90% transpiration. The actual partitioning depends on the energy supplied to the crop and soil, and the resistances to transport. A complete model which correctly partitions evapotranspiration is given by Norman and Campbell (1983), but it is too complex for the present analysis. A simpler approach, which is approximately correct, is to assume that the ratio of transpiration to evapotranspiration is the same as the ratio of radiation intercepted by the crop to total incident radiation. This is determined by the leaf area index of the crop, and, averaged over a day, can be approximated by

\[
T/ET = 1 - \exp(-0.82 F)
\]  

where \( F \) is the leaf area index of the crop. The ratio of potential evaporation to potential evapotranspiration is \( \exp(-0.82 F) \).

The partitioning of actual transpiration and evaporation is taken care of automatically in Prog. 11.1. It depends on the humidity of the soil surface and the stomatal resistance of leaves, as well as on potential transpiration and evaporation rates. If potential evaporation and transpiration are correctly modeled, it is likely that Prog. 11.1 will correctly determine actual evaporation and transpiration.
12.5 REFERENCES


12.6 PROBLEMS

1. Combine eqs. 12.29 and 11.18 eliminating E to give an implicit equation in leaf water potential which can be solved by the Newton-Raphson procedure. Also, find the derivative of the equation. Then modify and test the subroutine at line 2000 in Prog. 11.1 using these new equations. Compare simulated transpiration with and without these modifications to the program.
## APPENDIX

Table A1. Conversion factors for commonly used units in soil physics.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>SI units</th>
<th>Equivalent units</th>
</tr>
</thead>
<tbody>
<tr>
<td>length</td>
<td>1 m</td>
<td>= 3.281 ft</td>
</tr>
<tr>
<td>area</td>
<td>1 m&lt;sup&gt;2&lt;/sup&gt;</td>
<td>= 10.72 ft&lt;sup&gt;2&lt;/sup&gt;</td>
</tr>
<tr>
<td>area</td>
<td>1 m&lt;sup&gt;2&lt;/sup&gt;</td>
<td>= 2.469×10&lt;sup&gt;-4&lt;/sup&gt; acre</td>
</tr>
<tr>
<td>volume</td>
<td>1 m&lt;sup&gt;3&lt;/sup&gt;</td>
<td>= 35.31 ft&lt;sup&gt;3&lt;/sup&gt;</td>
</tr>
<tr>
<td>mass</td>
<td>1 kg</td>
<td>= 2.205 lb</td>
</tr>
<tr>
<td>density</td>
<td>1 Mg m&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>= 1.00 g cm&lt;sup&gt;-3&lt;/sup&gt;</td>
</tr>
<tr>
<td>force</td>
<td>1 N</td>
<td>= 10&lt;sup&gt;5&lt;/sup&gt; dynes</td>
</tr>
<tr>
<td>pressure</td>
<td>1 Pa</td>
<td>= 10&lt;sup&gt;-5&lt;/sup&gt; bar</td>
</tr>
<tr>
<td>pressure</td>
<td>1 Pa</td>
<td>= 9.9×10&lt;sup&gt;-6&lt;/sup&gt; atm</td>
</tr>
<tr>
<td>energy</td>
<td>1 J</td>
<td>= 0.2388 cal</td>
</tr>
<tr>
<td>energy density</td>
<td>1 J m&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>= 2.388×10&lt;sup&gt;-5&lt;/sup&gt; cal cm&lt;sup&gt;-2&lt;/sup&gt; (langley)</td>
</tr>
<tr>
<td>radiant flux density</td>
<td>1 W m&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>= 1.433×10&lt;sup&gt;-3&lt;/sup&gt; cal cm&lt;sup&gt;-2&lt;/sup&gt; min&lt;sup&gt;-1&lt;/sup&gt;</td>
</tr>
<tr>
<td>kinematic viscosity</td>
<td>1 m&lt;sup&gt;2&lt;/sup&gt;/s</td>
<td>= 10&lt;sup&gt;4&lt;/sup&gt; stokes</td>
</tr>
<tr>
<td>latent heat</td>
<td>1 J/kg</td>
<td>= 2.388×10&lt;sup&gt;-4&lt;/sup&gt; cal/g</td>
</tr>
<tr>
<td>specific heat</td>
<td>1 J kg&lt;sup&gt;-1&lt;/sup&gt; K&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>= 2.388×10&lt;sup&gt;-4&lt;/sup&gt; cal g&lt;sup&gt;-1&lt;/sup&gt; K&lt;sup&gt;-1&lt;/sup&gt;</td>
</tr>
<tr>
<td>thermal conductivity</td>
<td>1 W m&lt;sup&gt;-1&lt;/sup&gt; K&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>= 2.388×10&lt;sup&gt;-3&lt;/sup&gt; cal s&lt;sup&gt;-1&lt;/sup&gt; m&lt;sup&gt;-1&lt;/sup&gt; K&lt;sup&gt;-1&lt;/sup&gt;</td>
</tr>
<tr>
<td>water potential</td>
<td>1 J/kg</td>
<td>= 0.102 meters of water</td>
</tr>
<tr>
<td>water potential</td>
<td>1 J/kg</td>
<td>= 1 kPa</td>
</tr>
<tr>
<td>water potential</td>
<td>1 J/kg</td>
<td>= 0.01 bar</td>
</tr>
<tr>
<td>water flux density</td>
<td>1 kg m&lt;sup&gt;-2&lt;/sup&gt; s&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>= 1 mm m&lt;sup&gt;-2&lt;/sup&gt; s&lt;sup&gt;-1&lt;/sup&gt; (1 mm/s)</td>
</tr>
<tr>
<td>water flux density</td>
<td>1 kg m&lt;sup&gt;-2&lt;/sup&gt; s&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>= 360 cm/hr</td>
</tr>
<tr>
<td>water flux density</td>
<td>1 kg m&lt;sup&gt;-2&lt;/sup&gt; s&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>= 8.64×10&lt;sup&gt;3&lt;/sup&gt; cm/day</td>
</tr>
<tr>
<td>water flux density</td>
<td>1 kg m&lt;sup&gt;-2&lt;/sup&gt; s&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>= 3.40×10&lt;sup&gt;3&lt;/sup&gt; in/day</td>
</tr>
<tr>
<td>hydraulic conductivity</td>
<td>1 kg s m&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>= 9.8×10&lt;sup&gt;-3&lt;/sup&gt; m/s</td>
</tr>
<tr>
<td>hydraulic conductivity</td>
<td>1 kg s m&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>= 58.8 cm/min</td>
</tr>
<tr>
<td>hydraulic conductivity</td>
<td>1 kg s m&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>= 3.53×10&lt;sup&gt;3&lt;/sup&gt; cm/hr</td>
</tr>
<tr>
<td>electrical conductivity</td>
<td>1 dS/m</td>
<td>= 1.0 mmho/cm</td>
</tr>
</tbody>
</table>

