

Chapter 4: Time-dependent Boundary Settings: *Settddb*

Module

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This section describes boundary settings that depend only on time, not on the status of the soil surface or atmospheric conditions only. Dependencies on time of the boundary conditions are considered in this section. The next chapter, 5, describes soil-atmosphere boundaries where surface fluxes depend on atmospheric conditions.

4.1 Piece-wise boundary settings

2DSOIL recognizes two types of boundary values: fluxes or state variables. Thus, pressure head or water flux may be the boundary value for water flow, solute concentration or solute flux for solute transport, temperature or heat flux for heat movement, and gas content or gas flux for gas movement.

For heat movement one may specify either a boundary temperature or the parameters b_T and G_T in the general boundary heat flux equation:

$$Q_T = -b_T T_{surf} + G_T \quad (4.1)$$

where b_T and G_T are parameters that depend on the module used and T_{surf} is the temperature at the soil surface. This equation may be used in two cases:

- (1) When the surface heat flux is prescribed ($b_T=0$, G_T is the prescribed flux)
- (2) When conductive and/or radiative heat exchange occurs between the soil surface and the air above it. In this case $Q_T = -b_T(T_{surf} - T_a)$, where b_T is the heat transfer coefficient, T_{surf} is

the temperature of the boundary node, and T_a is the air temperature. This case is equivalent to the assumption that $G_T = b_T T_a$.

Gas boundary conditions are similar to those for heat movement, and also involve two possible formulations:

$$g_{surf,j} = \text{const}$$

or

$$Q_{g,j} = -b_{g,j} g_{surf,j} + G_{g,j} \quad (4.2)$$

where $b_{g,j}$ and $G_{g,j}$ are parameters that depend on the module used, $g_{surf,j}$ is the gas concentration at the soil surface, and the index, j , is the number of the gas under consideration.

The first formulation corresponds to a constant gas content at the boundary node. The second formulation corresponds to one of two cases:

- (1) When the potential surface gas flux is prescribed ($b_j = 0$, G_j is the prescribed gas flux)
- (2) When conductive gas exchange occurs between the soil surface and the air over it. Here $Q_{g,j} = -b_{g,j}(g_{surf,j} - g_{a,j})$, where b_g is the surface conductance of gas exchange, $g_{surf,j}$ is the content of the j th gas at the boundary node, and $g_{a,j}$ is the content of the j th gas in the atmospheric air. In this case $G_{g,j} = b_{g,j} g_{a,j}$.

The dependence of boundary values on time is assumed to be piece-wise. An example of such a dependence is shown in Fig. 4.1 for nodes 5 and 6 of the grid shown in Fig. 3.1. These nodes are at the bottom of a shallow furrow with constant water height but variable solute concentration and temperature. Boundary values change sharply several times, and boundary values are constant between those times. The program requires values of the boundary variable and times of boundary alterations for every boundary node that has code +3, +6, -3, or -6 (see section 3.2).

The time-dependent boundary information for every soil transport process under consideration is input from special data files. These data files contain the times $tTDB(I)$ as the end of the current time interval for the transport process I . Thus file **VarBW.dat** contains $tTDB(1)$ values for water transport, file **VarBS.dat** includes $tTDB(2)$ values for solute transport,

file **VarBH.dat** contains $tTDB(3)$ values for heat transport, and file **VarBG.dat** has $tTDB(4)$ for gas transport. Every file provides nodal numbers and boundary values for every time interval. The first interval begins at the time calculations are initiated ($Time$ in Table 2.2) and ends at the first of the $tTDB$ times. The second interval begins at the first $tTDB$ time and ends at the second $tTDB$ time, and so on.

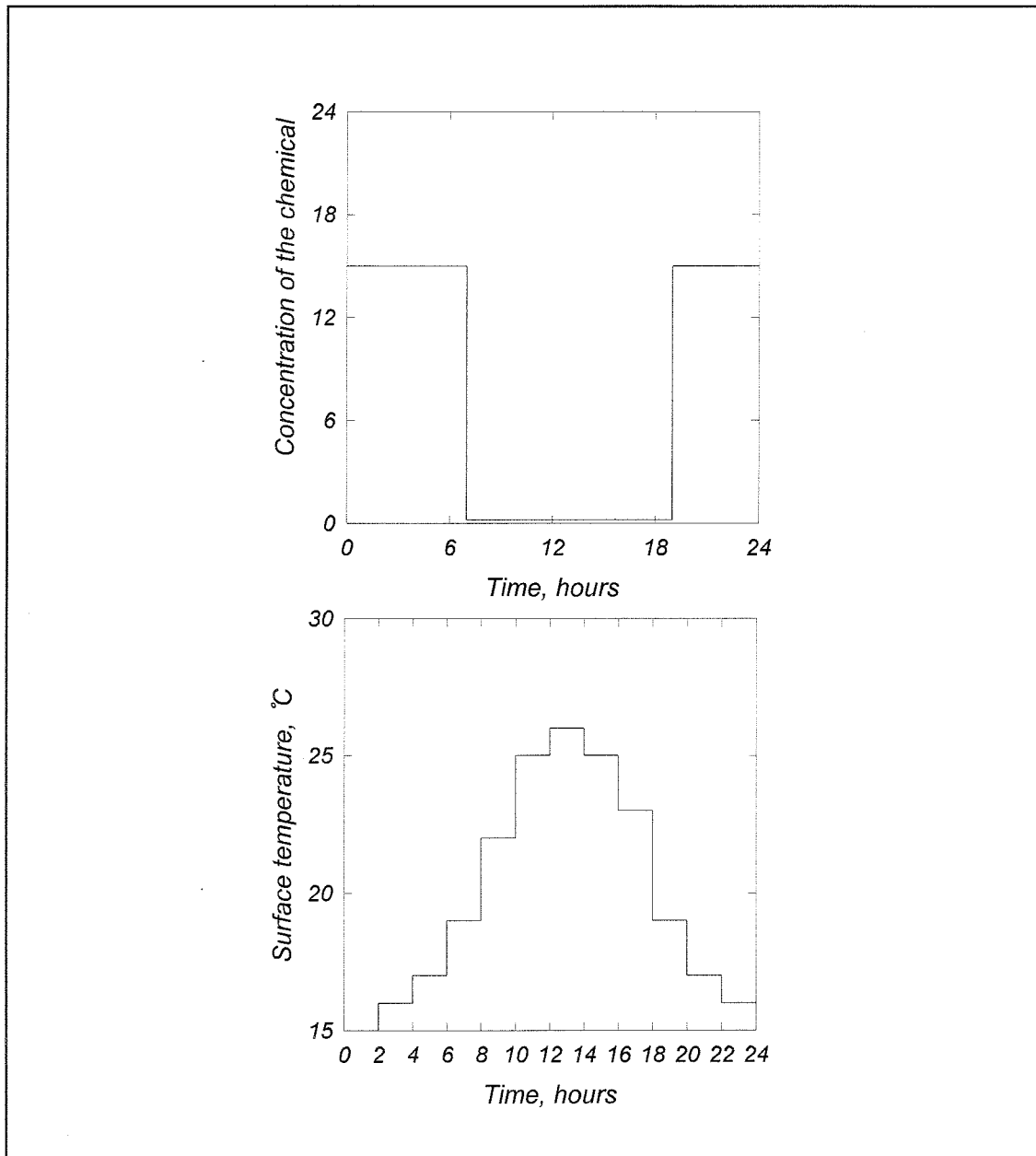


Figure 4.1 An example of piecewise dependencies of soil boundary solute concentration and temperature on time.

The *tTDB* values mark time intervals during which all time-dependent boundary values are constant. If some nodes do not change their boundary values at some *tTDB*, then these nodes need not be listed for this *tTDB*. It is only for the first value of *tTDB* that all time-dependent boundary nodes and boundary values in these nodes must be specified. However, it is preferable to give boundary values for all time-dependent boundary nodes at all tTDB to avoid mistakes.

When fluxes are given on the boundaries, it is important to use the correct dimensions. If the code of a boundary point is -3, then the flux has a dimension cm day^{-1} for water flow and $\text{J cm}^{-2} \text{ day}^{-1}$ for heat transport. In the latter case the flux per unit area is to be given. If the code of the boundary node is -6, then the nodal flux has dimension $\text{cm}^2 \text{ day}^{-1}$ for planar water flow and $\text{cm}^3 \text{ day}^{-1}$ for axisymmetrical water flow, $\text{J cm}^{-1} \text{ day}^{-1}$ for a planar heat flow and J day^{-1} for axisymmetrical heat flow, and $\text{g cm}^{-1} \text{ day}^{-1}$ for a planar gas flow and g day^{-1} for axisymmetrical gas flow. These examples assume that the units of time are given as days.

