Chapter 6: Water Flow: WaterMover Module

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The WaterMover module was extracted from the SWMS_2D model (Šimůnek et al., 1992). This water flow simulation code has several important computational advantages. Among these are: 1) the ability to adjust the iteration domain to only that region where convergence criteria are not met, 2) having a table look-up of soil water and hydraulic conductivity values as a function of soil water potential, 3) the possibility to use both triangular and rectangular grid cells to describe complex shapes of the soil surface.

The original code was slightly modified to handle abrupt changes in the water flux at the soil surface, root activity in a strongly non-equilibrium moisture regime, and root water uptake as determined for individual soil elements. The original algorithm could deal with scaled stochastic and/or anisotropic hydraulic soil properties. This option was excluded from 2DSoil to improve structure simplicity.

6.1 The two-dimensional model of water flow and its finite element implementation

The model considers two-dimensional Darcian water flow in a variably saturated soil. The code neglects deformations of a soil due to shrinking-swelling, assumes vapor transport to be negligibly small as compared to water flow in the liquid phase, treats soil as a locally isotropic medium, and allows temperature and solute concentrations to influence hydraulic parameters but not water potential gradients. The governing flow equation is given by the following appropriate form of the Richards' equation:

$$\frac{\partial \theta}{\partial t} - \frac{\partial}{\partial x}\left(k\frac{\partial h}{\partial x}\right) - \frac{\partial}{\partial z}\left[k\left(\frac{\partial h}{\partial z} + 1\right)\right] + S = 0 \qquad \textbf{(6.1)}$$

for water flow in a vertical soil cross-section, and by

$$\frac{\partial \theta}{\partial t} - \frac{1}{x}\frac{\partial}{\partial x}\left(kx\frac{\partial h}{\partial x}\right) - \frac{\partial}{\partial z}\left[k\left(\frac{\partial h}{\partial z} + 1\right)\right] + S = 0 \qquad \textbf{(6.2)}$$

for axisymmetrical water flow. Here, θ is the volumetric water content (cm^3 of water per cm^3 of soil), h is the pressure head (cm), S is an extraction term that describes the joint action of all factors contributing to removal of the water from the soil (cm^3 per cm^3 of soil per day), x either is the horizontal coordinate in case of water flow in a vertical soil cross-section, or the radial coordinate in case of axisymmetrical flow, cm; z is the vertical coordinate measured upward from a reference horizontal plane, (cm); t is time,(days); and k is soil hydraulic conductivity, (cm^3 of water per cm^2 of soil per day). The reference plane may be placed at any arbitrary depth.

The water content θ and hydraulic conductivity k depend on the pressure head h, and may also depend on the spatial coordinates x and z, time, the concentration of solutes, temperature, and other soil state variables. Two models describing the dependencies of θ and k on h are given in Sections 6.3 and 6.5 of this manual. The extraction term S is determined mainly by root water uptake. Chapter 10 of this manual describes submodels for root water uptake.

The governing equations (6.1) and (6.2) for water flow are solved numerically (Šimůnek et al., 1992) to obtain spatial and temporal distributions of the pressure head h within the soil domain. Numerical solution was accomplished using the Galerkin finite element method with linear basis functions and triangular elements (soil cells). The soil domain for this purpose is divided into a network of triangular elements. Nodal points are located at the corners of the different elements. For the example of the grid in Fig. 3.1, one possible subdivision is shown in Fig. 6.1. The pressure head at any point is expressed as a linear combination of nodal pressure head values:

$$\hat{h}(x,z,t) = \sum_{n=1}^{N_n} \phi_n(x,z) h_n(t) \qquad \textbf{(6.3)}$$

where N_n is the total number of nodes, $\phi_n(x,z)$ are basis functions for node n, and h_n is the pressure head at node n. Basis functions are interpolation functions for the element.

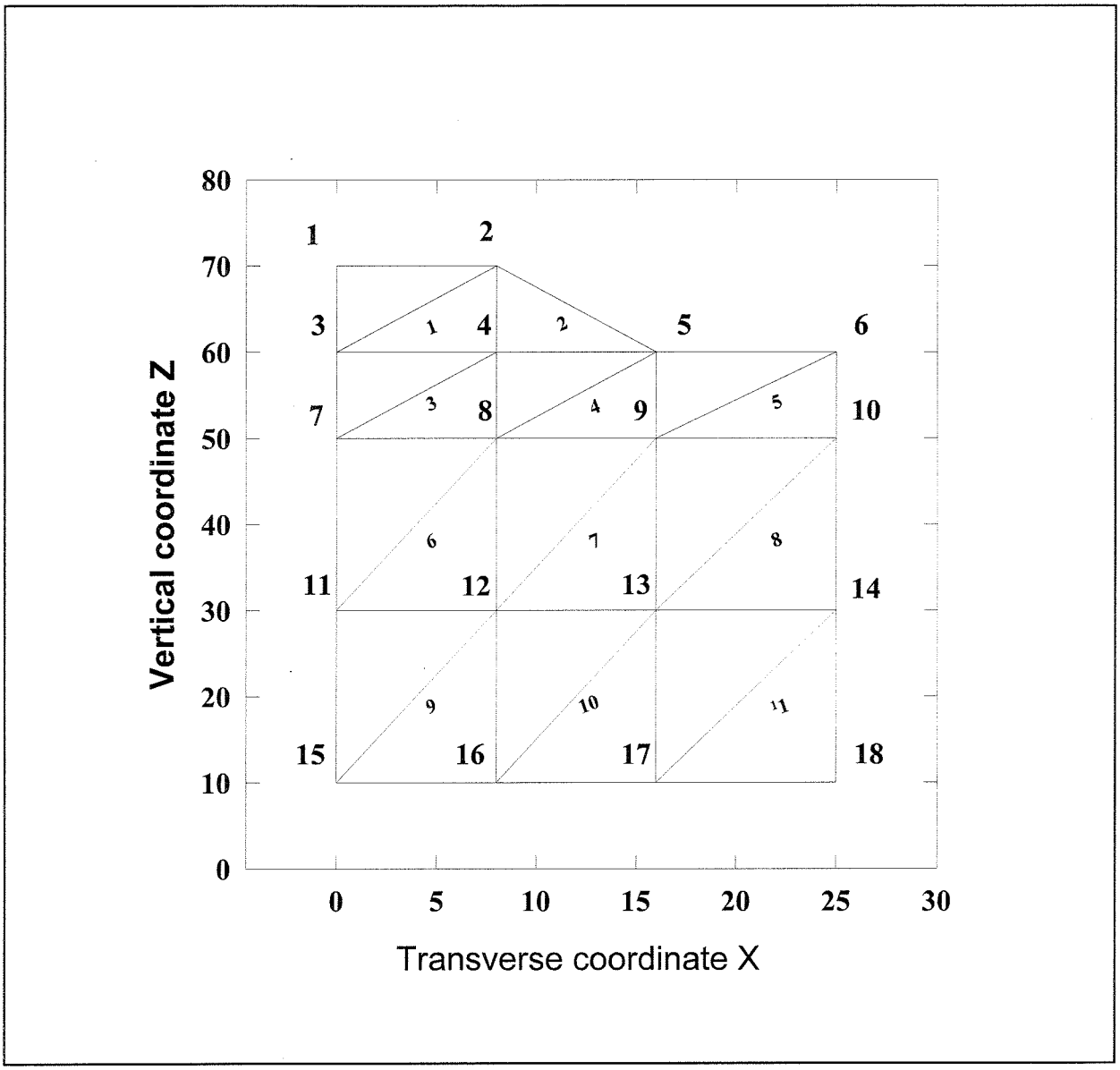

Figure 6.1 Subdivision of rectangular elements to triangular elements.

The triangular element, as shown in Fig. 6.2, has the following interpolation functions (Istok, 1989):

$$\phi(x,z)=\frac{1}{2A}(\hat{a}_s+\hat{b}_s x+\hat{c}_s z), \qquad s=i,j,k$$

$$\begin{aligned}
&\hat{a}_i=x_j z_k-x_k z_j, \quad \hat{b}_i=z_j-z_k, \quad \hat{c}_i=x_k-x_j \\
&\hat{a}_j=x_k z_i-x_i z_k, \quad \hat{b}_j=z_k-z_i, \quad \hat{c}_j=x_i-x_k \\
&\hat{a}_k=x_i z_j-x_j z_i, \quad \hat{b}_k=z_i-z_j, \quad \hat{c}_k=x_j-x_i \\
&A=\frac{1}{2}(\hat{a}_i+\hat{a}_j+\hat{a}_k)=\frac{1}{2}(\hat{c}_k\hat{b}_j-\hat{c}_j\hat{b}_k)
\end{aligned} \tag{6.4}$$

where A is the area of the element.

