Chapter 8: Heat Transport: HeatMover Module

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The **HeatMover** module calculates temperature changes in the soil due to diffusion of heat and movement of heat with water. This module has many features in common with the **SoluteMover** module described in Chapter 7.

8.1 The two-dimensional model of heat movement and its finite element implementation

The model considers two-dimensional transport of heat in a variably saturated soil. The governing heat transport equation is taken as

$$\frac{\partial(\hat{C}T)}{\partial t}-\frac{\partial}{\partial x}[\Lambda\frac{\partial T}{\partial x}]-\frac{\partial}{\partial z}[\Lambda\frac{\partial T}{\partial z}]+\frac{\partial(q_x C_w T)}{\partial x}+\frac{\partial(q_z C_w T)}{\partial z}=0 \qquad \textbf{(8.1)}$$

for heat transport in a vertical soil cross-section, and

$$\frac{\partial(CT)}{\partial t}-\frac{1}{x}\frac{\partial}{\partial x}[x\Lambda\frac{\partial T}{\partial x}]-\frac{\partial}{\partial z}[\Lambda\frac{\partial T}{\partial z}]$$
$$+\frac{1}{x}\frac{\partial(xq_X C_w T)}{\partial x}+\frac{\partial(q_z C_w T)}{\partial z}+C_w S T=0 \qquad \textbf{(8.2)}$$

for axisymmetrical heat transport. Sources or sinks of heat are not considered in these equations. T is the temperature (°C), and $\hat{C}$ is the total heat capacity of the soil system (solid material and water) given by $\hat{C}= C_{sm}X_m + C_{om}X_{om} + C_w\theta$. The units of $\hat{C}$ are Joules cm^{-3} $°C^{-1}$. Subscripted C's are the heat capacities of the mineral matter (sm), organic matter (om), and water (w) in the soil pores per unit volume, subscripted X's are the volume fractions, and θ is the volumetric water

content. $\hat{C}$ is not a constant because of its dependency on θ. DeVries (1966) gives C_{sm} =1.93 (0.46) and C_{om}=2.51 (0.6) and C_w =4.18 (1.0) as average values in Joules cm^{-3} $^oC^{-1}$ (cal cm^{-3} $^oC^{-1}$). Furthermore, x in Eq. 8.1 and 8.2 represents the horizontal coordinate in case of water flow in a vertical soil cross-section and the radial coordinate in case of axisymmetrical water flow, z is the vertical coordinate measured upward from the base of the soil profile; (z and x are both in cm), and t is time, days. The thermal conductivity, Λ, has units of Joules cm^{-1} day^{-1} $^oC^{-1}$, and depends on the moisture content. Modeling of these dependencies is discussed in the next section of this chapter.

Fluxes of heat are connected with rates of moisture content change ($\partial\theta/\partial t$) and water extraction ($S$) as follows

$$\begin{aligned} &\frac{\partial\theta}{\partial t}+\frac{\partial q_x}{\partial x}+\frac{\partial q_z}{\partial z}+S=0, \quad \text{planar symmetry} \\ &\frac{\partial\theta}{\partial t}+\frac{1}{x}\frac{\partial(xq_x)}{\partial x}+\frac{\partial q_z}{\partial z}+S=0, \quad \text{axial symmetry} \end{aligned} \tag{8.3}$$

Therefore, (8.1) may be recast as

$$\theta R\frac{\partial T}{\partial t}-\frac{1}{x}\frac{\partial}{\partial x}[\frac{\Lambda}{C_W}\frac{\partial T}{\partial x}]-\frac{\partial}{\partial z}[\frac{\Lambda}{C_W}\frac{\partial T}{\partial z}]+ +q_x\frac{\partial T}{\partial x}+q_z\frac{\partial T}{\partial z}=0 \tag{8.4}$$

and (8.2) becomes

$$\theta R\frac{\partial T}{\partial t}-\frac{\partial}{\partial x}[\frac{\Lambda}{C_W}\frac{\partial T}{\partial x}]-\frac{\partial}{\partial z}[\frac{\Lambda}{C_W}\frac{\partial T}{\partial z}] +q_x\frac{\partial T}{\partial x}+q_z\frac{\partial T}{\partial z}=0 \tag{8.5}$$

In these equations $R=1+\frac{C_{sm}X_{sm}+C_{om}X_{om}}{C_w\theta}$. The governing equations for heat transport (8.4) and (8.5) are solved numerically to obtain spatial and temporal distributions of the heat content as

measured by the temperature (T) within the soil profile. The Galerkin finite element method with linear basis functions and triangular elements is used.