4.2 Data files *VarBW.dat*, *VarBS.dat*, *VarBH.dat*, and *VarBG.dat*

The structures of these four files are shown in Tables 4.1-4.4. The tables are followed by examples of these files (Examples 4.1 and 4.2) that are given for time-dependent boundaries of Fig. 4.1. It is worth mentioning that the time intervals for heat and solute boundary conditions are different in the examples. Other examples can be found in Chapter 14 of this manual.

Table 4.1. Format of the file 'VarBW.dat'.

| Record | Variable | Description |
|--------|------------|--|
| 1,2 | - - | Comment lines. |
| 3 | $tTDB(1)$ | The <u>end</u> of the time interval for which the boundary information of record 4 is given. |
| 4 | n | Node number of the boundary point. |
| 4 | $VarBW(i)$ | value of pressure head for nodes with $CodeW(n)=3$ and $CodeW(n)=6$. |

Water flux per unit of area, cm day^{-1} (positive if into soil) for nodes with $CodeW(n)=-3$. Volumetric water flux at nodes with $CodeW(n)=-6$, $\text{cm}^3 \text{ day}^{-1}$ for planar flow, and $\text{cm}^2 \text{ day}^{-1}$ for axisymmetric flow. The value i is equal to the sequential number of the node n in the boundary node list of file 'Grid_bnd.dat'. Records 3,4 are both repeated for every time interval involving constant boundary variables. Record 4 is provided separately for each time-dependent boundary node.

Table 4.2. Format of the file 'VarBS.dat'.

| Record | Variable | Description |
|--------|--------------------|--|
| 1,2 | - - | Comment lines. |
| 3 | $tTDB(2)$ | The <u>end</u> of the time interval for which the boundary information of record 4 is given. |
| 4 | n | Node number of the boundary point. |
| 4 | $VarBS(i, 1)$ | Concentration of the 1st solute at the node n , g cm^{-3} . The value i is equal to the sequential number of the node n in the boundary node list of the file 'Grid_bnd.dat'. |
| 4 | $VarBS(i, 2)$ | Same as above for the 2nd solute. |
| . | . | . |
| 4 | $VarBS(i, NumSol)$ | Same as above for the last solute. |

Both records 3 and 4 are repeated for every time interval of constant boundary variables. Record 4 is given separately for each time-dependent boundary node.

Table 4.3. Format of the file 'VarBH.dat'.

| Record | Variable | Description |
|--------|---------------|---|
| 1,2 | - - | Comment lines. |
| 3 | $tTDB(3)$ | The <u>end</u> of the time interval for which the boundary information of record 4 is given. |
| 4 | n | Nodal number of the boundary point. |
| 4 | $VarBH(i, 1)$ | Temperature value for nodes with $CodeT(n)=3$ and $CodeT(n)=6$. If the boundary code is negative, then set this value to zero. |
| 4 | $VarBH(i, 2)$ | Coefficient b_T in Eq. (4.1), $\text{J cm}^{-2} \text{ day}^{-1} (\text{°C})^{-1}$ at nodes with $CodeT(n)=-3$, $\text{J cm}^{-1} \text{ day}^{-1} (\text{°C})^{-1}$ at nodes with $CodeT(n)=-6$ for planar flow, and $\text{J day}^{-1} (\text{°C})^{-1}$ at nodes with $CodeT(n)=-6$ for axisymmetrical flow. If the boundary code is positive, then set this value to zero. |

- 4 *VarBH(i,3)* Coefficient G_T in Eq. (4.1), $\text{J cm}^{-2} \text{ day}^{-1}$ at node with $\text{CodeT}(n)=-3$, $\text{J cm}^{-1} \text{ day}^{-1}$ at node with $\text{CodeT}(n)=-6$ for planar flow, and J day^{-1} at nodes with $\text{CodeT}(n)=-6$ for axisymmetrical flow. If the boundary code is positive, then set this value to zero.

The value i is equal to the sequential number of node n in the boundary node list of the file **Grid_bnd.dat**. Both records 3 and 4 are repeated for every time interval of constant boundary variables. Record 4 is given separately for each time-dependent boundary node.

Table 4.4. Format of the file 'VarBG.dat'.

| Record | Variable | Description |
|--------|-------------------|---|
| 1,2 | - | Comment lines. |
| 3 | $tTDB(4)$ | The <u>end</u> of the time interval for which the boundary information of record 4 is given. |
| 4 | n | Node number of the boundary point. |
| 4 | $VarBG(i,1,1)$ | Constant boundary content of the first gas $g_{surf,1}$ in Eq. (4.2). If the boundary code is negative, then set this value to zero. |
| 4 | $VarBG(i,1,2)$ | Coefficient $b_{g,1}$ in Eq.(4.3) for the first gas, $cm\ day^{-1}$ at nodes with $CodeG(n)=-3$, $cm^2\ day^{-1}$ at nodes with $CodeG(n)=-6$ for planar flow, and $cm^3\ day^{-1}$ at nodes with $CodeG(n)=-6$ for axisymmetrical flow. If the boundary code is positive, then set this value to zero. |
| 4 | $VarBG(i,1,3)$ | Coefficient $G_{g,1}$ in Eq. (4.3) for the first gas, $g\ cm^{-2}\ day^{-1}$ at nodes with $CodeG(n)=-3$, $g\ cm^{-1}\ day^{-1}$ at nodes with $CodeG(n)=-6$ for planar flow, and $g\ day^{-1}$ at nodes with $CodeG(n)=-6$ for axisymmetrical flow. If the boundary code is positive, then set this value to zero. |
| 4 | $VarBG(i,NumG,1)$ | Constant boundary content of the last gas $g_{surf, NumG}$ in Eq. (4.2). If the boundary code is negative, then set this value to zero. |
| 4 | $VarBG(i,NumG,2)$ | Coefficient $b_{g, NumG}$ in Eq.(4.3) for the first gas, $cm\ day^{-1}$ at nodes with $CodeG(n)=-3$, $cm^2\ day^{-1}$ at nodes with $CodeG(n)=-6$ for planar flow, and $cm^3\ day^{-1}$ at nodes with $CodeG(n)=-6$ for axisymmetrical flow. If the boundary code is positive, then set this value to zero. |
| 4 | $VarBG(i,NumG,3)$ | Coefficient $G_{g, NumG}$ in Eq. 4.2 for the first gas, $g\ cm^{-2}\ day^{-1}$ at nodes with $CodeG(n)=-3$, $g\ cm^{-1}\ day^{-1}$ at nodes with $CodeG(n)=-6$ for planar flow, and $g\ day^{-1}$ at nodes with $CodeG(n)=-6$ for axisymmetrical flow. If the boundary code is positive, then set this value to zero. |

The value i is equal to the sequential number of node n in the boundary node list of the file 'Grid_bnd.dat'. Both records 3 and 4 are repeated for every time interval of constant boundary variables. Record 4 is given separately for each time-dependent boundary node.

**** Example 4.1: TIME-DEPENDENT SOLUTE BOUNDARY: FILE 'VARBS.DAT'

End of the interval (days) Node number Boundary value

| | | |
|---------|---|-------|
| 0.29167 | 5 | 0.15 |
| | 6 | 0.15 |
| 0.79167 | 5 | 0.002 |
| | 6 | 0.002 |
| 1.00000 | 5 | 0.15 |
| | 6 | 0.15 |

END OF FILE 'VARBS.DAT'****

**** Example 4.2: TIME-DEPENDENT HEAT BOUNDARY: FILE 'VARBH.DAT'

End of the interval (days) Node number VarBH(1) VarBH(2) VarBH(3)

| | | | | |
|---------|---|----|---|---|
| 0.08333 | 5 | 15 | 0 | 0 |
| | 6 | 15 | 0 | 0 |
| 0.16667 | 5 | 16 | 0 | 0 |
| | 6 | 16 | 0 | 0 |
| 0.25 | 5 | 17 | 0 | 0 |
| | 6 | 17 | 0 | 0 |
| 0.33333 | . | . | . | . |
| . | . | . | . | . |
| 0.91667 | 5 | 17 | 0 | 0 |
| | 6 | 17 | 0 | 0 |
| 1.0 | 5 | 16 | 0 | 0 |
| | 6 | 16 | 0 | 0 |

END OF FILE 'VARBH.DAT'****

Chapter 5: Soil-atmosphere Boundary Setting: *SetSurf*

Modules

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Unlike the time-dependent boundaries discussed in the previous section, the soil-atmosphere boundary does not have set values of fluxes or concentrations. Potential values of fluxes or concentrations are generated for the soil-atmosphere boundary by the **SetSurf** module. Other modules may modify these potential values to provide physically possible - actual - fluxes or concentrations.