The Galerkin method is used to obtain equations for the nodal values of h. Area-averaged weighted residuals of Eq. (6.1) have to be equal to zero and must be true for every ϕ_n taken as a weight. Consequently, for the whole soil domain we obtain:

$$\sum_{e=1}^{N_e}\int_{\Omega_e}\left[\frac{\partial\theta}{\partial t}-\frac{\partial}{\partial x}(k\frac{\partial h}{\partial x})-\frac{\partial}{\partial z}[k(\frac{\partial h}{\partial z}+1)]+S\right]\phi_n d\omega=0 \tag{6.5}$$

where Ω_e designates the area of element e, and N_e is the total number of elements. After replacing h by $\hat{h}$ and using Green's first identity, one has:

$$\begin{aligned}
&\sum_{e=1}^{N_e}\int_{\Omega_e}\left[\frac{\partial\theta}{\partial t}\phi_n+k(\frac{\partial\hat{h}}{\partial x}\frac{\partial\phi_n}{\partial x}+\frac{\partial\hat{h}}{\partial z}\frac{\partial\phi_n}{\partial z})\right]d\omega= \\
&\quad\sum_{e=1}^{N_e}\int_{\Gamma_e}k\left[\frac{\partial\hat{h}}{\partial x}n_{\Gamma,x}+(\frac{\partial\hat{h}}{\partial z}+1)n_{\Gamma,z}\right]\phi_n d\Gamma \\
&\quad-\sum_{e=1}^{N_e}\int_{\Omega_e}k\frac{\partial\phi_n}{\partial z}d\omega-\sum_{e=1}^{N_e}\int_{\Omega_e}S\phi_n d\omega=0
\end{aligned} \tag{6.6}$$

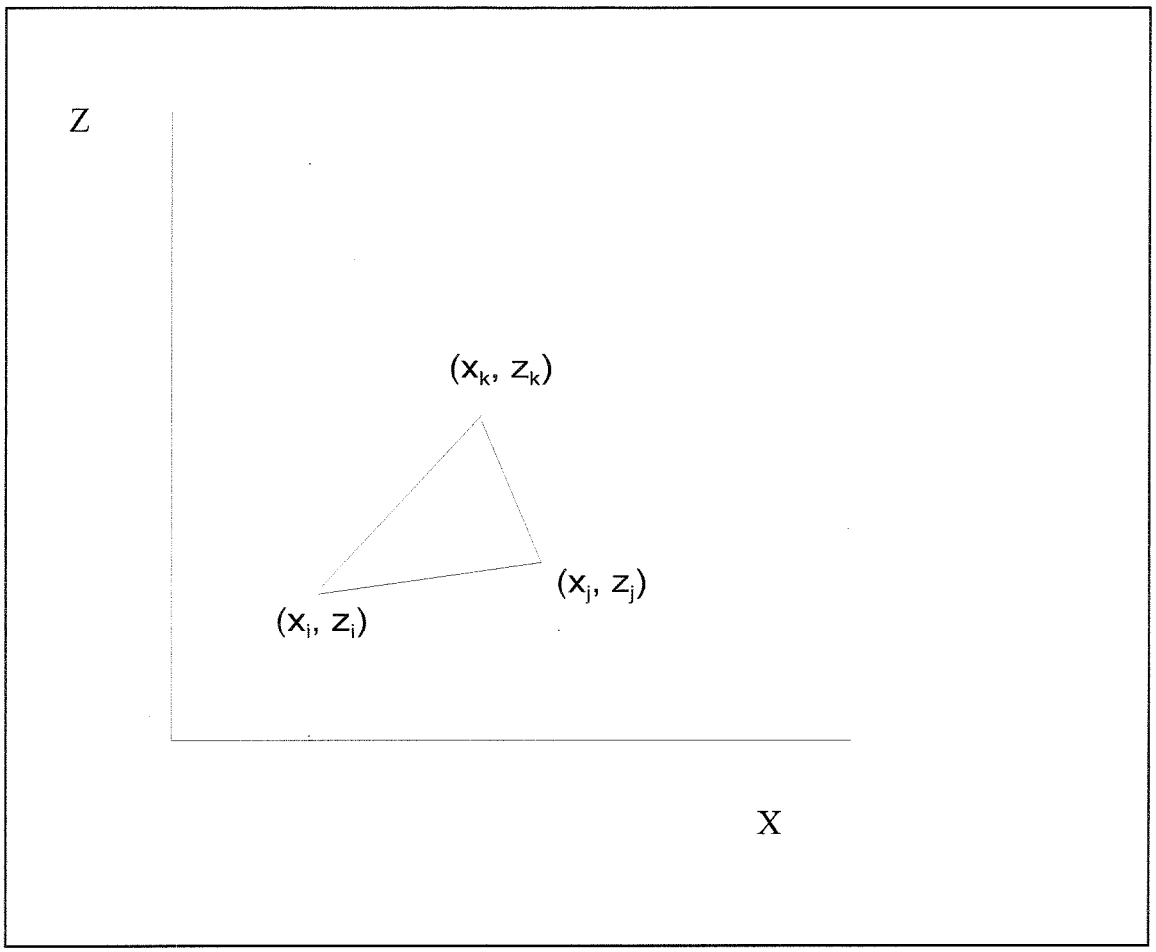

Figure 6.2 Triangular element as used for the finite element discretization of the flow equations in 2DSOIL.

where Γ_e is the boundary of element e, and $n_{\Gamma x}$, $n_{\Gamma z}$ designate components of the unit normal vector to the boundary.

Further simplifications are based on two important assumptions. First, moisture content θ, the soil hydraulic conductivity, the specific water capacity of the soil, and the water extraction rate S are assumed to vary linearly over each element. Second, nodal moisture content changes may be found as weighted averages of moisture content changes over an element according to the mass-lumping technique (Istok, 1989). Accepting these assumptions leads to a system of first-order ordinary differential equations for the nodal pressure head values:

$$[F]\frac{d\vec{\theta}}{dt}+[A]\vec{h}=\vec{Q}-\vec{B}-\vec{D} \qquad \textbf{(6.7)}$$

where the vectors $\vec{h}$, and $\vec{\theta}$ include all nodal values of h, and θ. The matrices $[A]$ and $[F]$ have as elements

$$A_{m,n}=\sum_e \frac{1}{4A_e}\bar{k}_e(\hat{b}_m\hat{b}_n+\hat{c}_m\hat{c}_n), \quad F_{m,n}=\delta_{mn}\sum_e \frac{A_e}{3} \tag{6.8}$$

where the summation involves all elements that have the nodes m and n among their corner nodes. The vectors $\vec{B},\vec{Q},$, and $\vec{D}$ are given by

$$B_n=\sum_e \frac{\bar{k}_e}{2}\hat{c}_n, \quad Q_n=-\sum_e q_{e,n}\frac{d_{e,n}}{2}, \quad D_n=\sum_e \frac{1}{12}A_e(3\bar{S}_e+S_n) \tag{6.9}$$

where the summation involves all elements adjacent to node n. The parameters $\hat{b}_n$, $\hat{c}_n$, A_e have the same meaning as in Eq. (6.4); $\bar{k}_e$ is the average hydraulic conductivity over the element; $d_{e,n}$ is the length of the soil domain boundary segment that serves as the boundary of the element e and ends at the node n; and $q_{e,n}$ is the water flux through the soil domain boundary to/from element e near node n, such that $q_{e,n}$ is positive when water flows out of the soil domain (cm per day).

Nodal water extraction rates are calculated as $S_n=\Sigma A_e S_e / \Sigma A_e$ where the summation includes all elements that have node n at one of their corners. The average nodal water extraction rate, $\bar{S}$, of an element is found as the mean of 5 at its nodal values. A method of solution of system (6.7) is described in detail by Šimůnek et al. (1992). After every time step water flow velocities are calculated in accordance with Darcy's law, and derivatives of the pressure head are obtained directly from Eq. (6.3).

Slight modifications of the coefficients in Eqs. (6.8) and (6.9) allow axisymmetrical cases as described by Eq. (6.2) to be solved (Šimůnek et al., 1992). Boundary and initial conditions must be set to solve Eq. (6.7). Methods of time-dependent boundary settings are presented in Chapters 4 and 5 of this manual. Time-independent boundary pressure heads must be included in the initial distribution data as described in the next section.