As with water and solutes, the heat content is approximated by a linear combination of nodal concentration values:

$$\hat{T}(x,z,t)=\sum_{n=1}^{N_n}\phi_n(x,z)T_n(t) \tag{8.6}$$

where N_n is the total number of nodes, $\phi_n(x,z)$ are basis functions for node n and T_n is the temperature in node n. Basis functions may be derived from interpolation functions for the elements. Interpolation functions for triangular elements are given in (6.4).

The Galerkin method gives equations for the nodal values of T. Area-averaged weighted residuals of (8.4) and (8.5) have to be equal to zero for every ϕ_n taken as a weight. Consequently for the whole soil domain we have

$$\sum_{e=1}^{N_e}\int_{\Omega_e}\left[\theta R\frac{\partial T}{\partial t}-\frac{\partial}{\partial x}\left(\frac{\Lambda}{C_W}\frac{\partial T}{\partial x}\right)-\frac{\partial}{\partial z}\left(\frac{\Lambda}{C_W}\frac{\partial T}{\partial z}\right)+q_x\frac{\partial T}{\partial x}+q_z\frac{\partial T}{\partial z}\right]\phi_n d\omega=0 \tag{8.7}$$

where Ω_e designates the area of element e and N_e is the total number of elements. After replacing T by $\hat{T}$ and using Green's first identity, one has:

$$\begin{aligned}&\sum_{e=1}^{N_e}\int_{\Omega_e}\left(-\theta R\frac{\partial \hat{T}}{\partial t}\right)\phi_n d\omega\\ &+\sum_{e=1}^{N_e}\int_{\Omega_e}\left[-\frac{\partial \hat{T}}{\partial x}\left(q_x\phi_n+\frac{\Lambda}{C_W}\frac{\partial \phi_n}{\partial x}\right)-\frac{\partial \hat{T}}{\partial z}\left(q_z\phi_n+\frac{\Lambda}{C_W}\frac{\partial \phi_n}{\partial z}\right)\right]d\omega+\\ &+\sum_{e=1}^{N_e}\int_{\Gamma_e}\left(\frac{\partial \hat{T}}{\partial x}n_{\Gamma,x}+\frac{\partial \hat{T}}{\partial z}n_{\Gamma,z}\right)\frac{\Lambda}{C_W}\phi_n d\Gamma\end{aligned} \tag{8.8}$$

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

Further simplifications are based on two important assumptions. First, the moisture content, θ, and soil water fluxes, q_x, and q_z vary linearly over each element. Second, nodal

temperature changes may be found as weighted averages of temperature changes over an element according to a mass-lumping technique (Istok, 1989).

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

$$[Q]\frac{d\vec{T}}{dt}+[G]\{T\}=\{Q\}^D \tag{8.9}$$

where the vector $\{T\}$ includes all nodal values of T. Matrices Q and G have elements

$$\begin{aligned} Q_{m,n} &= \delta_{mn}\sum_e \frac{A_e}{12}(3\bar{\theta}\bar{R}+\theta_n R_n) \\ G_{m,n} &= \left[-\frac{\hat{b}_m}{24}[3\bar{q}_x+(q_x)_n]-\frac{\hat{c}_m}{24}[3\bar{q}_z+(q_z)_n] \right. \\ &\quad \left. -\frac{1}{4A_e}\frac{\Lambda}{C_w}[\hat{b}_m\hat{b}_n+\hat{c}_m\hat{c}_n] \right] \end{aligned} \tag{8.10}$$

where the summation involves elements which have the nodes m and n among their corner nodes. Nodal water extraction rates are calculated as $S_n=\Sigma A_e S_e/\Sigma A_e$ where the summation covers all elements that have node n at one of their corners. Values of the parameters $\hat{b}_n$, $\hat{c}_n$, and A_e have the same meaning as in (6.4), while overlined values indicate average values over the element.

The vector $\{Q^D\}$ has non-zero components only for boundary nodes. This variable represents the convective heat flux and is given by:

$$\{Q\}_n^D=-\sum_{m=1}^{M_n} S_{m,n}T_m \tag{8.11}$$

If the temperature is constant along a boundary, then $dT_n/dt=0$ and, in accordance with (8.9), if the heat flux is constant at the boundary, then $\{Q^D\}$ is replaced by the known total boundary flux divided by C_W.