Existing soil models and submodels use two different methods to set the soil-atmosphere boundary. Some, e.g., LEACHM (Wagenet and Hudson, 1987), SESP (Timlin et al., 1989), and GRASP (Tillotson and Fontaine, 1991), rely on daily meteorological data. Others, e.g., an alfalfa growth model (Thompson and Fick, 1980), RZWQM (Ahuja et al., 1991), and SHAW (Flerchinger and Saxton, 1989), require more detailed information, including precise durations and intensities of the precipitation/infiltration events. The two approaches each have their own advantages and disadvantages. Data for the former approach are easier to obtain, and long-term changes in the soil environment during plant growth and development are easier calculated. Use of the latter approach can provide a much more realistic description of transport in soils during short time intervals but the data are more difficult to obtain. Combining the two approaches presents an important future task. Both are available separately in 2DSOIL at the present stage of development. The module **SetSurf01** reads detailed boundary information but does not generate other information; the values are simply used in the form they are read in. The module **SetSurf02** reads daily data but can generate evapotranspiration on an hourly basis.

5.1 Using daily meteorological data: SetSurf02 module

This module uses daily meteorological information. It transforms these data to hourly updated soil surface boundary conditions for water, solute, heat, and gas within the soil domain. Several parameters of the crop canopy are used to distinguish bare soil from soil covered by the canopy.

The module reads in the following standard meteorological data:

J - day of the year (Julian date),

R_I - daily solar radiation integral,

T_{max} - maximum air temperature during the day,

T_{min} - minimum air temperature during the day,

II - precipitation (or irrigation),

V - wind speed at 2 m height,

T_{wet} - wet bulb temperature,

T_{dry} - dry bulb temperature,

$c_1, c_2, \dots, c_{NumSol}$ - concentrations of solutes in the precipitation or irrigation

water,

$g_1, g_2, \dots, g_{NumG}$ - contents of gases in the atmosphere.

The model of soil-atmosphere interaction uses relationships of celestial geometry, crop canopy geometry, and radiation balance theory. This model is described below as a sequence of submodels. Before any calculations are performed, the model changes the units of the input data: R_I to $J \cdot m^{-2}$; T_{max} , T_{min} , T_{wet} and T_{dry} to $^{\circ}C$; II to cm ; V to $km \cdot h^{-1}$; $c_1, c_2, \dots, c_{NumSol}$ and $g_1, g_2, \dots, g_{NumG}$ to $g \cdot cm^{-3}$.

5.1.1 Incident radiation submodel.

This submodel produces values of

δ - solar declination,

- t_d - daylength, hours,
 $R_{00,n}$ - radiation incident at the top of the atmosphere at noon, $W \cdot m^{-2}$,
 a - atmospheric transmission coefficient,
 $R_{0,n}$ - potential radiation incident at earth's surface at noon, $W \cdot m^{-2}$,
 R_n - actual radiation incident at earth's surface at noon, $W \cdot m^{-2}$,
 η - cloud cover factor,
 f_{cl} - proportion of sky covered with cloud (1=full cover),
 t_{dn} - time of dawn, hours,
 t_{dk} - time of dusk, hours,
 R - actual radiation incident at earth's surface, $W \cdot m^{-2}$.

Index I indicates that the value is found at time $t_I = (I-0.5)$ hours. Input values are J , Julian day number; ϕ , local latitude; and R_I , daily solar radiation integral.

Table 5.1 shows dependencies among the variables and the corresponding equation numbers in this chapter.

Table 5.1. Dependencies among variables of the incident radiation submodel and the corresponding equation numbers in the submodel.

| Input values | Output values | | | | | | | | | | |
|--------------|---------------|------|------------|-----|-----------|-------|----------|----------|----------|----------|-----|
| | δ | td | $R_{00,n}$ | a | $R_{0,n}$ | R_n | η_1 | f_{cl} | t_{dn} | t_{dk} | R |
| J | 1 | . | 3 | 4 | . | . | . | . | . | . | . |
| φ | 2 | 3 | 4 | 5 | . | 7 | . | . | . | . | . |
| R_l | . | . | . | . | . | 6 | . | . | . | . | . |
| δ | . | 2 | 3 | . | 5 | . | . | . | . | . | . |
| t_d | . | . | . | . | . | 6 | . | . | . | 9 | 11 |
| $R_{00,n}$ | . | . | . | 5 | . | . | . | . | . | . | . |
| a | . | . | . | . | 5 | . | . | . | . | . | . |
| $R_{0,n}$ | . | . | . | . | . | . | . | . | 8 | . | . |
| R_n | . | . | . | . | . | . | . | . | 8 | . | 11 |
| η | . | . | . | . | . | . | . | . | 8 | . | . |
| f_{cl} | . | . | . | . | . | . | . | . | . | . | . |
| t_{dn} | . | 9 | . | . | . | . | . | . | . | . | . |
| t_{dk} | . | 10 | . | . | . | . | . | . | . | . | . |
| R | . | . | . | . | . | . | . | . | . | . | . |

Solar declination is calculated using the algorithm of Robertson and Russelo (1968)

$$\delta = \beta_1 + \sum_{i=2}^{i=5} [\beta_i \sin(0.01721(i-1)J) + \beta_{i+4} \cos(0.01721(i-1)J)] \quad (5.1)$$

where the coefficients β_i are equal to

$$\beta_1 = 0.3964; \beta_2 = 3.631; \beta_3 = 0.03838; \beta_4 = 0.07659; \beta_5 = 0.0; \beta_6 = -22.97;$$

$$\beta_7 = -0.3885; \beta_8 = -0.1587; \beta_9 = -0.01021.$$

The equation relating solar altitude and declination to latitude and hour angle is commonly found in books on celestial mechanics, and is also given in the Smithsonian Meteorological Tables (1966, p. 495). Daylength is defined (p. 506) as the interval between sunrise and sunset; at both of these times the center of the sun's disk is 50° below the horizon. Setting solar altitude equal to -50° , we solve for the hour angle and then convert this to hours from solar noon. Doubling the answer gives daylength:

$$t_d = \frac{\pi}{24} \arccos\left(-\frac{0.014544 + \sin \varphi \sin \delta}{\cos \varphi \cos \delta}\right) \quad (5.2)$$

The equations for solar radiation incident on top of the earth's atmosphere are given in the Smithsonian Meteorological Tables (1966, p. 417). The conditional solar constant, i. e., the

$$R_{00,n} = 1325.4 \frac{\cos(\varphi - \delta)}{Z^2} \quad (5.3)$$

radiation flux on the top of the troposphere is assumed to be $1325.4 \text{ W} \cdot \text{m}^{-2}$ (Budyko, 1974):

where $Z = 1 + 0.01674 \sin[0.01721(J - 93.5)]$ is the radius-vector of the earth.

The atmospheric transmission coefficient is estimated for different latitudes and times of year from the data of Budyko (1974):

$$\begin{aligned}
 a &= 0.68 + (1.57\xi - 0.1) \frac{145 - J}{1000}, & J \leq 145 \\
 a &= 0.68 + [\xi(2.04 - 0.37\xi) - 0.19] \frac{J - 237}{1000}, & J \geq 237 \\
 a &= 0.68 & 145 < J < 237
 \end{aligned} \tag{5.4}$$

where $\xi = \varphi/30$, with φ in degrees.

Potential radiation incident on the earth's surface at noon is found as

$$R_{0,n} = \frac{1}{2} R_{00,n} \left[(0.93 - \frac{0.02}{\cos(\varphi - \delta)} + a^{1/\cos(\varphi - \delta)}) \right] \tag{5.5}$$

This equation essentially reconstitutes the data given in Budyko (1974, Table 3) and was derived from an equation given in the Smithsonian Meteorological Tables (1966, p. 420). Instead of assuming that a constant 9% of extra-terrestrial radiation is adsorbed by water vapor and ozone, the percent adsorption was allowed to vary with atmospheric path length, i.e., solar altitude, according to the data given by Miller (1981).