6.2 Data files '*Param_W.dat*' and '*Nodal_W.dat*'

Computations within the WaterMover module may be affected by several iteration and time-stepping parameters that are read from the file **'Param_W.dat'**. It is difficult to recommend specific values for these parameters as they are dependent on the water redistribution pattern and especially on the values of boundary fluxes for the problem under consideration. Therefore, only ranges and/or limits are presented below.

The parameter *MaxIt* determines the maximum allowable number of iterations. Our experience suggests that this parameter is best set between 10 and 20. The rate of convergence (number of iterations) and the precision of computations is affected by the tolerance limits *TolAbs* and *TolRel*. Iterations may be stopped when the difference between the pressure heads of the previous iteration, h^{temp}, and the current iteration, h^{new}, obeys the inequality

$$|h^{new} - h^{temp}| \le TolAbs + TolRel * |h^{new}| \qquad \textbf{(6.10)}$$

everywhere in the soil domain. Recently Huang et al., (1996) proposed the use of a convergence criterion based on water content rather than matric potential. The advantage of this criterion is that convergence is much more rapid in dry soils. The convergence criterion is:

$$Tolth = \frac{d\theta}{dh}\frac{(hNew - hTemp)}{\theta_{sat} - \theta_r} \qquad \textbf{(6.11)}$$

The value of *TolAbs* influences the precision and rate of convergence mainly for nodes where the soil is close to saturation. The value of *TolRel* does the same for nodes where the soil has a low moisture content. Values of *TolAbs* between 0.005 and 0.05 cm and values of *TolRel* between 0.005 and 0.0005 seem to be reasonable for the majority of problems. For *TolTh*, the value 0.001 usually works well.

The model does not allow evaporation to create arbitrarily low negative pressure heads on the soil-atmosphere boundary. When the pressure head decreases to the *hCritA* value, a further decrease in pressure head will be prevented, and the pressure head is forced to remain at *hCritA*

(the pressure head potential that corresponds to the air-dry soil water content). At the next time step the program will inspect potential fluxes across the surface. If the soil continues to dry (positive flux), then the pressure head is maintained at the *hCritA* level. Real fluxes will then be less than potential. If potential fluxes tend to rewet the soil, then they are allowed to act as real fluxes, and the pressure head becomes greater than *hCritA*. A range from -30,000 to -100,000 cm seems to be reasonable for *hCritA*.

The model can handle positive pressure heads along the soil-atmosphere boundary only in cases where the water flux on the surface is directed into the soil (or equal to zero). Therefore, it is advisable to avoid positive surface pressure heads if ponding due to rainfall may be changed to evaporation during a time step. The variable *hCritS* may be used for this purpose. This variable may be arbitrarily made positive if no 'rainfall ponding-evaporation' alterations will occur, but must be set to zero if such alterations will occur.

Time steps are regulated mainly by the *Synchronizer* module. The WaterMover module itself may decrease the time step if convergence is not reached within *MaxIt* iterations. The WaterMover cannot make the time step larger than *Synchronizer* does. However, it is advisable to set a reasonable upper limit for the time step in the WaterMover so as to prevent drastic changes in time steps during the calculations. This upper limit is assigned to a variable *DtMx(1)*, which may have values between 0.001 and 0.01 of the total simulated time.

Variables *hTab1* and *hTabN* mark the range of pressure head values that are most likely during the calculations. Dependencies of the moisture content and the hydraulic conductivity on the pressure head in this range will be tabulated at the very beginning of the calculations. Thereafter, interpolation between tabular values will avoid the time-consuming calculations of hydraulic properties from approximation formulas. Appropriate values for the hydraulic properties will be computed directly from the approximation formulas only if the absolute value of the pressure head during program execution lies outside the interval [*-hTabN,-hTab1*].

The structure of data for the computational parameters is presented in Table 6.1. An example is given immediately after the table. Besides the computational parameters, *WaterMover* reads data on the initial pressure head distribution from the file **'Nodal_W.dat'**. If there are constant head boundaries, then the values of the boundary heads must be given in the

file. Table 6.2 shows the structure of data in the **'Nodal_W.dat'** file, with our example following the table. The example corresponds to the grid of Fig. 3.1 and to the file **'Grid_bnd.dat'** of Example 3.3. The reference plane of the vertical coordinate is placed at the 270-cm depth.

6.3 The unsaturated soil hydraulic properties: Using closed-form approximations in the submodule SetMat01

A widespread approach for describing the unsaturated soil hydraulic properties is to use closed-form equations. The approach used here was introduced by van Genuchten (1980) who used the statistical pore-size distribution model of Mualem (1976) to obtain a predictive equation for the unsaturated hydraulic conductivity function. Later, the original van Genuchten

Table 6.1. WaterMover module information on computational parameters - file **'Param_w.dat'**.

Record	Variable	Description
1,2	-	Comment line.
3	*MaxIt*	Maximum number of iterations allowed during any time step.
3	*TolAbs*	Absolute pressure head tolerance.
3	*TolRel*	Relative pressure head tolerance.
3	*hCritA*	Value of the minimum allowed pressure head at the soil-atmosphere boundary (usually a value of matric potential for air-dry water content).
3	*hCritS*	Maximum allowed pressure head at the soil-atmosphere boundary (to allow runoff, a value of -1 will cause less numerical problems than a value of 0 or greater).
3	*dtMx(1)*	Maximum allowed time step in water transport calculations.
3	*hTab1*	Absolute value of lower limit of the pressure head interval for which a table of hydraulic properties will be generated internally for each material (must be greater the 0.0, e.g., 0.001 cm).
3	*hTabN*	Absolute value of the upper limit of the pressure head interval for which a table of hydraulic properties will be generated internally for each material (e.g., 1000 cm).

*** Example 6.1: WATERMOVER COMPUTATIONAL PARAMETERS: file 'Param_W.dat'
MaxIt TolAbs TolRel hCritA hCritS DtMx(1) hTab1 hTabN
20 .50 0.001 -1.E+05 1.E+06 1.0 0.001 100

Table 6.2. Format of file **'Nodal_W.dat'**.

Record	Variable	Description
1,2	-	Comment lines.
3	*n*	Nodal number.
3	*hOld(n)*	Initial value of the pressure head at node *n*.

Record 3 is provided for every node of the grid. If a 'constant head' boundary condition is to be Imposed in some nodes, then the corresponding boundary values of the pressure head must be present in this table.

```
**** Example 6.2: INITIAL PRESSURE HEAD DISTRIBUTION - file 'Nodal_w.dat'
 n  hOld
 1  -270
 2  -270
 3  -260
 4  -260
 5   2.5
 6   2.5
 7  -250
 8  -250
 9  -250
10  -250
11  -230
12  -230
13  -230
14  -230
15  -210
16  -210
17  -210
18  -210
```

equations were modified to add extra flexibility to the description of the hydraulic properties near saturation (Vogel and Cislerova, 1988). The most recent formulation may be found in the report of Šimůnek et al. (1992) in which the soil water retention, $\theta(h)$, and hydraulic conductivity, $k(h)$, functions are given by

$$\theta(h)=\begin{cases}\theta_a+\dfrac{\theta_m-\theta_a}{(1+|\alpha h|^n)^m}, & h<h_s\\ \theta_s, & h\geq h_s\end{cases} \qquad \textbf{(6.12)}$$

and

$$k(h)=\begin{cases} K_s[K_r(h)], & h\le h_k \\ K_k+\dfrac{(h-h_k)(K_s-K_k)}{h_s-h_k}, & h_k<h<h_s \\ K_s & h\ge h_s \end{cases} \qquad \textbf{(6.13)}$$

respectively, where

$$K_r=\frac{K_k}{K_s}\left(\frac{S_\theta}{S_{\theta k}}\right)^{1/2}\left[\frac{F(\theta_r)-F(\theta)}{F(\theta_r)-F(\theta_k)}\right]^2, \qquad F(\theta)=\left[1-\left(\frac{\theta-\theta_a}{\theta_m-\theta_a}\right)^{1/m}\right]^m$$
$$S_\theta=\frac{\theta-\theta_r}{\theta_s-\theta_r}, \qquad S_{\theta k}=\frac{\theta_k-\theta_r}{\theta_s-\theta_r}, \qquad m=1-\frac{1}{n}, \qquad n>1 \qquad \textbf{(6.14)}$$

Here, θ_r and θ_s denote the residual and saturated water contents, respectively, and K_s is the saturated hydraulic conductivity. To allow for a non-zero air-entry value, h_s, Vogel and Cislerova (1988) replaced the parameters θ_r and θ_s in the retention function by the fictitious (extrapolated) parameters $\theta_a \le \theta_r$ and $\theta_m \ge \theta_s$ as shown in Fig. 6.3. The value, θ_m, can be considered a measure of soil macroporosity. The approach maintains the physical meaning of θ_r and θ_s as measurable quantities. Equation (6.12) assumes that the predicted hydraulic conductivity function is matched to a measured value of the hydraulic conductivity at some water content θ_k less than the saturated water content, θ_s. The above set of soil hydraulic functions contains nine unknown parameters: θ_r, θ_s, θ_a, θ_m, α, n, K_s, K_k, θ_k. When $\theta_a=\theta_r$, $\theta_m=\theta_k=\theta_s$, and $K_k=K_s$, the soil hydraulic functions reduce to the original expressions of van Genuchten (1980). To find the parameters from experimental data, one can use the program **GENPAR**, which is not included in this release of 2DSOIL but is available upon request from the authors.