To convert from SI units to the indicated units, multiply by the indicated value. To convert from the indicated units to SI, divide by the indicated value. Some conversions have assumed nominal values of 1.0 Mg m<sup>-3</sup> for the density of water and 9.8 m s<sup>-2</sup> for the gravitational constant, and are therefore only approximate.
Table A2. Properties of water and water vapor.

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>Density ρ/ kg m⁻³</th>
<th>L  / MJ/kg</th>
<th>Viscosity μ  / m²/s</th>
<th>σ  / J m⁻² K⁻¹</th>
<th>cᵥ  / g m⁻³</th>
<th>s  / g m⁻³ K⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.99987</td>
<td>2.50</td>
<td>1.79×10⁻⁶</td>
<td>7.56×10⁻²</td>
<td>4.85</td>
<td>0.33</td>
</tr>
<tr>
<td>4</td>
<td>1.00000</td>
<td>2.49</td>
<td>1.57×10⁻⁶</td>
<td>7.50×10⁻²</td>
<td>6.36</td>
<td>0.43</td>
</tr>
<tr>
<td>10</td>
<td>0.99973</td>
<td>2.48</td>
<td>1.31×10⁻⁶</td>
<td>7.42×10⁻²</td>
<td>9.40</td>
<td>0.60</td>
</tr>
<tr>
<td>20</td>
<td>0.99823</td>
<td>2.45</td>
<td>1.01×10⁻⁶</td>
<td>7.27×10⁻²</td>
<td>17.30</td>
<td>1.01</td>
</tr>
<tr>
<td>30</td>
<td>0.99568</td>
<td>2.43</td>
<td>0.80×10⁻⁶</td>
<td>7.11×10⁻²</td>
<td>30.38</td>
<td>1.65</td>
</tr>
<tr>
<td>40</td>
<td>0.99225</td>
<td>2.41</td>
<td>0.66×10⁻⁶</td>
<td>6.95×10⁻²</td>
<td>51.19</td>
<td>2.57</td>
</tr>
<tr>
<td>50</td>
<td>0.98807</td>
<td>2.38</td>
<td>0.56×10⁻⁶</td>
<td>6.79×10⁻²</td>
<td>83.06</td>
<td>3.88</td>
</tr>
</tbody>
</table>

Diffusion coefficients for gases in water at 20°C:
D(O₂) = 2.1×10⁻⁹ m²/s
D(CO₂) = 1.8×10⁻⁹ m²/s

Latent heat of fusion = 334 kJ/kg
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