Actual radiation incident at the earth's surface at noon (R_n) under a cloudless sky is calculated from the given daily integral, and the assumption that the radiation flux density varies as a half sine wave over the photoperiod:

$$R_n = \frac{\pi}{3600} \frac{R_I}{t_d} \frac{1}{2} \tag{5.6}$$

Cloud cover is accounted for by a factor η taken from Budyko (1974, Table 4). The following equation gives good estimates within the range of latitude from 10 to 55° N:

$$\eta = \begin{cases} 0.45 - 0.004\varphi, & \varphi \leq 25 \\ 0.30 + 0.002\varphi, & \varphi > 25 \end{cases} \tag{5.7}$$

The proportion of sky covered with cloud, f_{cl} , is calculated from the ratio of actual to potential radiation at noon using the cloud cover factor η :

$$f_{cl} = \frac{\sqrt{(\eta^2 + 1.52(1 - \frac{R_n}{R_{0,n}})) - \eta}}{0.76} \quad (5.8)$$

Berliand's equation (Budyko, 1974) for actual incident radiation, $R_n = R_{0,n} [1 - (\eta + 0.38f_{cl})f_{cl}]$ has been solved for f_{cl} to obtain eq 5.8. This equation gives a good fit of radiation data for the north central region of the U.S. (Baker, 1975).

Both time of dawn, t_{dn} , and time of dusk, t_{dk} , are derived from daylength, t_d :

$$t_{dn} = 12 - t_d/2 \quad (5.9)$$

$$t_{dk} = 12 + t_d/2 \quad (5.10)$$

Actual radiation incident at the earth's surface at time t_i is found according to the half sine wave pattern:

$$R_i = R_n \sin\left(\frac{\pi(i-0.5)}{t_d}\right) \quad (5.11)$$

Corrections are made for incomplete hours after dawn and before dusk.

5.1.2 Temperature-vapor pressure submodel

The temperature-vapor submodel produces values of:

t_{maxhr} - time of maximum air temperature measured from dawn, hr,

T_{dk} - air temperature at dusk, °C,

ε - actual water vapor pressure for day (assumed constant), kPa

γ - psychrometric constant, $\text{kPa}\cdot(^{\circ}\text{C})^{-1}$,

T_a - air temperature, °C,

b_{ε} - slope of saturation water pressure curve, $\text{kPa}\cdot(^{\circ}\text{C})^{-1}$,

$\Delta\varepsilon$ - vapor pressure deficit, kPa.

Index i indicates that the value is found for time $t_i=(i-0.5)$ hours.

Input values are maximum air temperature for the day, T_{max} ; minimum air temperature for the day, T_{min} ; wet bulb temperature, T_{wet} ; dry bulb temperature, T_{dry} ; minimum air temperature for the following day, T_{mint} ; air temperature at sunset on the previous day, T_y , °C; time of dawn, t_{dn} (hours); time of dusk, t_{dk} (hours); actual radiation incident at earth's surface at noon, R_n ($\text{W}\cdot\text{m}^{-2}$); and daylength, hours, t_d .

Variables and the corresponding equation numbers that describe their dependencies are given in Table 5.2.

Table 5.2. Variables of the temperature-vapor pressure submodel and corresponding equation numbers included in the submodel.

| Input values | Output values | | | | | | |
|---------------------|---------------|----------|-------|---------------|----------|-----------------|---------------------|
| | t_{maxhr} | T_{dk} | T_a | ε | γ | b_ε | $\Delta\varepsilon$ |
| T_{max} | 12 | 13 | 14 | . | . | . | . |
| T_{min} | . | 13 | 14 | 15 | . | . | . |
| T_{dry} | . | . | . | 16 | . | . | . |
| T_{wet} | . | . | . | 16 | 16 | . | . |
| t_{dn} | . | . | 14 | . | . | . | . |
| t_{dk} | . | . | 14 | . | . | . | . |
| R_n | 12 | . | . | . | . | . | . |
| t_d | 12 | 13 | 14 | . | . | . | . |
| t_{mint} | . | . | 14 | . | . | . | . |
| t_y | . | . | 14 | . | . | . | . |
| t_{maxhr} | . | 13 | 14 | . | . | . | . |
| t_{dk} | . | . | 14 | . | . | . | . |
| T_a | . | . | . | . | . | 17 | 17 |
| ε | . | . | . | . | . | . | 17 |
| γ | . | . | . | . | . | . | . |
| b_ε | . | . | . | . | . | . | . |
| $\Delta\varepsilon$ | . | . | . | . | . | . | . |

The time of maximum air temperature measured from dawn was found by empirically fitting local data. For Mississippi conditions, for example, the equation is:

$$t_{maxhr} = \frac{t_d}{\pi} \left| \pi - \arcsin \left(\frac{T_{max}}{R_n(0.0945 - 8.06 \cdot 10^{-5} R_n + 6.77 \cdot 10^{-4} T_{max})} \right) \right| \quad (5.12)$$

where the expression after 'arcsin' is less than one. The air temperature at sunset is:

$$T_{dk} = \frac{T_{max} - T_{min}}{2} \left| 1 + \sin \left(\frac{\pi t_d}{t_{maxhr}} + \frac{3\pi}{2} \right) \right| + T_{min} \quad (5.13)$$

Diurnal temperature variation approximated by a half sine wave during the day and by a logarithmic or linear dependency at night. At time $t=t_i$ we have:

$$\begin{aligned}
T_{a,i} &= T_{\min} + \frac{T_{\max} - T_{\min}}{2} \left[1 + \sin\left(\frac{\pi t_d}{t_{\max hr}} + \frac{3\pi}{2}\right) \right], \quad t_{dn} \leq t_i \leq t_{dk}, \\
T_{a,i} &= T_{\min} + T_* \left[\left(1 + \frac{T_y - T_{\min}}{T_*} \right)^{\frac{t_{dn} - t_i}{2t_{dn}}} - 1 \right], \quad t_i < t_{dn}, \quad T_y > T_{\min}, \\
T_{a,i} &= T_{\min} + (T_y - T_{\min}) \frac{t_{dn} - t_i}{2t_{dn}}, \quad t_i < t_{dn}, \quad T_y \leq T_{\min}, \\
T_{a,i} &= T_{dk} + T_* \left(1 + \frac{T_{dk} - T_{mint}}{T_*} \right) \left[\left(1 + \frac{T_{dk} - T_{mint}}{T_*} \right)^{-\frac{t_i - t_{dk}}{2(24 - t_{dk})}} - 1 \right], \quad t_i > t_{dk}, \quad T_{mint} < T_{dk}, \\
T_{a,i} &= T_{dk} + (T_{mint} - T_{dk}) \frac{t_i - t_{dk}}{2(24 - t_{dk})}, \quad t_i > t_{dk}, \quad T_{mint} \geq T_{dk}
\end{aligned}
\tag{5.14}$$

These equations have given a good fit to data sets from Arizona and Mississippi, when the parameter T_* was set at 5°C.

Calculations of actual water vapor pressure for the day depend on the availability of wet and dry bulb temperature values. If those are not available, dew point temperature is assumed to be the minimum temperature and the algorithm of Weiss (1977) is used. The psychrometric constant depends on T_{\min} :

$$\varepsilon = 0.61 \frac{\exp(17.27T_{\min})}{(T_{\min} + 237.3)}; \quad \gamma = 0.0645 \tag{5.15}$$

If wet and dry bulb temperatures are known, then calculations include the value of the saturated water vapor pressure at wet bulb temperature ε_w , humidity ratio ν , and latent heat of evaporation F_L :

$$\begin{aligned}
\varepsilon_w &= 0.61 \frac{\exp(17.27T_{wet})}{T_{wet} + 237.3}; & v &= \frac{0.622\varepsilon_w}{101.3 - \varepsilon_w}; \\
F_L &= 2500.8 - 2.37T_{wet}; & \gamma &= 62.81 \frac{1.006 + 1.846v}{L(0.622 + v)^2}; \\
\varepsilon &= \varepsilon_w - \gamma(T_{dry} - T_{wet})
\end{aligned} \tag{5.16}$$

The slope, b_ε of the saturation water vapor pressure curve is estimated using the dry bulb temperature ε_a . The vapor pressure deficit, $\Delta\varepsilon$, is then calculated from:

$$\begin{aligned}
\varepsilon_a &= 0.61 \frac{\exp(17.27T_a)}{(T_a + 237.3)} \\
b_\varepsilon &= 0.61 \frac{\exp[17.27(T_a + 1)]}{[(T_a + 1) + 237.3]} - \varepsilon_a \\
\Delta\varepsilon &= \varepsilon_a - \varepsilon
\end{aligned} \tag{5.17}$$

5.1.3 Radiation interception submodel

This submodel works only if there is a crop cover. The submodel produces hourly values of

α_ϕ - solar altitude,

ζ - solar azimuth,

f_D - proportion of total radiation that is diffuse

β - angle between row orientation and solar azimuth

d_{sh} - width of shadow cast by row crop measured at right angles to the row, cm,

f_{di} - proportion of direct radiation intercepted by rows of plants assuming they are opaque cylinders,

f_{Di} - proportion of diffuse radiation intercepted by "solid" rows,

f_c - fraction of the solar radiation intercepted by the crop.

Index i indicates that the value is for time $t_i = (i - 0.5)$ hours.