The method for solving the system (8.9) is similar to those for systems (6.9) and (8.9). The axisymmetrical cases described by (8.5) can be calculated by making slight modifications to the coefficients in (8.10) and (8.11). Boundary and initial conditions must be set to solve (8.9). Methods of implementing time-dependent boundary settings are presented in Chapters 4 and 5 of this manual. Time-independent boundary temperature must be included in the initial distribution data as described in Section 8.3.

8.2 Parameters of the HeatMover module

The thermal conductivity of a soil controls the diffusion of heat in soil. The overall thermal conductivity is an average of the thermal conductivities of the different soil components and depends on the relative proportions of these components. The method of calculating the average thermal conductivity is taken from DeVries (1966):

$$\Lambda = \frac{\sum_{i=1}^{N} \omega_i X_i \Lambda_i}{\sum_{i=1}^{N} \omega_i X_i} \qquad \textbf{(8.12)}$$

where N is the number of components, Λ is the thermal conductivity of the soil, ω_i is a weighing factor that depends on the ratios of the thermal conductivities of the component, the medium in which heat transport occurs (air or water) and the size and relative shapes of the granules, X_i is the volume fraction of the i'th component, and Λ_i is the thermal conductivity of the ith component. Values of ω_i are calculated as:

$$\omega_i = \frac{1}{3}\sum_{j=1}^{3} \left| 1 + \left(\frac{\Lambda_i}{\Lambda_o} - 1 \right) \Upsilon_j \right|^{-1} \qquad \textbf{(8.13)}$$

where Υ_j (j=1,2,3) are shape factors that depend on the shapes of the particles. The sum of the three shape factors is unity so that for spherical particles $\Upsilon_1 = \Upsilon_2 = \Upsilon_3 = 1/3$. The parameter Λ_o

represents the thermal conductivity of the reference medium (water for a moist soil, and air for a dry soil). The components of the system that affect the thermal conductivities are the soil mineral particles, soil organic matter, soil air (containing water vapor), and soil water. The thermal conductivity of air containing water vapor is calculated as:

$$\Lambda_a = \Lambda_{da} + \Lambda_v \frac{\theta}{\theta_s} \tag{8.14}$$

Where, Λ_{da} is the thermal conductivity of dry air, and Λ_v is the thermal conductivity of water vapor. These two parameters are calculated as

$$\begin{aligned} \Lambda_{da} &= 0.058 + 1.74 \cdot 10^{-3} T_a \\ \Lambda_v &= 0.052 \cdot e^{(0.058 T_{surf})} \end{aligned} \tag{8.15}$$

The two equations were taken from figure 7.2, page 217 of De Vries (1966). The units for the conductivities in these equations are millicalories cm^{-1} day^{-1} $°C^{-1}$. In the program they are converted to Joules cm^{-1} day^{-1} $°C^{-1}$.

8.3 Data files '*Param_T.dat*' and '*Nodal_T.dat*'

Parameters needed for calculations of heat transport are read from the file **'Param_T.dat'**. One parameter is the time-weighting factor *epsi* used in the final matrix equation for heat flow. See Section 7 (**SoluteMover**) for more information . Reasonable values of *epsi* are between 0.5 and 0.8. Another parameter is *HCritA* which is described in more detail in Section 6 (**WaterMover**) and should be that same as the value used in the WaterMover module. Parameters needed to calculate heat capacities are also included in the data file **'Param_T.dat'**. These are the mass percentages of sand, silt and clay particles. These parameters are provided separately for every soil layer. Materials are identified by the material number, *MatNumN*, specified for every node in the Grid_and_Boundary information file **'Grid_Bnd.dat'**. The structure of the data file for the heat transport parameters is given Table 8.1. The example

following the table holds for two soil materials. In addition to the computational parameters, **HeatMover** reads data about the initial temperature distribution from file **'Nodal_T.dat'**. If there are constant temperature boundaries, then the values of the boundary temperatures must be given in this file. Table 8.2 shows the structure of the **'Nodal_T.dat'** file. The example following the table corresponds to the grid of Fig. 3.1 and to file **'Grid_bnd.dat'** of Example 3.3.