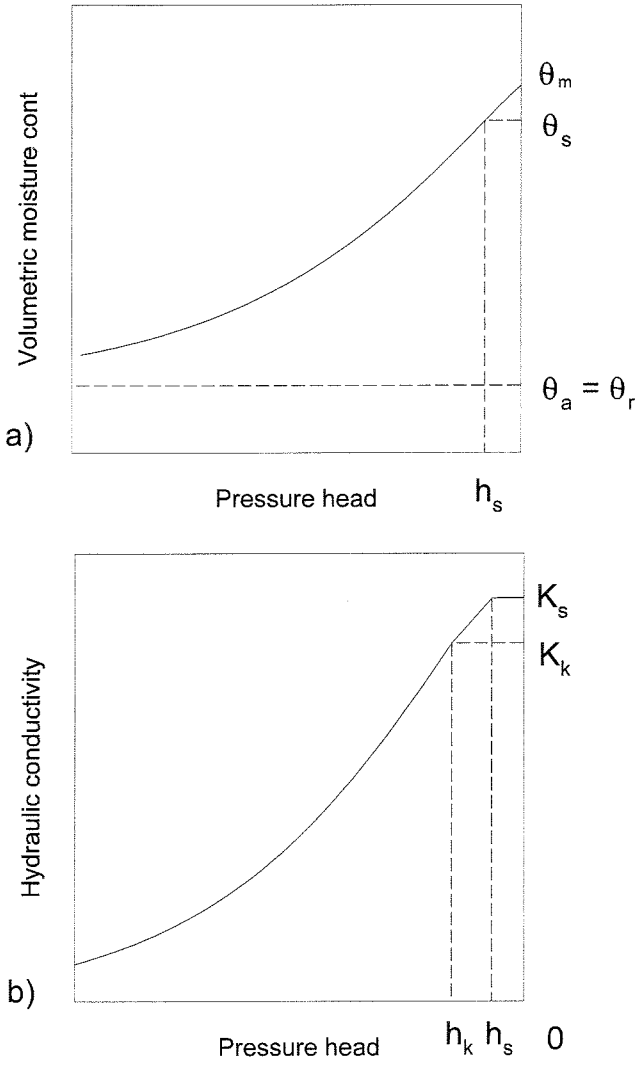

Figure 6.3 Schematic of the relationship between pressure head and water content and pressure head and hydraulic conductivity as expressed in equations 6.11 and 6.12

6.4 Data file '*Closefrm.dat*'

This file contains parameters that appear in the closed-form soil hydraulic equations for all soil materials that differ in their properties. The structure of data file **'Closefrm.dat'** is given in Table 6.3. This table is followed by an example data file for a soil profile with three layers.

6.5 The unsaturated soil hydraulic properties: Using piece-wise polynomial approximations in the submodule SetMat02

Continuous and smooth relationships between the hydraulic conductivity and pressure head, and between moisture content and matric pressure head, may be constructed from a limited number of data points by using some method of interpolation or approximation that smooths the data. This process may result in a significant loss of information since the derivatives of the moisture content and hydraulic conductivity with respect to pressure head are very important for the water flow simulation. This loss of information can be illustrated by recasting Eq. (6.1) into the following form:

$$\frac{d\theta}{dH}\frac{\partial H}{\partial t}+k\left\{\frac{d\ln(k)}{dH}\left[\left(\frac{\partial H}{\partial z}+1\right)\frac{\partial H}{\partial z}+\left(\frac{\partial H}{\partial x}\right)^2\right]+\frac{\partial^2 H}{\partial z^2}+\frac{\partial^2 H}{\partial x^2}\right\}+S=0 \qquad \textbf{(6.15)}$$

Table 6.3. WaterMover module information for parameters in close-form equations of the soil hydraulic properties- **file 'Closefrm.dat'**.

Record	Variable	Description
1,2	-	Comment lines.
3	*Par(1,M)*	Parameter θ_r for material *M*.
3	*Par(2,M)*	Parameter θ_s for material *M*.
3	*Par(3,M)*	Parameter θ_a for material *M*.
3	*Par(4,M)*	Parameter θ_m for material *M*.
3	*Par(5,M)*	Parameter α for material *M*.
3	*Par(6,M)*	Parameter n for material *M*.
3	*Par(7,M)*	Parameter K_s for material *M*.
3	*Par(8,M)*	Parameter K_k for material *M*.
3	*Par(9,M)*	Parameter θ_k for material *M*.
	Record 3 information is provided for each material *M* (from 1 to *NMat*).	

```
*** Example 6.3: SOIL HYDRAULIC PARAMETERS - file 'Closefrm.dat'
 thr      ths      tha      thm      Alfa     n        Ks       Kk       thk
.0001    .399     .0001    .399     .0174    1.3757   10       10       .399
.02      .450     .01      .551     .0093    1.567    1.2      0.7      .420
.01      .411     .005     .490     .0120    1.440    3.5      2.4      .391
```

where the matric suction H is used instead of the pressure head h, *i.e.*, $H=-h$ in unsaturated soil. This form of the Richards' equation clearly shows the coefficients that govern changes in the matric suction and hence the water content. These coefficients are the derivatives of the moisture content and hydraulic conductivity with respect to matric suction, i.e., the specific soil water capacity $\sigma=d\theta/dH$, and $\mu=d\ln k/dH$, respectively. We require that values of σ, μ, and k, as well as the values of the moisture content and H, be as close to the experimental data as possible, and still are situated on a continuous curve.

Although the use of analytical formulas to approximate hydraulic parameters can, to a certain extent, guarantee a reasonable closeness between calculated and measured θ and H, or k and H values, analytical approximations do not guarantee that calculated and actual values of the derivatives, σ and μ, are always close. This in turn can have an impact on the results of models that use these smoothed data in water flow simulations. We describe now a method for utilizing a piecewise continuous polynomial to interpolate water contents from soil matric potentials at the midpoints between pairs of measured data. The interpolating curve consists of a sequence of

cubic polynomials. Because splines are shape preserving, the shape of the piecewise polynomial function is close to the shape of measured water retention curves. Since cubic splines preserves first-order continuity, the derivatives are better preserved.

The method is illustrated in Fig. 6.4 for the water retention curve. Interpolation is done between midpoints of segments that connect neighboring pairs of the measurement points. If A_1, A_2, A_3 are sequentially measured points and $\hat{A}_2$, $\hat{A}_3$ are midpoints of the segments $[A_1A_2]$ and $[A_2A_3]$, then the interpolating curve will join points the $\hat{A}_2$ and $\hat{A}_3$. The interpolating curve is tangent to f$[A_1A_2]$ at the point $\hat{A}_2$, and tangent to $[A_2A_3]$ at the point $\hat{A}_3$.

In the region close to saturation the interpolating curve goes through saturation at $H=0$ and the first measured data point after saturation. This first piece has a zero derivative at saturation and is tangent to the segment connecting the first and second measured unsaturated data points. The calculations are carried out according to the following equations. Let the water content be measured for N values of the suction, i.e., at $H_{i,j+1...N,...}:=0, H_1, H_2,...,H_N$.