Input values are local latitude, φ (degrees), row spacing, d_{rs} (cm), row orientation measured eastward from north, ν (degrees), canopy extinction coefficient, ϵ , height of top leaves above soil, H_c (cm), leaf area per unit soil area covered by crop canopy, A_c , solar declination, δ , daylength, t_d (hours), atmospheric transmission coefficient, a , cloud cover factor, η , and proportion of sky covered with cloud, f_{cl} , (1=full cover).

Table 5.3 shows dependencies between variables and the corresponding equation numbers.

Table 5.3. Dependencies between variables of the radiation interception submodel and corresponding equation numbers in the submodel.

| Input values | Output values | | | | | | |
|---------------|---------------------|-------|---------|----------|----------|----------|-------|
| | $\alpha_\phi \zeta$ | f_D | β | d_{sh} | f_{di} | f_{Di} | f_c |
| φ | 18 | . | . | . | . | . | . |
| d_{rs} | . | . | . | . | . | 23 | 24 |
| ν | . | . | . | 22 | . | . | . |
| ϵ | . | . | . | . | . | . | 26-27 |
| H_c | . | . | . | . | 23 | . | 24 |
| A_c | . | . | . | . | . | . | 26-27 |
| δ | 18 | 19 | . | . | . | . | . |
| t_d | . | . | . | . | . | . | . |
| a | . | . | 21 | . | . | . | . |
| η | . | . | 21 | . | . | . | . |
| f_{cl} | . | . | 21 | . | . | . | . |
| α_ϕ | . | 19 | 21 | 22 | 23 | . | . |
| ζ | . | . | . | . | . | . | 26-27 |
| f_D | . | . | . | . | . | . | 26-27 |
| ν | . | . | . | . | 23 | . | . |
| d_{sh} | . | . | . | . | . | 23 | . |
| f_{di} | . | . | . | . | . | . | 26-27 |
| f_{Di} | . | . | . | . | . | . | 26-27 |
| f_c | . | . | . | . | . | . | . |

The equation relating solar altitude to solar declination, latitude, and hour angle is commonly found in books on celestial mechanics, and is also given in the Smithsonian Meteorological Tables (1966, p. 495). For hour angles at $t=t_i$, it gives

$$(\alpha_{\diamond})_i = \arcsin \left| \sin \varphi \sin \delta + \cos \varphi \cos \delta \cos \left| \frac{\pi}{12} \left(i - 12 - \frac{1}{2} \right) \right| \right| \quad (5.18)$$

The equation for solar azimuth may be found in the Smithsonian Meteorological Tables (1966, p. 497). For hour angles at $t=t_i$

$$\zeta_i = \pi + \arcsin \left\{ - \frac{\cos \delta \sin \left| \frac{\pi}{12} \left(12 - i + \frac{1}{2} \right) \right|}{\cos(\alpha_{\diamond})_i} \right\}, \quad i=1, 2, \dots, 12, \quad (5.19)$$

$$\zeta_i = 2\pi - \zeta_{25-i}, \quad i=13, 14, \dots, 24$$

According to equations and procedures given in the Smithsonian Meteorological Tables (1966, p. 420), direct solar radiation flux at the earth's surface is calculated as:

$$R_d = R_{00,n} a^{\frac{1}{\sin \alpha_{\diamond}}} \quad (5.20)$$

Diffuse radiation at the earth's surface $R_D = (f_R R_{00,n} - R_d)/2$, where f_R is the proportion of radiation not adsorbed by ozone or water vapor, $R_{00,n}$ is the radiation incident at the top of the atmosphere at noon, and a is the atmospheric transmission coefficient. Instead of assuming that a is a constant 9% of extra-terrestrial radiation adsorbed by water vapor and ozone, the percent adsorption is allowed to vary with atmospheric path length (i.e., solar altitude) according to data given by Miller (1981). As a result, we have for the proportion of diffuse radiation:

$$f_D^{\sim} = 1 - \frac{\sim}{1 + (0.93 - \frac{0.02}{\sin \alpha_{\diamond}}) a^{\frac{1}{\sin \alpha_{\diamond}}}} \quad (5.21)$$

$$f_D = 1 - \frac{(1 - f_{cl})(1 - f_D^0)}{1 - f_{cl} + f_D}$$

where f_D^0 is the proportion of diffuse radiation on cloudless days, and where direct radiation is assumed to be inversely proportional to the percentage of the sky covered by clouds.

Canopy radiation interception is calculated for rowcrops that are approximated as opaque cylinders. The interception of diffuse and direct radiation by these cylinders is calculated for every hour of the day by a method proposed by Acock and Trent (1991). First, solar position and row orientation are used to calculate an apparent solar elevation, α'_ϕ , at right angles to the row that would give the same shadow length:

$$\alpha' = \arctan \left(\frac{\tan \alpha_\phi}{\sin |\beta|} \right) \quad (5.22)$$

The angle β is calculated as the difference between the solar azimuth and the row orientation (see Chapter 10). Next, the proportion of direct radiation intercepted is shadow width (d_{sh}) divided by row width (d_{rs}):

$$d_{sh} = \frac{H_c}{\sin \alpha'_\phi}; \quad f_{di} = \frac{d_{sh}}{d_{rs}} \quad (5.23)$$

The proportion of sky, $f_{Di,d}$, obscured by "opaque" rows at the distance d from the row is (Acock and Trent, 1991):

$$f_{Di,d} = \frac{2}{\pi} \left[\arctan \left(\frac{H_c}{2(d_{rs} - d)} \right) + \arctan \left(\frac{H_c}{2d} \right) \right],$$

$$f_{Di} = \min \left(1, \frac{1}{d_{rs}} \int_0^{d_{rs}} f_{Di,x} dx \right) = \min \left[1, \frac{1}{\pi} \left(4 \arctan \frac{H_c}{2d_{rs}} - \frac{H_c}{d_{rs}} \ln \frac{1}{1 + \left(\frac{2d_{rs}}{H_c} \right)^2} \right) \right] \quad (5.24)$$

The values of $f_{Di,d}$ averaged from row to mid-row give f_{Di} .

The proportion of total radiation intercepted by the crop is made dependent on sun altitude. If $\alpha_\phi > 0$, effective leaf canopy area index $A_{c,e}$ replaces the original leaf area canopy index, A_c , allowing for the fact that light at low angles traverses more leaves to reach the soil:

$$A_{c,e} = \frac{A_c \max(1, \frac{d_{sh}}{d_{rs}})}{\sin[\arccos(\cos\beta\cos\alpha_\phi)]} \quad (5.25)$$

The value of $A_{c,e}$ is used to calculate Beer's law correction for radiation interception: $f_{Beer} = 1 - \exp(-A_{c,e})$. Further, f_c is the fraction of solar radiation intercepted by the crop:

$$f_c = [f_{Di}f_D + f_{di}(1 - f_D)]f_{Beer} \quad (5.26)$$

If $\alpha_\phi \leq 0$, $A_{c,e}$ coincides with A_c and

$$f_c = \min(\frac{H_c}{d_{rs}}, 1)f_{Beer} \quad (5.27)$$

5.1.4 Potential evapotranspiration submodel

The evapotranspiration submodel produces hourly values of

R_u - net upward long wave radiation, $W \cdot m^{-2}$,

ν_s - albedo of soil,

R_{Ns} - net radiation on a bare soil surface, $W \cdot m^{-2}$,

E_s - potential evaporation rate from soil surface, $cm \cdot day^{-1}$,

r_c - a crop surface roughness parameter,

R_{Nc} - net radiation on the crop assuming complete cover, $W \cdot m^{-2}$,

E_c - potential transpiration rate from the crop, $cm \cdot day^{-1}$.

Input values are, wind speed at 2 m height, V ($km \cdot h^{-1}$); row spacing, d_{rs} (cm); height of the topmost leaves above the soil, H_c (cm); potential radiation incident at the earth's surface at noon, $R_{0,n}$ ($W \cdot m^{-2}$); actual radiation incident at the earth's surface at noon, R_n ($W \cdot m^{-2}$); actual radiation incident at the earth's surface at time t, R , ($W \cdot m^{-2}$); soil moisture content for the grid nodes at the soil surface, θ ; psychrometric constant, γ ($kPa \cdot (^\circ C)^{-1}$); air temperature, T_a ($^\circ C$); slope of the saturation water vapor pressure curve, b_ϵ ($kPa \cdot (^\circ C)^{-1}$); vapor pressure deficit, $\Delta\epsilon$ (kPa); and

fraction of the solar radiation intercepted by the crop, f_c . The index, i , indicates that the value is found at time $t_i = (i-0.5)$ hours.