Table 8.1 Format of the file **'Param_T.dat'**

Record	Variable	Description
1,2	-	Comment line
	Computational Information	
3	*epsi*	Temporal weighting coefficient.
3	*HcritA*	A threshold matric potential of soil. When the soil is drier than this, actual evaporation is less that potential evaporation. It should correspond to the value of hCritA used in the **Param_w.dat** file (Table 6.1).
	Material information	
4,5	-	Comment lines.
6	*BulD(M)*	Bulk density of soil material in subdomain # M, g cm^{-3}
6	*FracOm(M)*	Mass fraction of Organic matter in soil material in subdomain # M
6	*FracSind(M)*	Same as above for sand+silt
6	*FracClay(M)*	Same as above for clay

Record 6 is made for each soil material *M, M=1,2,... Nmat* and is given as a percentage.

```
*** Example 8.1:  HEAT MOVER PARAMETER INFORMATION ******************
***  EPSI    HCritA
     0.5     1.E+06
Soil materaial information
(BulD)     (FracOm)  (FracSind)  (FracClay)
  1.59         0           95         05      (Soil material # 1)·
  1.66         0           56         44      (Soil material # 2)
```

Table 8.2 Format of the file **'Nodal_T.dat'**

Record	Variable	Description
1,2	-	Comment lines.
3	*n*	Nodal number
3	*T(n)*	Initial value of temperature at node *n*, °C

Record 3 is provided for every node of the grid.
Constant boundary temperature, if used, must be present in this file.

```
*** Example 8.2: HEAT MOVER NODAL INFORMATION
   n      Tmpr
1         25
2         25
3         20
4         20
5         25
6         25
7         20
8         20
9         20
10         20
11         20
12         20
13         20
14         20
15         20
16         20
17         20
18         20
```

Chapter 9: Gas Transport: GasMover Module

Yakov Pachepsky and Dennis Timlin

The **GasMover** module was written especially for 2DSOIL and has many features in common with the **SoluteMover** module described in Chapter 7. This module considers gas movement in the liquid-free pore space as caused by diffusion and gas production/extraction by biological activity in the soil.

9.1 The two-dimensional model of solute movement and its finite element implementation

The model considers two-dimensional transport of several gases in variably saturated soil. The code neglects deformation of soil due to shrinking-swelling, and allows temperature and gas values to influence transport parameters. Molecular diffusion is the main process governing gas transport in this model; pneumatic effects are not considered. The governing gas transport equation is:

$$\frac{\partial(\vartheta g)}{\partial t}-\frac{\partial}{\partial x}[\vartheta D_g\frac{\partial g}{\partial x}]-\frac{\partial}{\partial z}[\vartheta D_g\frac{\partial g}{\partial z}]+S_g=0 \qquad \textbf{(9.1)}$$

for gas transport in a vertical soil cross-section and

$$\frac{\partial(\vartheta g)}{\partial t}-\frac{1}{x}\frac{\partial}{\partial x}[x\vartheta D_g\frac{\partial g}{\partial x}]-\frac{\partial}{\partial z}[\vartheta D_g\frac{\partial g}{\partial z}]+S_g=0 \qquad \textbf{(9.2)}$$

for axisymmetric gas transport. Here ϑ is the air-filled porosity, cm^3 per cm^3 of soil; g is the gas content, g per cm^3 of soil air; S_g is an extraction term that describes the joint action of all factors contributing to removal of the gas from the air-filled pore space, g per cm^3 of soil per day; x is the horizontal coordinate in the case of planar water transport, and the radial coordinate for the case of axisymmetric water transport, cm; z is the vertical coordinate measured upward from a reference plane, cm; t is time, days; and D_g is the gas molecular diffusion coefficient in soil air,

cm^2 day^{-1}. The molecular diffusion coefficient D_g depends on moisture content, the spatial coordinates x and z, time, and concentrations of gases and temperature. The modeling of the molecular diffusion coefficient is discussed in a later section of this chapter. The extraction term, S_g, includes gas uptake and production by roots, chemical interactions, and microbiological activity. Chapter 15 of this manual describes an example of incorporating root respiration into 2DSOIL.