1. An auxiliary set of intermediate values of H is introduced:

$$\bar{H}_0=H_0;\ \bar{H}_1=H_1;\ \bar{H}_i=[H_{i-1}H_i]^{\frac{1}{2}},\ i=2,3,...,N;\ \bar{H}_{N+1}=H_N \qquad \textbf{(6.16)}$$

2. Approximate values of θ and σ are calculated for values of $\hat{H}$ from Eq. (6.16):

$$\bar{\theta}_0=\theta_0;\ \bar{\theta}_1=\theta_1;\qquad \bar{\theta}_i=\frac{1}{2}(\theta_{i-1}+\theta_i),\qquad i=2,3,...,N;\ \bar{\theta}_{N+1}=$$

$$\bar{\sigma}_0=0;\ \bar{\sigma}_1=\left(\frac{\theta_2-\theta_1}{\ln H_2-\ln H_1}\right)\frac{1}{H_1};\ \bar{\sigma}_i=\left(\frac{\theta_i-\theta_{i-1}}{\ln H_i-\ln H_{i-1}}\right)\frac{1}{\bar{H}_i},\ i=2,3,... \qquad \textbf{(6.17)}$$

$$\bar{\sigma}_{N+1}=\left(\frac{\theta_N-\theta_{N-1}}{\ln H_N-\ln H_{N-1}}\right)\frac{1}{H_N}$$

where $\bar{\sigma}\ (I=2,3,...,N)$ are values of the specific water capacity at midpoints $\bar{\theta}_I$ between measured data.

3. On intervals between H_I and H_{I+1} (I=1,2,...,N) the dependency of moisture content on suction is represented by cubic polynomials with cubics on these intervals being dependent on ln$H$:, i.e., $\theta=f_{\theta,i}(\ln H)$. The interval $[H_0,H_1]$ has also a cubic polynomial, but this curve is dependent on H as: $\theta=f_{\theta,0}(H)$. Cubic polynomials provide for the following equalities at points H_I and H_{I+1}:

$$f_{\theta,i}|_{\bar{H}_i}=\bar{\theta}_i,\ \frac{df_{\theta,i}}{dH}|_{\bar{H}_i}=\bar{\sigma}_i,\ f_{\theta,i}|_{\bar{H}_{i+1}}=\bar{\theta}_{i+1},\ \frac{df_{\theta,i}}{dH}|_{\bar{H}_{i+1}}=\bar{\sigma}_{i+1} \qquad \textbf{(6.18)}$$

In principle, the above cubic spline method is not to be used for extrapolation, i.e., for

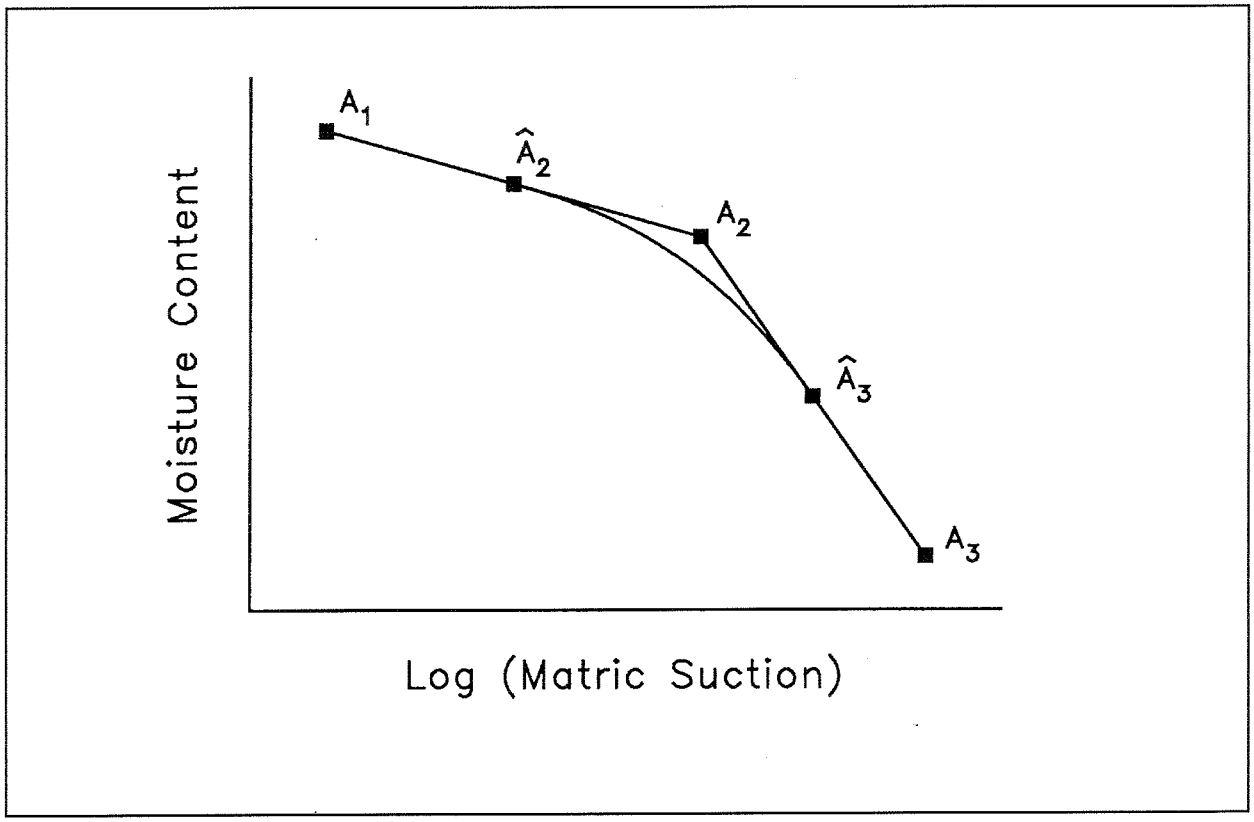

Figure 6.4 Schematic of the piecewise polynomial method for approximation of water retention and hydraulic conductivity data.

calculation of water content or conductivity values outside the measurement range $[H_0,H_N]$. One

cannot exclude, however, the possibility of crossing these limits during iterative water flow calculations. For such cases we have:

$$\theta=\theta_0, \text{ if } H<0; \quad \theta=\theta_N(H_N/H)^{-\bar{\sigma}_{N+1}H_N/\theta_N}, \quad \text{if } H>H_N \tag{6.19}$$

Starting from the second point (the first measured point below saturation), the interpolating curve using this method is that of a cubic spline. Unlike the regular use of splines, here the interpolating curve goes through the estimated midpoints ($\bar{H},\bar{\theta}$), but not through the measured points (H, θ).

If θ is replaced by $\ln k$ and σ by B, then the above formulas can be used also for calculating hydraulic conductivity values. They are coded in the FORTRAN subroutine HYDSUB, which uses measured θ, H, and k values to find the polynomial coefficients to calculate θ, σ, and k for given H values, and also to calculate H for given θ.

6.6 Data file '*Hydprop.dat*'

This file contains measured dependencies of the moisture content and hydraulic conductivity on matric suction for all soil layers that differ in there properties. The dependencies are presented in tabular form. The first pairs of values for both 'moisture content-matric suction' and 'hydraulic conductivity - matric suction' are for a water-saturated soil, i.e., the matric suction must be equal to zero in the first pair. The structure of the data file **'Hydprop.dat'** is given in Table 6.4. The table is followed by an example for a soil profile having two layers. Intermediate lines are replaced by periods for the sake of brevity.

Table 6.4. Format of the file **'Hydprop.dat'**.

Record	Variable	Description
1	-	Comment line.
2,3	-	Comment lines.
4	*NOBR*	Number of measured pairs of moisture content and pressure head values.
5	$\Psi(I)$	Measured value of the pressure head.
5	$\Theta(I)$	Corresponding measured volumetric soil moisture content.
	Record 5 is provided for all measured pairs of soil material, *I=1,2,...,NOBR*.	
6,7	-	Comment lines.
8	*NOBC*	Number of measured pairs of hydraulic conductivity and pressure head values.
9	$\Psi(I)$	Measured value of the pressure head.
9	*HYCON(I)*	Corresponding measured value of the soil hydraulic conductivity.
	Record 9 is provided for all measured pairs of the soil material, *I=1,2,...,NOBC*.	