Table 5.4 shows dependencies among the variables and the corresponding equation numbers.

Table 5.4. Dependencies among variables of the evapotranspiration submodel and corresponding numbers of equations included in the potential evapotranspiration submodel.

| Input values | Output values | | | | | | |
|------------------|---------------|-------|----------|-------|-------|----------|-------|
| | R_u | v_s | R_{Ns} | E_s | r_c | R_{Nc} | E_c |
| f_{ET} | . | . | . | 32 | . | . | 36 |
| V | . | . | . | 32 | . | . | 36 |
| d_{rs} | . | . | 30 | 32 | 32 | 34 | 36 |
| H_c | . | . | 30 | 32 | 32 | 34 | 36 |
| $R_{0,n}$ | 28 | . | . | . | . | . | . |
| R_n | 28 | . | . | . | . | . | . |
| R | . | . | 30 | . | . | . | . |
| θ | . | 29 | . | . | . | . | . |
| γ | . | . | . | 32 | . | . | 36 |
| T_a | 28 | . | . | 32 | . | . | 36 |
| b_e | . | . | . | 32 | . | . | 36 |
| $\Delta\epsilon$ | . | . | . | 32 | . | . | 36 |
| f_c | . | . | 30 | . | . | 34 | . |
| R_u | . | . | 31 | . | . | 35 | . |
| v_s | . | . | 31 | . | . | . | . |
| R_{Ns} | . | . | . | 32 | . | . | . |
| E_s | . | . | . | . | . | . | . |
| r_c | . | . | . | . | . | . | . |
| R_{Nc} | . | . | . | . | . | . | 36 |
| E_c | . | . | . | . | . | . | . |

Most equations for calculation of evapotranspiration are largely empirical, but the Penman (1963) equation is at least semi-mechanistic and has been widely tested. Penman's equation is used here to calculate potential water loss from both soil and plant. Penman's equation is assumed that after the crop canopy closes, water evaporation from soil will be negligible.

Net upward long-wave radiation is calculated using an approximation derived by Linacre (1968) multiplied by the ratio of potential and actual radiation at noon:

$$R_u = 11.2 * (100 - T_a) \frac{R_n}{R_{0,n}} \quad (5.28)$$

The albedo of exposed soil cells is estimated from the data of Bower (1971) as a function of soil water content (θ):

$$v_s = 0.3 - 0.5\theta \quad (5.29)$$

The sum of total radiation falling on the soil is assumed to be concentrated on the bare soil, and the equivalent total radiation R_s^e is calculated as:

$$R_s^e = R \left[\frac{1 - f_c}{1 - \frac{H_c}{d_{rs}}} \right], \quad H_c < d_{rs} \quad (5.30)$$

$$R_s^e = 0, \quad H_c \geq d_{rs}$$

Radiation impinging on the soil is assumed to be spread uniformly over the bare soil between crop rows. The net radiation on the exposed soil cells is derived as:

$$R_{Ns} = (1 - v_s)R_s^e - R_u \quad (5.31)$$

Penman's equation gives the potential evaporation rate from the soil:

$$E_s = f_{ET} \frac{24}{10000} \frac{\frac{b_e}{\gamma} \frac{3600}{2500.8 - 2.37T_a} R_{Ns} + 109.375(1 + 0.149V f_v^s) \Delta \epsilon}{\frac{b_e}{\gamma} + 1},$$

$$f_v^s = \min[1, 2(1 - \frac{\min(d_{rs}, H_c)}{d_{rs}})] \quad (5.32)$$

The correction factor f_v^s is used to gradually alter windspeed at the soil surface as the crop grows and the canopy closes. As the crop grows, turbulence increases at the soil surface and wind is gradually excluded.

Potential transpiration is calculated if a crop is growing. The crop surface roughness parameter, r_c , is assumed to gradually increase from 1 to 2 as the crop grows until half the soil surface is covered, after which it decreases to 1 as the canopy closes:

$$r_c = \max \left(1, \frac{1}{\left| \frac{H_c}{d_{rs}} - \frac{1}{2} \right| + \frac{1}{2}} \right) \quad (5.33)$$

Crop albedo v_c is chosen to be constant and equal to 0.23. This value has been used in many other studies, e.g., (Fritschen, 1967; Linacre, 1968; Ritchie, 1971).

Total radiation intercepted by the crop is assumed to be spread uniformly over the area covered by the crop, and an equivalent total radiation R_c^e is calculated as:

$$R_c^e = R \frac{f_c}{\min \left(1, \frac{H_c}{d_{rs}} \right)} \quad (5.34)$$

Net radiation on the crop is given by:

$$R_{Nc} = (1 - v_c) R_c^e - R_u \quad (5.35)$$

Potential transpiration rate is found from Penman's equation as follows:

$$E_c = f_{ET} \frac{24}{10000} \min \left(1, \frac{H_c}{d_{rs}} \right) \frac{\frac{b_e}{\gamma} \frac{3600}{2500.8 - 2.37T} R_{Nc} + 109.375(1 + 0.149V f_v^c) \Delta \epsilon}{\frac{b_e}{\gamma} + 1},$$

$$f_v^c = \begin{cases} \max(0.36/V, 1), & T_a > 25^\circ \\ 1, & T_a \leq 25^\circ \end{cases} \quad (5.36)$$

Here, the correction factor f_v^c is derived from the idea of a minimum effective wind speed caused by convection on hot, still days (Gates, 1968).

5.1.5 Precipitation-Irrigation Submodel.

This submodel calculates the rain intensity using a locally established relationship between the amount of rain/irrigation water and the duration of a precipitation/irrigation event. 2DSOIL uses a constant daily value of the mean intensity, I_R , which is an input parameter. Chemical concentrations of the irrigation or rain water can be given here also. Concentrations of chemicals in the precipitation/irrigation water are assumed to be constant during each event but may vary from one event to another.

For simulation of flood and/or furrow irrigation, a prescribed small negative pressure of head -1 cm is maintained at certain surface nodes until the prescribed amount of water has infiltrated.

5.1.6 Heat movement submodel

This submodel produces hourly values of the parameters b_T and G_T in the boundary condition equation:

$$Q_T = -b_T T_{surf} + G_T \quad (5.37)$$

Here Q_T is the total heat flux into the soil, $\text{J}\cdot\text{cm}^{-2}\cdot\text{day}^{-1}$, and T_{surf} is soil surface temperature, $^{\circ}\text{C}$. The module **HeatMover** may further modify values of G_T as described in Chapter 8. These coefficients are also described in Chapter 3.

The input values are potential evaporation, $(E_s, \text{cm}\cdot\text{d}^{-1})$ from exposed soil cells, as calculated in Eq. (5.32); air temperature, T_a ; windspeed at 2 m height, V (km hr^{-1}); height of the crop, H_c (cm); and row spacing, d_{rs} (cm). Parameters b_T and G_T are obtained as combinations of parameters of submodels for components of the surface heat balance equation:

$$Q_T = \begin{cases} F_L E_s - F_L E_a - R_{conv} + R_{rain}, & \text{bare soil} \\ -R_{cond} + R_{rain}, & \text{under canopy} \end{cases} \quad (5.38)$$

where $F_L E_s$ is energy for potentially available for evaporation of water, $F_L E_a$ is energy actually used for evaporation of water, R_{conv} is the heat flux between soil and air due to a temperature difference and air movement, R_{rain} is the heat flux caused by rainfall, R_{cond} is the conductive heat flux; all fluxes are given in $\text{J}\cdot\text{cm}^{-2}\text{ day}^{-1}$. Equation 5.38 expresses the dependence of the heat flux into or out of the soil, on soil and air temperature, net radiation incident on the exposed soil surface, water evaporation rate, and rainfall. Under a plant, only the conductive heat flux and heat influx with rain water are considered.

Submodels for components of the heat balance are described next where we will show how b_T and G_T may be derived. For bare soil, convective heat transfer, R_{conv} , between the soil and atmosphere occurs when the soil surface is warmer than the air:

$$R_{conv} = b_{conv}(T_a - T_{surf}) \quad (5.39)$$

where b_{conv} is the coefficient of heat conduction between the soil and the atmosphere. This coefficient is calculated as (Linacre, 1968, Appendix 2):

$$b_{conv} = (0.0040 + 0.00139 V f_v^c) \cdot 6027.26 \quad (5.40)$$

where V is windspeed at 2 m (km hr^{-1}), and f_v^c is a correction factor for windspeed given by Eq. (5.36). The numerical factor 6027.26 changes units from cal cm^{-2} as used in the formulation of Linacre. Heat influx R_{rain} due to rainfall is calculated based on the intensity and temperature of the rainwater (the latter assumed to be equal to the air temperature):

$$R_{rain} = I_R C_W T_a \quad (5.41)$$

where I_R is rain intensity, cm day^{-1} , and C_W is the specific heat capacity of water, $\text{J g}^{-1} (\text{°C})^{-1}$.