Air-filled porosity changes at a rate that is opposite to the rate of change of moisture content:

$$\frac{\partial \vartheta}{\partial t} = -\frac{\partial \theta}{\partial t} \tag{9.3}$$

where the sum of θ and ϑ is assummed constant and equal to θ_s, i.e. saturated moisture content. Therefore, Eqs. (9.1) and (9.2) may be recast to

$$\vartheta \frac{\partial g}{\partial t} - \frac{\partial}{\partial x}(\vartheta D_g \frac{\partial g}{\partial x}) - \frac{\partial}{\partial z}(\vartheta D_g \frac{\partial g}{\partial z}) + S_g + \frac{\partial \theta}{\partial t} g = 0 \tag{9.4}$$

and

$$\vartheta \frac{\partial g}{\partial t} - \frac{1}{x}\frac{\partial}{\partial x}(\vartheta D_g x \frac{\partial g}{\partial x}) - \frac{\partial}{\partial z}(\vartheta D_g \frac{\partial g}{\partial z}) + S_g + \frac{\partial \theta}{\partial t} g = 0 \tag{9.5}$$

The governing equations of gas transport (9.4) and (9.5) are solved numerically to obtain spatial and temporal distributions of the gas content, g, within the soil domain. The soil domain for this purpose is divided into a network of triangular elements with nodal points representing corners of elements. One possible subdivision is shown in Fig. 6.1 which applies to the grid in Fig. 3.1. The gas content is approximated by a linear combination of nodal concentration values:

$$\hat{g}(x,z,t) = \sum_{n=1}^{N_e} \phi_n(x,z) g_n(t) \tag{9.6}$$

where N_n is the total number of nodes, $\phi_n(x,z)$ are basis functions for node n, and g_n is the gas content at the node n. The basis functions are linear and are derived from interpolation functions which are given for triangular elements in Eq. (6.4). The Galerkin method is used to obtain equations for nodal values of g. Area-averaged weighted residuals of Eq. (9.4) must equal zero for every ϕ_n taken as a weight. Consequently, for the whole soil domain we obtain:

$$\sum_{e=1}^{N_e} \int_{\Omega_e} \left[\vartheta \frac{\partial g}{\partial t} - \frac{\partial}{\partial x}(\vartheta D_g \frac{\partial g}{\partial x}) - \frac{\partial}{\partial z}(\vartheta D_g \frac{\partial g}{\partial z}) + S_g + \frac{\partial \theta}{\partial t} g \right] \phi_n d\omega = 0 \tag{9.7}$$

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

$$\begin{aligned} &\sum_{e=1}^{N_e} \int_{\Omega_e} (-\vartheta \frac{\partial \hat{g}}{\partial t}) \phi_n d\omega - \sum_{e=1}^{N_e} \int_{\Omega_e} \frac{\partial \theta}{\partial t} \hat{g} \phi_n d\omega \\ &+ \sum_{e=1}^{N_e} \int_{\Omega_e} [-\frac{\partial \hat{g}}{\partial x} \frac{\partial \phi_n}{\partial x} - \frac{\partial \hat{g}}{\partial z} \frac{\partial \phi_n}{\partial z}] \vartheta D_g d\omega \\ &+ \sum_{e=1}^{N_e} \int_{\Gamma_e} (\frac{\partial \hat{g}}{\partial x} n_{\Gamma,x} + \frac{\partial \hat{g}}{\partial z} n_{\Gamma,z}) \vartheta D_g \phi_n d\Gamma \\ &- \sum_{e=1}^{N_e} \int_{\Omega_e} S_g \phi_n d\omega = 0 \end{aligned} \tag{9.8}$$

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

Further simplifications are based on two important assumptions. First, the air-filled porosity, ϑ, varies linearly over each element and S_g, the gas extraction rate, is constant over an element. Second, changes of nodal gas content are calculated as weighted averages of gas content changes over the element according to the mass-lumping technique (Istok, 1989). These assumptions lead to a system of first-order ordinary differential equations for the values of gas concentration:

$$[Q]\frac{d\{g\}}{dt}+[G]\{g\}+\{f\}=\{Q\}^D \tag{9.9}$$

where vector $\{g\}$ includes all nodal values of g. The matrices Q and G have elements

$$\begin{aligned} Q_{m,n}&=\delta_{mn}\sum_e \frac{A_e}{3}\vartheta_n \\ G_{m,n}&=\sum_e [-\frac{A_e}{3}(\frac{\partial\theta}{\partial t})_n\delta_{mn}-\frac{\overline{\vartheta D_g}}{4A_e}(\hat{b}_m\hat{b}_n+\hat{c}_m\hat{c}_n)] \end{aligned} \tag{9.10}$$

where summation is over elements having nodes m and n. Vector $\{\vec{f}\}$ has components

$$f_n=\sum_e \frac{1}{12}A_e[(\overline{S_g})_e+(S_g')_n] \tag{9.11}$$

where summation is over elements having the node n. Gas extraction rates at the nodes are calculated as $(S_g')_n=\Sigma A_e(S_g)_e/\Sigma A_e$ where summation is over all elements that contain the node n. The average nodal gas extraction rate of element S_e is found as a mean of the nodal values for that element. The parameters $\hat{b}_n$, $\hat{c}_n$, A_e have the same meaning as in Eq. (6.4). Parameters with over lines are averaged over elements.