Records 2-9 must be provided for every soil material *M, M=1,2...,NMat,* where *NMat* is the total number of soil materials.

```
****Example 6.4: MEASURED SOIL HYDRAULIC PROPERTIES - FILE 'Hydprop.dat'
Water retention of  soil material # 1
NOBR  H      Theta
 8
   0.000    0.419
   .....    .....
 500.000    0.098
Hydraulic conductivity of the material # 1
NOBC  H      k
 17
   0.000   12.220
   2.266    6.295
   .....    .....
  80.243    0.045
Water retention of the material # 2
NOB  H      theta
8
   0.000    0.311
   .....    .....
 500.000    0.079
Hydraulic conductivity of the material # 2
NOB  H      k
17
   0.000    6.200
   0.698    1.860
   .....    .....
  71.337    0.051
```

Chapter 7: Solute Transport: SoluteMover module

Jirka Šimůnek, Martinus Th. van Genuchten, and Yakov Pachepsky

The **SoluteMover** module was extracted from the SWMS_2D model (Šimůnek et al., 1992) and modified to provide better mass conservation for large surface fluxes. The solute is considered to be a dissolved substance that obeys the law of mass conservation. The original code was expanded to handle several solutes. However, the interdependence of mobilities of solute is not described, and interaction of solutes may occur only due to interactions between liquid and non-liquid soil phases.

The original SWMS_2D code considers linear adsorption, and first and zero-order biological transformation and/or decay. These processes are described by other modules in 2DSOIL. Therefore, the relevant adsorption and decay options have been removed, and **SoluteMover** describes solute transport as affected only by solute extraction. Extraction combines the effects of transformations, decay, interactions with solid phases, and production/uptake. Where it may be numerically more efficient to include the transformations terms directly in the solute transport equations, this approach is not appealing from the standpoint of modularity. Hence, the transformation terms are included in 2DSOIL as separate modules.

7.1 Two-dimensional model for solute transport and its finite element implementation

The model considers two-dimensional solute transport in variably saturated soil. 2DSOIL neglects deformations of a soil due to shrinking-swelling, and allows temperature and solute concentrations to influence hydraulic parameters but not solute concentration gradients. Molecular diffusion, hydrodynamic dispersion, and advection are the main processes causing solute transport in this model.

The governing solute transport equation is

$$\frac{\partial(\theta c)}{\partial t}-\frac{\partial}{\partial x}\left[\theta(D_{xx}\frac{\partial c}{\partial x}+D_{xz}\frac{\partial c}{\partial z})\right]-\frac{\partial}{\partial z}\left[\theta(D_{xz}\frac{\partial c}{\partial x}+D_{zz}\frac{\partial c}{\partial z})\right] + \frac{\partial(q_x C)}{\partial x}+\frac{\partial(q_z c)}{\partial z}+S_c=0 \tag{6.20}$$

for planar solute transport in a vertical soil cross-section, and

$$\frac{\partial(\theta c)}{\partial t}-\frac{1}{x}\frac{\partial}{\partial x}\left[x\theta(D_{xx}\frac{\partial c}{\partial x}+D_{xz}\frac{\partial c}{\partial z})\right]-\frac{\partial}{\partial z}\left[\theta(D_{xz}\frac{\partial c}{\partial x}+D_{zz}\frac{\partial c}{\partial z})\right] + \frac{1}{x}\frac{\partial(xq_x C)}{\partial x}+\frac{\partial(q_z c)}{\partial z}+S_c=0 \tag{6.21}$$

for axisymmetrical solute transport. Here, as before, θ is the volumetric water content (cm^3 of water per cm^3 of soil), c is the solute concentration (g per cm^3 of soil solution), S_c is an extraction term that describes the joint action of all factors contributing to removal of solute from the soil solution, g per cm^3 of soil per day; x is either the horizontal coordinate in case of transport in a vertical soil cross-section, or the radial coordinate in case of axisymmetrical transport, cm; z is the vertical coordinate measured upward from a reference plane, cm; t is time, days; D_{xx}, D_{xz} and D_{zz} are dispersion coefficients, cm^2 per day; and q_x and q_z are volumetric flux densities, cm^3 of water per cm^2 of soil per day.

The dispersion coefficients D_{xx}, D_{xz} and D_{zz} depend on the values of the fluxes q_x and q_z, the molecular diffusion coefficient D_0, the moisture content, the longitudinal and transverse dispersivities λ_L and λ_T, the coordinates x and z, time, concentrations of solutes, temperature, and other soil state variables. We assume that

$$q_x = -k\frac{\partial h}{\partial x}, \qquad q_z = -k(\frac{\partial h}{\partial z} + 1),$$

$$\theta D_{xx} = \theta\tau_c D_{mol} + \lambda_L \frac{q_x^2}{|q|} + \lambda_T \frac{q_z^2}{|q|},$$

$$\theta D_{xz} = (\lambda_L - \lambda_T)\frac{q_x q_z}{|q|}, \tag{6.22}$$

$$\theta D_{zz} = \theta\tau_c D_{mol} + \lambda_L \frac{q_z^2}{|q|} + \lambda_T \frac{q_x^2}{|q|},$$

$$|q| = \sqrt{q_x^2 + q_z^2}$$

where h is the pressure head, k is hydraulic conductivity, D_{mol} is the molecular diffusion coefficient in a free solution, τ_c is tortuosity factor, λ_L is the longitudinal dispersivity, and λ_T is transverse dispersivity.

The governing solute transport equations, Eqs. (7.1) and (7.2), are solved numerically to obtain spatial and temporal distributions of the concentration c within the soil domain following Šimůnek et al. (1992). We used the Galerkin finite element method with linear basis functions and triangular elements. The pressure head h, the hydraulic conductivity k, the molecular diffusion coefficient, and the concentration c are assumed to vary linearly over each element (Fig 3.1) as follows

$$\tilde{h}(x,z,t) = \sum_{n=1}^{N_n} \phi_n(x,z) h_n(t),$$
$$\tilde{c}(x,z,t) = \sum_{n=1}^{N_n} \phi_n(x,z) c_n(t), \tag{6.23}$$
$$\tilde{k}(x,y,t) = \sum_{n=1}^{N_n} \phi_n(x,y) k_n(t)$$

where N_n is the total number of nodes, $\phi_n(x,z)$ are the basis functions for node n; and h_n, k_n, and c_n are the pressure head, hydraulic conductivity, and concentration at node n, respectively.

The Galerkin method leads to equations for the nodal values of c. Area-averaged weighted residuals of Eq. (7.1) have to be equal to zero for every ϕ_n taken as a weight. Consequently, for the whole soil domain we obtain

$$\sum_{e=1}^{N_e}\int_{\Omega_e}\left[-\frac{\partial(\theta c)}{\partial t}+\frac{\partial}{\partial x}(\theta D_{xx}\frac{\partial c}{\partial x}+\theta D_{xz}\frac{\partial c}{\partial z}-q_x c)+\frac{\partial}{\partial z}(\theta D_{xz}\frac{\partial c}{\partial x}+\theta D_{zz}\frac{\partial c}{\partial z}-q_z c)+S_c\right]\phi_n d\omega=0 \qquad \textbf{(6.24)}$$

where Ω_e designates the area of the element e, and N_e is the total number of elements. After replacing c by $\tilde{c}$ and using Green's first identity, Eq (7.5) becomes

$$\begin{aligned}
&\sum_{e=1}^{N_e}\int_{\Omega_e}(-\frac{\partial(\theta c)}{\partial t})\phi_n d\omega \\
&+\sum_{e=1}^{N_e}\int_{\Omega_e}[-(-q_x\tilde{c}+\theta D_{xx}\frac{\partial\tilde{c}}{\partial x}+\theta D_{xz}\frac{\partial\tilde{c}}{\partial z})\frac{\partial\Phi_n}{\partial x}-(-q_z\tilde{c}+\theta D_{xz}\frac{\partial\tilde{c}}{\partial x}+\theta D_{zz}\frac{\partial\tilde{c}}{\partial z})\frac{\partial\phi_n}{\partial z}]d\omega \\
&+\sum_{e=1}^{N_e}\int_{\Gamma_e}[(-q_x\tilde{c}+\theta D_{xx}\frac{\partial\tilde{c}}{\partial x}+\theta D_{xz}\frac{\partial\tilde{c}}{\partial z})n_{\Gamma,x}+(-q_z\tilde{c}+\theta D_{xz}\frac{\partial\tilde{c}}{\partial x}+\theta D_{zz}\frac{\partial\tilde{c}}{\partial z})n_{\Gamma,z}]\phi_n d\Gamma \\
&-\sum_{e=1}^{N_e}\int_{\Omega_e}S_c\phi_n d\omega=0
\end{aligned} \qquad \textbf{(6.25)}$$

where Γ_e is the boundary of element e, and $n_{\Gamma,x}$, and $n_{\Gamma,z}$ designate components of the unit vector is normal to the boundary.