Beneath the crop canopy, conduction and rain heat transfer are assumed to be the only modes of heat transfer. Conduction is driven by the difference between air and soil surface temperature, and is limited by the conductance of the air boundary layer above the soil. This air layer is assumed to be 1 cm thick and saturated with water vapor. The component R_{cond} of heat flux due to conduction is calculated as:

$$R_{cond} = \Lambda_a (T_{surf} - T_a) \quad (5.42)$$

where Λ_a is the thermal conductivity of air saturated with water vapor. The thermal conductivity of saturated air is calculated from a regression equation fitted to a graph of conductivity vs. temperature as prepared by De Vries (1966):

$$\Lambda_a = \left(\frac{0.058 + 0.00017T_a + 0.052e^{0.058 T_a}}{1000} \right) 6027.26 \quad (5.43)$$

The numeric factor changes from units $\text{cal cm}^{-2} \text{min}^{-1} \text{°C}^{-1}$ in the original formulation of Acock and Trent (1991) to $\text{J cm}^{-1} \text{k}^{-1} \text{day}^{-1}$. Substituting the heat balance components given by (5.39), (5.41), (5.42) into (5.37) and gathering coefficients of T_{surf} , we have for a base soil

$$\begin{aligned} b_T &= b_{conv} \\ G_T &= b_{conv} T_{surf} + I_R C_W T_a + F_L E_S - F_L E_a \end{aligned} \quad (5.44)$$

For soil beneath the plant, substituting components of the heat balance from (5.41) and (5.42) into (5.37), we have:

$$\begin{aligned} b_T &= \Lambda_a \\ G_T &= \Lambda_a T_a + I_R C_W T_a \end{aligned} \quad (5.45)$$

The *SetSurf02* module does not include the term $F_L E_a$ in G_T for a bare soil. The value is subtracted from G_T by the **HeatMover** module since this parameter depends on the soil water status.

5.1.7 Gas movement submodel.

We assume that gas flux through the soil surface may be found as

$$Q_j = -b_j(g_{surfj} - g_{aj}) = -b_j g_{surfj} + G_j \quad (5.46)$$

Where Q_j is the flux of gas j to atmosphere, ($\text{g cm}^{-2} \text{ day}^{-1}$), g_{aj} is content of this gas in the atmosphere, b_j is the conductance of the surface air layer for gas j , and G_j is the component of the surface gas flux that depends on gas sources other than concentration in the soil air at the surface. This approach has been successfully applied by Kirk and Nye (1991).

5.2 Data files 'Weather.dat' and 'Furnod.dat'

The '**Weather.dat**' file, used by the **SetSurf02** module, is described in Table 5.5. Units are converted immediately after the data are read, if necessary by using specific conversion factors. The *BSOLAR* factor is equal to radiation in $\text{J}\cdot\text{m}^{-2}$ divided by radiation in units used in the '**Weather.dat**' file. The *BTEMP* factor is equal to the change in temperature (in the units used in the '**Weather.dat**' file) equivalent to a 1 °C change. The *ATEMP* factor is equal to the temperature used in the '**Weather.dat**' file that is equivalent to 0 °C. The *ERAIN* factor equals rainfall in $\text{cm}\cdot\text{day}^{-1}$ divided by rainfall in the units used in the '**Weather.dat**' file. The *BWIND* factor is equal to windspeed in $\text{km}\cdot\text{hr}^{-1}$ divided by windspeed in units used in the '**Weather.dat**' file.

An illustration of the use of these factors is shown in Example 5.1 following Table 5.5. Radiation data are expressed in langleys so that $BSOLAR=41680$, whereas *BTEMP* and *ATEMP*

convert temperatures from °F to °C. *ERAIN* is set to change inches of rainfall to cm and *BWIND* values convert windspeed values from miles-hr⁻¹ to km-d⁻¹. The *parameter IRAV*, which converts rainfall intensity values from in d⁻¹ to cm d⁻¹, is given in the file but not used because of the switch, *MSW3*, being equal to 1 and since daily rain intensities are available.

The '**Furnod.dat**' data file is read only if furrow and/or flood irrigation is to be simulated. The description of the file in Table 5.6 is self-explanatory.

Table 5.5. Format of the file '**Weather.dat**'.

| Record | Variable | Description |
|--------|-------------------|--|
| 1,2 | - | Comment lines. |
| 3 | <i>LATUDE</i> | Latitude of the site, degrees N. |
| 4 | - | Comment line. |
| 5 | <i>MSW1</i> | Switch to indicate if daily wet bulb temperatures are available (= 1 if yes). |
| 5 | <i>MSW2</i> | Switch to indicate if daily wind is available (= 1 if yes). |
| 5 | <i>MSW3</i> | Switch to indicate if daily rain intensities are available (= 1 if yes). |
| 5 | <i>MSW4</i> | Switch to indicate if daily concentrations of the chemicals in the rain water are available (= 1 if yes). |
| 5 | <i>MSW5</i> | Switch to indicate if flood irrigation will be applied (=1 if yes). |
| 5 | <i>MSW6</i> | Switch to indicate if daily values of relative humidity are available (=1 if yes) |
| 6,7 | - | Comment lines. |
| 8 | <i>BSOLAR</i> | Factor for changing solar radiation units. |
| 8 | <i>BTEMP</i> | Factor for changing temperature units. |
| 8 | <i>ATEMP</i> | Factor for changing temperature units. |
| 8 | <i>ERAIN</i> | Factor for changing rainfall units. |
| 8 | <i>BWIND</i> | Factor for changing windspeed units. |
| 8 | <i>BIR</i> | Factor for changing rainfall intensity units. |
| 9,10 | - | Comment lines. |
| 11 | <i>WINDA</i> | The average windspeed for the site. Not used if <i>MSW2</i> =0. |
| 11 | <i>IRAV</i> | The average rain intensity for the site. Not used if <i>MSW3</i> =0. |
| 11 | <i>C(1)</i> | Concentration of the first solute in the rain water. Not used if <i>MSW4</i> =0. |
| 11 | <i>C(2)</i> | Same as above for the second solute. |
| 11 | <i>C(NumSol)</i> | Same as above for the last solute. |
| 11 | <i>PG</i> | Conductance of surface air layer to gas flow. Leave this record blank if gas movement will not be simulated and go to record 12. |
| 11 | <i>GAIR(1)</i> | Content of the first gas in the atmosphere. Leave this record blank if gas movement will not be simulated. |
| 11 | <i>GAIR(2)</i> | Same as above for the second gas |
| 11 | <i>GAIR(NumG)</i> | Same as above for the last gas. |
| 12,13 | - | Comment line. |
| 14 | <i>JDAY</i> | Julian day number. |
| 14 | <i>RI</i> | Daily solar radiation integral. |
| 14 | <i>TMAX</i> | Maximum air temperature of the day. |
| 14 | <i>TMIN</i> | Minimum air temperature of the day. |
| 14 | <i>RAIN</i> | Rainfall/irrigation during the day (use a negative value if flood irrigation is used) |
| 14 | <i>WIND</i> | Windspeed at 2 meters if <i>MSW2</i> =1. |
| 14 | <i>TWET</i> | Wet bulb temperature if <i>MSW1</i> =1. |
| 14 | <i>TDRY</i> | Dry bulb temperature if <i>MSW1</i> =1. |
| 14 | <i>IR</i> | Rainfall intensity if <i>MSW3</i> =10. |
| 14 | <i>C(1)</i> | Concentration of the first solute in the rain water if <i>MSW4</i> =1. |
| 14 | <i>C(2)</i> | Same as above for the second solute. |
| 14 | <i>C(NumSol)</i> | Same as above for the last solute. |

Record 14 is provided for every day of the period modeled.

**** Example 5.1: WEATHER DATA FOR SETSURF02: FILE 'WEATHER.DAT'

Latitude, deg

40

MSW1 MSW2 MSW3 MSW4 MSW5 MSW6

0 1 0 0 0 0

--Factors for changing units-----

BSOLAR BTEMP ATEMP ERAIN BWIND IRAV

41680 0.5556 32 0.394 0.625 0.394

--Average values for site-----

WINDA IRAV C(1) C(2) PG GAIR(1)

7.5 0.011 0.001 0.17 0.21

--Daily weather parameters -----

JDAY RI TMAX TMIN RAIN WIND TWET TDRY IR C(1) C(2)....

177 600.6 78.6 62.0 0.5 6.0

178 553.1 81.3 59.1 0.0 0.0

.....