Vector $\vec{Q}^D$ has non-zero components only for boundary nodes. It represents the total gas flux. If the concentration is constant at the boundary, then $dg_n/dt=0$ and, in accordance with Eq. (9.9),

$$Q_n^D=-\sum_{m=1}^{N_n} G_{m,n}g_m-f_n \tag{9.12}$$

If the gas flux is constant at the boundary, then Q^D is replaced by the known total boundary flux. This flux is added to components of the vector $\vec{f}$ in Eq. (9.9) and Q^D is zeroed.

Methods used for solving Eq. (9.9) are similar to those described in sections 7.9 and 8.9. Slight modifications of the coefficients in Eqs. (9.10) and (9.11) allows the solution of

axisymmetric cases described by Eq. (9.5). Boundary and initial conditions must be defined to solve Eq. (9.9). Information on time-dependent boundary settings are presented in Chapters 4 and 5 of this manual. Time-independent boundary concentrations are specified as initial data. The initialization file is described in section 9.3.

9.2 Parameters of the GasMover module.

Molecular diffusion in soil air is the only mechanism that governs gas movement in the model. The gas diffusion coefficient in soils, D_g, depends on the diffusion coefficient in air D_0 and on the soil conditions according to:

$$D_g = D_0 \tau_g = D_{0,st} \left(\frac{T}{273.15} + 1\right)^{n_g} \tau_g \qquad \textbf{(9.13)}$$

where $D_{0,st}$ is the molecular diffusion coefficient at standard conditions (760 mm Hg and 273.15 K), and n_g is an exponent between 1.75 and 2.0 (American Institute of Physics Handbook, 1972). Here, n_g=2 applies for all gases. The tortuosity factor τ_g strongly depends on soil structure and texture as well as on soil moisture content. This relationship is illustrated in Fig. 9.1, where the averaged data for different gases have been compiled from various sources. The data indicate that there is a threshold level of air-filled porosity below which diffusion does not occur. The dependence of the tortuosity factor on air-filled porosity may be expressed as

$$\tau_g = \begin{cases} b_{Tort}(\vartheta - \vartheta_{Thr}), & \vartheta > \vartheta_{Thr} \\ 0, & \vartheta \le \vartheta_{Thr} \end{cases} \qquad \textbf{(9.14)}$$

where ϑ_{Thr} is a threshold value of air-filled porosity, and b_{Tort} is a tortuosity change per unit of air-filled porosity. Reasonable values for the variables in Eq 9.14 are: ϑ_{Thr}=0.12 and b_{Tort}=0.65.