Further simplifications are based on the assumptions that nodal mass changes may be found as weighted averages of mass changes over the element according to mass-lumping techniques:

$$\frac{d(\theta_n c_n)}{dt}=\frac{\sum_{e=1}^{N_e}\int_{\Omega_e}\frac{\partial(\theta c)}{\partial t}\phi_n d\omega}{\sum_{e=1}^{N_e}\int_{\Omega_e}\phi_n d\omega} \qquad \textbf{(6.26)}$$

Accepting these assumptions leads to a system of first-order ordinary differential equations for the concentration values:

$$[Q]\frac{d\{\theta c\}}{dt}+[G]\{c\}+\{f\}=-\{Q_S^B\} \tag{6.27}$$

where the vector $\{\theta c\}$ includes all nodal values of θc. The matrices $[Q]$ and $[G]$ have as elements:

$$Q_{m,n}=-\delta_{mn}\sum_e \int_{\Omega_e}\phi_n d\omega=-\sum_{e=1}\frac{\Delta_e}{3}\delta_{mn}$$

$$G_{m,n}=-\sum_e\left\{\int_{\Omega_e}\left[\tilde{k}\frac{\partial\tilde{h}}{\partial x}\phi_m+D_{xx}\frac{\hat{b}_m}{2A_e}+D_{xz}\frac{\hat{c}_m}{2A_e}\right]\frac{\hat{b}_n}{2A_e}\right.$$

$$\left.+\left[(\tilde{k}(\frac{\partial\tilde{h}}{\partial z}+1)\phi_m+D_{xz}\frac{\hat{b}_m}{2A_e}+D_{zz}\frac{\hat{c}_m}{2A_e}\right]\frac{\hat{c}_n}{2A_e}\right\}d\omega= \tag{6.28}$$

$$-\sum_e\frac{1}{4A_e}\left\{\frac{\bar{k}_e+k_m/3}{4}[\hat{b}_n\Upsilon_b+\hat{c}_n\Upsilon_c]+D_{mol}(\hat{b}_m\hat{b}_n+\hat{c}_m\hat{c}_n)\overline{(\theta\tau)}\right.$$

$$\left.-\bar{k}\frac{b_m b_n(\lambda_L\Upsilon_b^2+\lambda_T\Upsilon_c^2)+(b_m c_n+b_n c_m)(\lambda_L-\lambda_T)\Upsilon_b\Upsilon_c+c_m c_n(\lambda_L\Upsilon_c^2+\lambda_T\Upsilon_b^2)]}{\overline{\omega^2\ \omega^2}}\right.$$

where

$$\Upsilon_b=\sum_{p=1}^{3}h_p b_p,\qquad \Upsilon_c=\sum_{p=1}^{3}h_p c_p+2A \tag{6.29}$$

for an element, overlined symbols denote average values over an element, and where summation occurs over elements which have the nodes m and n among their corner nodes.

Because the solute extraction rate, S_c, in 2DSOIL is constant over an element, the vector $\{f\}$ has components

$$f_n = \sum_e \frac{1}{3} A_e (S_c)_e \tag{6.30}$$

where summation involves elements that have the node n among its corner nodes.

Vector $\{Q_S^B\}$ has non-zero components only for boundary nodes. This vector represents total solute fluxes. If the concentration is constant at a boundary, then $dc_n/dt=0$ and, in accordance with (7.8),

$$(Q_S^B)_n = -\sum_{m=1}^{N_n} G_{m,n} c_m - f_n \tag{6.31}$$

If the solute flux is known at the boundary, then $\{Q_S^B\}$ is included in vector $\{f\}$. If the dispersive flux is assumed to be zero at the boundary, then $(Q_S^B)_n = Q_n c_n$ and the value of Q_n must be added to G_{nn}.

Methods used for solving (7.8) are similar to those described in detail by Šimůnek et al. (1992). A first-order finite difference approximation of the time derivatives leads to the following set of algebraic equations:

$$[Q]\frac{\{\theta c\}_{j+1} - \{\theta c\}_j}{\Delta t} + \epsilon_t [G]_{j+1}\{c\}_{j+1} (1-\epsilon_t)[G]_j c_j + \epsilon_t \{f\}_{j+1} + (1-\epsilon_t)\{f\}_j = 0 \tag{6.32}$$

where j and $j+1$ denote the previous and current time levels, respectively; Δt is the time increment and ϵ_t is a time weighing factor. Equation (7.13) can be rewritten in the form

$$[A]\{c\}_{j+1} = \{b\} \tag{6.33}$$

where

$$[A]=\frac{1}{\Delta t}[Q][\theta]_{j+1}+\epsilon_t[G]_{j+1}$$
$$\{b\}=\frac{1}{\Delta t}[Q]\{\theta c\}_j-(1-\epsilon_t)[G]_j\{c\}_j-\epsilon_t\{f\}_{j+1}-(1-\epsilon_t)\{f\}_j \qquad \textbf{(6.34)}$$

Slight modifications of the coefficients in Eqs. (7.9), (7.10) and (7.11) allows the axisymmetrical case described by Eq. (7.2) to be solved (Šimůnek et al., 1992). Boundary and initial conditions must be defined to solve Eq. (7.8). Methods of setting the time-dependent boundary are presented in Chapters 4 and 5 of this manual. Time-independent boundary concentrations must be included as part of the initial distribution data as described in section 7.3.

7.2 Parameters of the SoluteMover module

Equation (7.3) shows that dispersion, as manifested by solute spreading during transport in the subsurface, is a result of the joint action of ionic or molecular diffusion and hydrodynamic dispersion [Bear, 1972; Simunek et al., 1992]. A good rule of thumb for groundwater is that the transverse and longitudinal dispersivities in (7.3) are related by $\lambda_T = 0.1\ \lambda_L$. The ratio may be higher in soils.

For practical problems we make use of the fact that, in general, λ_T is significantly less then λ_L (Bear, 1972). Having $\lambda_T=0$, one must know the value of λ_L, which strongly depends on soil structure at high velocities and on soil texture at low velocities. The value of λ_L is also known to have high spatial variability. As a first approximation the following power dependence may be used:

$$\lambda_L=0.012(\text{clay percentage})^2 \qquad \textbf{(6.35)}$$

which appears reasonable for clay percentages between 20 and 60 percent(Pachepsky, 1992).

The tortuosity factor, τ_c, in (7.3) strongly depends on soil structure and texture as well as on soil moisture content. Its value may be estimated as (Pachepsky, 1990)

$$\tau_c = \begin{cases} 0.59 - 0.12\log_{10}|h|, & h < -0.2cm \\ 0.67, & h \geq -0.2cm \end{cases} \qquad \textbf{(6.36)}$$

This equation has proved to be a reasonable approximation for soils of different textures, and has been incorporated into the 2D SOIL code. Molecular diffusion coefficients in solution are tabulated in many sources. A summary of these as derived from a table in Beven et al. (1993), is given in Table 7.1. The concise review of Nye and Tinker (1977) also provides information necessary for estimating the value of D_{mol}.

Table 7.1 Representative values of dispersion parameters from published undisturbed core experiments (from Beven et al., 1993)

Study	Dispersion coefficient $cm^2\ h^{-1}$)	Dispersivity (m)	Mean pore water velocity (cm h^{-1})	θ_m/θ
Elrick and French (1966)				
undisturbed	1.404	-	1.52	
Anderson and Bouma (1977)				
medium sand/sub-angular blocky	4.17	-	0.0417	
clay loam/prismatic	0.417	-	0.0417	
Cassel et al. (1974)				
Aberdeen undisturbed	0.197	-	0.0151	
Boetia undisturbed	0.161	-	0.0151	
Smettem (1984)	24.0	0.077	2.3	
	(102.8/1.2)	(0.218/0.013)	(5.8/0.6)	
Seyfried and Rao (1987)	4.04	150.6	2.709	
	(6.44/ 1.65)	(r84.4/95.3)	(4.1/1.7)	

Table 7.1 Representative values of dispersion parameters from published undisturbed core experiments (from Beven et al., 1993)

Study	Dispersion coefficient $cm^2\ h^{-1}$)	Dispersivity (m)	Mean pore water velocity (cm h^{-1})	θ_m/θ
Jury and Sposito (1985)				
Core—highest value	5.642	0.251	0.225	
Core—lowest value	3.367	0.197	0.171	
Dyson and White (1987)	23.075	0.066	2.941	
	(75.5/2.55)	(0.139/0.029)	(6.34/0.74)	
Abdulkabir (1989)				
Grass soil	0.230	-	1.409	0.41
	(0.57/0.06)	-	(1.76/0.77)	(0.58/0.32)
Forest soil	5.55	-	52.4	0.38
	(7.58/2.79)	-	(57.6/46.7)	(0.59)/0.27)
Lancaster core	160.4	0.526	3.04	0.68
	54.2	0.357	1.52	0.95
	18.6	0.243	0.76	1.0
Slapton Wood core				
Upward flux	370.0	1.217	3.04	0.61
	31.5	0.706	1.53	0.44
	15.5	0.203	0.76	0.33
Downward flux	13.5	0.177	0.76	0.42
	8.4	0.220	0.38	0.47
Wierenga and van Genuchten (1989)				
Small cores	20.9	0.0087	1.01	
	(46.2/3.9)	(0.0094/0.0077)	(2.22/0.18)	
Large core	2.71	34.0	0.08	

Figures in parentheses are highest and lowest quoted values for each parameter

Table 7.2 Representative values of dispersion parameters from published field plot experiments (from Beven et al., 1993).