287 451.2 62.6 45.2 0.1 3.0

END OF FILE 'WEATHER.DAT'****

Table 5.6. File 'Furnod.dat'.

| Record | Variable | Description |
|--------|-------------|--|
| 1,2 | - | Comment lines. |
| 3 | NumFP | Total umber of nodes under flood water during irrigation. |
| 4 | - | Comment line. |
| 5 | NumF(1) | Number of the first node under flood irrigation. |
| 5 | NumF(2) | Same as above for the second node. |
| 5 | NumF(NumFP) | Same as above for the last node. |
| 6 | - | Comment line. |
| 7 | hNod(1) | Pressure head at the first flooded node during irrigation. |
| 7 | hNod(2) | Same as above for the second node. |
| 7 | hNod(NumFP) | Same as above for the last node. |

**** Example 5.2: FURROW DATA FOR SETSURF2: FILE 'FURNOD.DAT'

NumFP

3

NumF(1) NumF(2) NumF(3)

15 16 17

hNod(1) hNod(2) hNod(3)

-0.1 -0.1 -0.1

5.3 Using customized agro-meteorological data: *SetSurf01* module

The frequency of meteorological data collection may be more detailed than daily. This may occur in field experiments as well as in simulation runs with diurnal weather generators. The *Setsurf01* module will read such weather information but will not change units.

The data file, '**Setsurf.dat**', for the module **SetSurf01** is described in Table 5.7. The data file contains values of precipitation, evaporation from bare soil, and solute concentrations in rainfall and/or irrigation water. '**Setsurf.dat**' also contains boundary parameters for heat and gas movement.

Boundary condition parameter for heat movement reflect two possible formulations of the surface boundary conditions:

$$T_{surf} = \text{const} \quad (5.47)$$

or

$$Q_T = -b_T T_{surf} + G_T \quad (5.48)$$

Where T_{surf} is the surface temperature, Q_T is the heat flux, $\text{J cm}^{-2} \text{ d}^{-1}$, and b_T and G_T are coefficients described below. The first formulation corresponds to a constant temperature at the boundary node. The second formulation may be used in the following two cases:

- (1) Surface heat flux is prescribed ($b_T=0$, G_T is prescribed flux)
- (2) Conductive heat exchange occurs between soil and air, $Q_T = -b_T (T_{surf} - T_a)$, where b_T is the conductance for heat exchange, T_{surf} is the temperature in the boundary node, and T_a is the air temperature. This case is equivalent to the assumption $G_T = b_T T_a$.

Gas movement boundary parameters are introduced very much like those for heat movement parameters. As for heat there are two formulations of the surface boundary conditions:

$$g_{surfj} = \text{const} \quad (5.49)$$

or

$$Q_{gj} = -b_{gj} g_{surfj} + G_j \quad (5.50)$$

where index j is the number of the gas under consideration, Q_{gj} is gas flux, $\text{cm}^{-2} \text{d}^{-1}$, and the parameters, b_{gj} and G_j are described below. The first formulation corresponds to a constant gas content at the boundary node. The second formulation may correspond to the following two cases:

- (1) The potential surface gas flux is prescribed ($b_{gj}=0$, G_j is prescribed flux)
- (2) Convective gas exchange occurs between soil and air, in which case $Q_{gj} = -b_{gj}(g_{surfj} - g_j)$, where b_{gj} is the gas transfer coefficient, g_{surfj} is the content of the j th gas at the boundary node, and g_j is the content of the j th gas in the atmospheric. This case is equivalent to the assumption, $G_j = b_{gj}g_j$.

If some of the above processes are not included in the simulation, the corresponding data must be omitted from the data file. Units of solute concentration and gas content are the same as in the corresponding **SoluteMover** and **GasMover** modules.

The surface data may be set at each node separately or at all nodes simultaneously, as shown in Example 5.3. For the first time interval, $nCode=0$ and all nodes get the same values of boundary concentrations and fluxes. For the second time interval $nCode \neq 0$, indicating that the boundary data for the two boundary nodes are set separately. Heat movement is not simulated in this example; hence, so surface parameters for heat movement are absent in this example.

Table 5.7. File 'Setsurf.dat'.

| Record | Variable | Description |
|--------|-------------------|--|
| 1,2 | - | Comment lines. |
| 3 | t_{Atm} | Time at the end of the time interval. |
| 3 | $nCode$ | Code indicating the surface nodes: $nCode=0$ means that data are valid for all nodes of the surface. $nCode \neq 0$ means that data are given separately for every surface node. |
| 4 | n | Nodal number of the surface node. Set it arbitrary if $nCode=0$. |
| 4 | $VarBW(*,1)$ | Precipitation rate during the time interval, cm day^{-1} . The asterisk means that this value is valid for node n if $nCode \neq 0$ and for all surface nodes if $nCode=0$. |
| 4 | $VarBW(*,2)$ | Potential evaporation rate, cm day^{-1} . The asterisk means that this value is valid for node n if $nCode \neq 0$ and for all surface nodes if $nCode=0$. |
| 4 | $VarBS(1)$ | Concentration of the first solute in the rain/irrigation water. The asterisk means that the value is valid for node n if $nCode \neq 0$ and for all surface nodes if $nCode=0$. |
| 4 | $VarBS(2)$ | Same as above for the second solute. |
| 4 | $VarBS(NumSol)$ | Same as above for the last solute. |
| 4 | $VarBT(*,1)$ | Constant boundary temperature T_{surf} . If the boundary code is -4, then set this value to zero. Asterisk means that the $VarBT(*,1)$ value must be given for node n if $nCode \neq 0$ and for all surface nodes if $nCode=0$. |
| 4 | $VarBT(*,2)$ | Coefficient b_T in Eq. (5.48), $\text{J cm}^{-2} \text{ day}^{-1} (\text{°C})^{-1}$. If the boundary code is 4, then set this value to 0. Asterisk means that the $VarBT(*,2)$ value must be given for node n if $nCode \neq 0$ and for all surface nodes if $nCode=0$. |
| 4 | $VarBT(*,3)$ | Coefficient G_T in Eq. (5.48). If the boundary code is 4, then set this value to zero. Asterisk means that the $VarBT(*,2)$ value must be given for node n if $nCode \neq 0$ and for all surface nodes if $nCode=0$. |
| 4 | $VarBG(*,1,1)$ | Constant boundary content of the first gas $g_{1,surf}$ in Eq.(5.49), g cm^{-2} . If the boundary code is -4, then set this value to zero. Asterisk means that the $VarBG(*,1,1)$ value must be given for node n if $nCode \neq 0$ and for all surface nodes if $nCode=0$. |
| 4 | $VarBG(*,1,2)$ | Coefficient $b_{g,j}$ in Eq.(5.50) for the first gas, cm day^{-1} . If the boundary code is 4, then set this value to zero. Asterisk means that the $VarBG(*,1,2)$ value must be given for node n if $nCode \neq 0$ and for all surface nodes if $nCode=0$. |
| 4 | $VarBG(*,1,3)$ | Coefficient $G_{g,j}$ in Eq.(5.50) for the first gas, $\text{g cm}^{-2} \text{ day}^{-1}$. If the boundary code is 4, then set this value to zero. Asterisk means that the $VarBG(*,1,3)$ value must be given for node n if $nCode \neq 0$ and for all surface nodes if $nCode=0$. |
| 4 | $VarBG(*,2,1)$ | Same as $VarBG(*,1,1)$ for the second gas. |
| 4 | $VarBG(*,2,2)$ | Same as $VarBG(*,1,2)$ for the second gas. |
| 4 | $VarBG(*,2,3)$ | Same as $VarBG(*,1,3)$ for the second gas. |
| 4 | $VarBG(*,NumG,1)$ | Same as $VarBG(*,1,1)$ for the last gas. |
| 4 | $VarBG(*,NumG,2)$ | Same as $VarBG(*,1,2)$ for the last gas. |
| 4 | $VarBG(*,NumG,3)$ | Same as $VarBG(*,1,3)$ for the last gas. |

The asterisk means that the record 4 is provided for all boundary nodes if $nCode \neq 0$. Records 3 and 4 are provided for sequential time intervals that cover the simulation interval altogether.

```

*** Example 5.3: DATA FOR SETSURF1: FILE 'SETSURF.DAT'
tAtm  nCode  n    Prec  rSoil    c(1) Ts    bT GT    g1  bg1 Gg1 g2  bg2 Gg2
0.29      0      0    0.00   0.001    600  0.003 0.   0.   0.21   0.   0.
0.75      1      1    0.00   0.008    100  0.005 0.   0.   0.205  0.   0.
          2    0.50   0.002    600  0.003 0.   0.   0.210  0.   0.

```