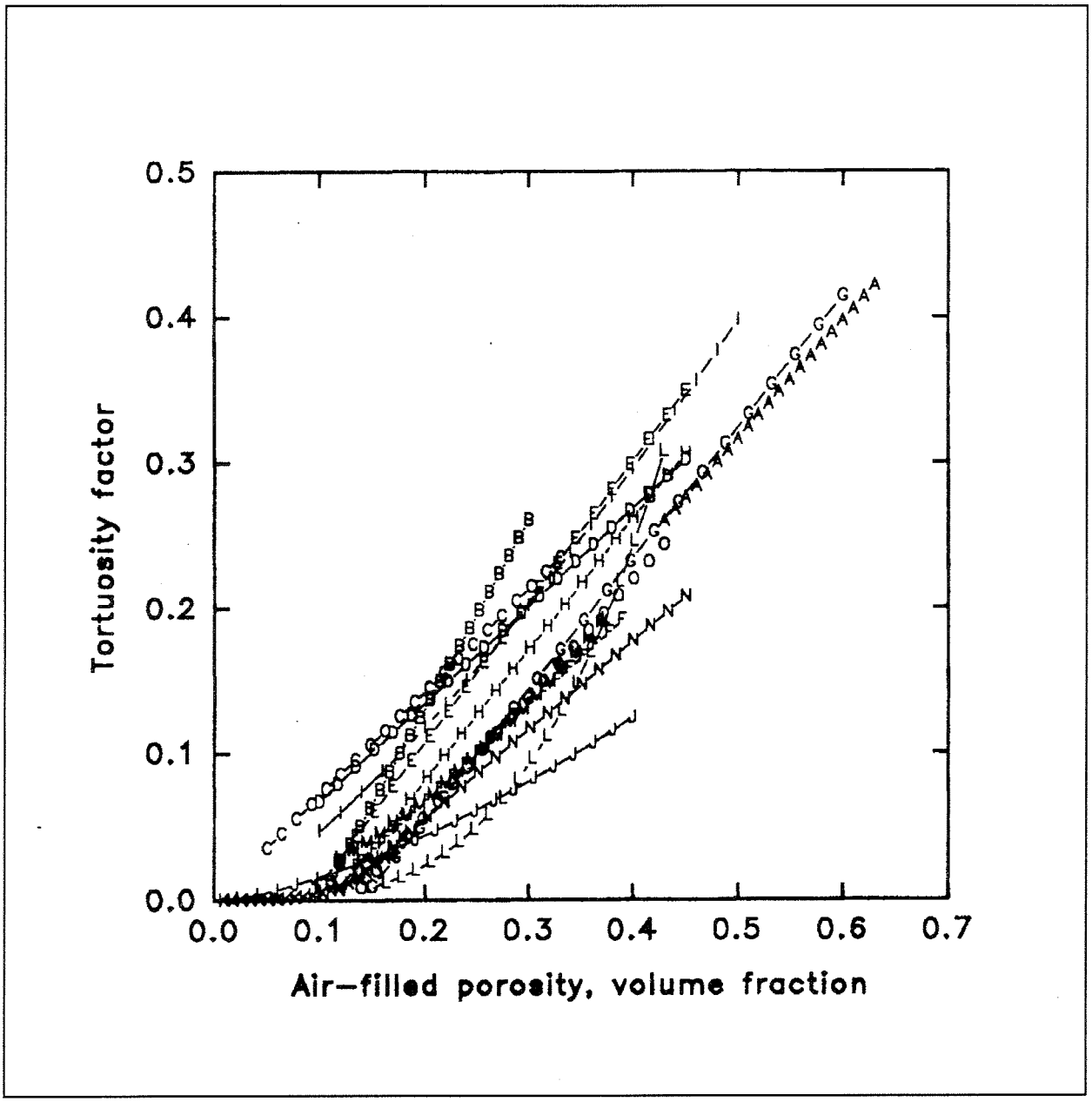

Figure 9.1 Soil tortuosity from gaseous diffusion data. Averaged data of (A) Penman, 1940, (B) Blake and Page, 1948, (C,D) Taylor, 1949, (E) Call, 1957, (F) Wesseling and van Wijk, 1957, (G) Wesseling, 1962, (H) Ritchie, 1964, (I) Millington and Quirk, 1960, (J) Gradwell, 1961, (K) Kimball, 1965, (L) Kimball, 1965, (M) Grable and Siemer, 1968, (N) Currie, 1984, and (O) Bruckler et al., 1989.

We suggest that some non-zero value of air-filled porosity exists near saturation. This value corresponds to entrapped air and is denoted as ϑ_{min}. Consequently, air-filled porosity is calculated as

$$\vartheta = \begin{cases} \theta_s - \theta + \vartheta_{min}, & \theta < \theta_s \\ \vartheta_{min}, & \theta = \theta_s \end{cases} \qquad \textbf{(9.15)}$$

9.3 Data files '*Param_G.dat*' and '*Nodal_G.dat*'

Parameters for the **GasMover** module are read from the file **'Param_G.dat'**. The first parameter is a time-weighing factor, *epsi*, used in the final matrix equation for gas transport. Values of *epsi* between 0.5 and 0.8 usually give good results. See Section 7 for a full description of this parameter. The other transport parameters are functions of soil conditions and are given separately for every soil material in the soil domain. The materials are identified by the material number, *MatNumN*, specified for every node in the Grid_and_Boundary information file **'Grid_Bnd.dat'**. The parameters are fully described in Table 9.1 which also shows the structure of this file.