Study	Dispersion coefficient	Dispersivity (m)	Mean pore water velocity ($cm^2\ h^{-1}$)
Biggar and Nielsen (1976)	8.776	0.0547	1.826
	(66.5/0.35)	(0.257/0.017)	(15.28/0.008)
Van de Pol et al. (1977)	1.531	0.0942	0.1625
	(3 54/0.925)	(2.72/0.04)	(0.218/0.130
Bowman and Rice (1986)			
Water applied semi-weekly	16.14	0.524	0.290
	(47.9/6.5)	(1.41/0.208)	(0.367/0.197)
Water applied bi-weekly	21.759	0.445	0.293
	(107.9/1.558)	(0.952/0.094)	(0.533/0.162)
Schulin et al. (1987)			
Br^- as tracer	0.0604	0.0393	0.0163
Cl- as tracer	0.0471	0.0214	0.0220
Rice et al. (1986)	2:229	0.165	0.146
	(6.67/1.13)	(0.21/0.14)	(0.46/0.071)
Jaynes et al. (1988)	88.90	0.178	5.00
	(99.9/79.2)	(0.228/0.138)	(5.75/4.38)
Jaynes (1991)	149.6	0.288	4.75
	(920.8/1.9)	0.658/0.045)	(29.99/0.42)
Jury and Sposito (1985)	2.488	0. 1 73	0.146
	(3.00/1.313)	(0.257/0.197)	(0.179/0.117)
Buttcrs and Jury (1989)			
Field Scale	-	0.102	-
Local scale	-	0.177	-

Figures in parenthesis are highest and lowest quoted for each parameter when available.

7.3 Data files '*Param_S.dat*' and '*Nodal_S.dat*'

Parameters needed for computations by the **SoluteMover** module are read from the file **'Param_S.dat'**. One of these parameters is the time-weighing factor *epsi* (ϵ in Eq 7.13). Values of *epsi* between 0.5 and 0.8 usually give good results. When *epsi* = *0*, calculations for the next time step become faster, but the time step in general must be much smaller than for *epsi* > 0.5. The second parameter, *lUpW*, is a switch that allows upstream weighing. Upstream weighing has been shown to diminish or eliminate numerical oscillations that often arise near steep concentration fronts and in areas with high flow velocities relative to dispersion (Yeh and Tripathi, 1990). It seems reasonable to always use this method in the algorithm when sharp concentration fronts are expected. A third parameter, *CourMax*, is the upper limit of the so-called Courant number, which is the ratio between the amount of water within an element and the amount of water brought to the element through boundaries during the current time step. Values of 0.3-0.5 have proved to be satisfactory.

Solute transport parameters are provided separately for each soil subdomain. For current calculations, materials are identified by the material number, *MatNumN*, specified for every node in the Grid_and_Boundary information file **'Grid_Bnd.dat'**. Parameter values are discussed in the next section.

The structure of the data for the computational parameters is presented in Table 7.3. The example following the table holds for two soil materials and three solutes. In addition to the computational parameters, **SoluteMover** reads data about the initial concentration distribution from the file **'Nodal_S.dat'**. If there are constant concentration boundaries, then the values of the boundary concentrations must be given in the file. Table 7.4 shows the structure of data in the **'Nodal_S.dat'** file. The example following the table corresponds to the grid shown in Fig. 3.1 and to the file **'Grid_Bnd.dat'** of Example 3.3.

Table 7.3. Format of the file **'Param_S.dat'**.

Record	Variable	Description
1	-	Comment line.
		Computational Information
2	-	Comment line.
3	*NumSol*	Number of solutes under consideration.
4,5	-	Comment lines.
6	*epsi*	Temporal weighing coefficient.
6	*lUpW*	1 - upstream weighing formulation, 0 - original Galerkin formulation.
6	*CourMax*	Maximum allowed Courant number.
		Material information
7-9	-	Comment lines.
10	*Dmol(1)*	Ionic or molecular diffusion coefficient in free water for solute 1.
10	*Dmol(2)*	Same as above for solute 2.
. .	. .	. .
10	*Dmol(NumSol)*	Same as above for the last solute.
11,12	-	Comment lines.
13	*Dlng(M,1)*	Longitudinal dispersivity of solute 1of the material in subdomain *M*.
13	*Dlng(M,2)*	Same as above for solute 2.
. .	. .	. .
13	*Dlng(M,NumSol)*	Same as above for the last solute.
		Record 13 is given for the soil material of each subdomain *M* (from 1 to *NMat*).
14,15	-	Comment lines.
16	*Dtrn(M,1)*	Transverse dispersivity of solute *j* for the soil material in subdomain *M*.
16	*Dtrn(M,2)*	Same as above for solute 2.
. .	. .	. .
16	*Dtrn(M,NumSol)*	Same as above for the last solute.
		Record 16 is given for the soil material in each subdomain *M* (from 1 to *NMat*).

```
** Example 7.1: SOLUTEMOVER PARAMETERS: file 'Param_S.dat'
Number of solutes
        3
Computational parameters
epsi    lUpW     CourMax
0.55     1            0.5
Soil material and solute parameters
Diffusion coefficients
 Solute #1     Solute #2     Solute #3
 1.73       1.25       0.12
Longitudinal dispersivities of soil materials
   Sol # 1  Sol # 2  Sol # 3
     5         5        20          (material in subdomain # 1)
    10        10        40          (material in subdomain # 2)
Transverse dispersivities of soil layers
   Sol # 1  Sol # 2  Sol # 3
      2         2        20          (material in subdomain # 1)
      2         2        10          (material in subdomain # 2)
```

Table 7.4. Format of the file **'Nodal_S.dat'**.

Record	Variable	Description
1,2	-	Comment lines.
3	*n*	Nodal number.
3	*Conc(n,1)*	Initial value of the concentration of the first solute at node *n*, mg L^{-1}
3	*Conc(n,2)*	Same as above for the 2nd solute.
.	.	.
3	*Conc(n,NumSol)*	Same as above for the last solute.

Record 3 is provided for every node of the grid. If some boundary nodes have constant concentrations, the concentration values must be present in this file.

```
**** Example 7.2: INITIAL SOLUTE CONCENTRATION DISTRIBUTION - file
 'Nodal_S.dat'
 n  Conc(n,1)  Conc(n,2)  Conc(n,3)
 1    0.17E-03    0.045E-03    1.3E-03
 2    0.18E-03    0.047E-03    1.4E-03
 3    0.41E-03    0.049E-03    0.0
 4    0.45E-03    0.051E-03    0.0
 5    0.23E-03    0.054E-03    0.0
 6    0.27E-03    0.072E-03    0.0
 7    0.29E-03    0.077E-03    0.0
 8    0.33E-03    0.106E-03    0.0
 9    0.35E-03    0.111E-03    0.0
10    0.37E-03    0.115E-03    0.0
11    0.29E-03    0.125E-03    0.0
12    0.44E-03    0.134E-03    0.0
13    0.44E-03    0.144E-03    0.0
14    0.56E-03    0.171E-03    0.0
15    0.57E-03    0.172E-03    0.0
16    0.59E-03    0.172E-03    0.0
17    0.60E-03    0.172E-03    0.0
18    0.63E-03    0.172E-03    0.0
```