GasMover reads data on the initial gas contents from the file **'Nodal_G.dat'**. If constant boundary value for gas content is used, then the values must be given in this file. Table 9.2 shows the format for the file **'Nodal_G.dat'**. The example following the table corresponds to the grid in Fig. 3.1 and to the file **'Grid_bnd.dat'** of Example 3.3.

Table 9.1. Format of the file **'Param_G.dat'.**

Record	Variable	Description
1	-	Comment line.
	Computational Information	
2	-	Comment line.
3	*NumG*	Number of gases under consideration.
4	-	Comment lines.
5	*epsi*	Temporal weighing coefficient.
	Material information	
6-8	-	Comment lines.
9	*ThTot(1)*	Porosity of soil material in subdomain #1.
9	*ThTot(2)*	Same as above for soil material in subdomain #2.
.	.	.
9	*ThTot(NMat)*	Same as above for the soil material in the last subdomain.
10,11	-	Comment lines.
12	*ThATr(1)*	Threshold value of air-filled porosity for the soil material in subdomain #1.
12	*ThATr(2)*	Same as above for material in subdomain #2.
.	.	.
12	*ThATr(NMat)*	Same as above for the soil material in the last subdomain.
13,14	-	Comment lines.
15	*bTort(1)*	Tortuosity change per unit of the air-filled porosity for soil material in subdomain #1.
15	*bTort(2)*	Same as above for material in subdomain #2.
.	.	.
15	*bTort(NMat)*	Same as above for the soil material in the last subdomain.
16,17	-	Comment lines.
18	*ThAMin(1)*	Minimum value of the air-filled porosity for the soil material in subdomain #1.
18	*ThAMin(2)*	Same as above for material in subdomain #2.
.	.	.
18	*ThAMin(NMat)*	Same as above for the soil material in the last subdomain.
19,20	-	Comment lines.
21	*Dair(1)*	Diffusion coefficient in air for gas 1 in standard conditions, cm^2 per day
21	*Dair(2)*	Same as above for gas 2.
.	.	.
21	*Dair(NumG)*	Same as above for the last gas.

```
*** Example 9.1: GASMOVER PARAMETERS: file 'Param_G.dat'
Number of gases
        3
epsi
0.55
Soil material and gas parameters
Total porosities of soil materials (ThTot)
 Subdomain #1    Subdomain #2
 0.470         0.420
Treshold values of soil air-filled porosity (ThATr)
 Subdomain # 1   Subdomain # 2
    0.12        0.05
Reduced tortuosity changes (bTort)
 Subdomain # 1   Subdomain # 2
   0.60         0.80
Minimum air filled porosities
  Subdomain # 1  Subdomain # 2
   0.02         0.01
Gas diffusion coefficients in air at standard conditions, cm/day
 Gas # 1 (CO2)    Gas # 2 (Oxygen)    Gas # 3 (Methane)
  11920             15400                 16900
```

Table 9.2. Format of the file **'Nodal_G.dat'**.

Record	Variable	Description
1,2	-	Comment lines.
3	*n*	Nodal number.
3	*g(n,1)*	Initial value of the content for the first gas in soil air at node *n*, g cm^{-3}.
3	*g(n,2)*	Same as above for the second gas.
.	.	.
3	*g(n,NumG)*	Same as above for the last gas.

Record 3 is provided for every node of the grid. Constant boundary gas content, if used, must be present in this file.

```
**** Example 9.2: INITIAL GAS CONTENT DISTRIBUTION - file 'Nodal_G.dat'
 n  g(n,1)      g(n,2)        g(n,3)
 1  1.3E-05     3.0E-04       0.0
 2  1.3E-05     3.0E-04       0.0
 3  1.3E-05     3.0E-04       0.0
 4  1.3E-05     3.0E-04       0.0
 5  1.3E-05     3.0E-04       0.0
 6  1.3E-05     3.0E-04       0.0
 7  1.3E-05     3.0E-04       0.0
 8  1.3E-05     3.0E-04       0.0
 9  1.3E-05     3.0E-04       0.0
10  1.3E-05     3.0E-04       0.0
11  1.3E-05     3.0E-04       0.0
12  1.3E-05     3.0E-04       0.0
13  1.3E-05     3.0E-04       0.0
14  1.3E-05     3.0E-04       0.0
15  1.3E-05     3.0E-04       0.0
16  1.3E-05     3.0E-04       0.0
17  1.3E-05     3.0E-04       0.0
18  1.3E-05     3.0E-04       0.0
```