Chapter 11: Intrasoil Chemical Reactions: *MacroChem* Module

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The soil chemistry of Ca^{2+}, Mg^{2+}, Na^{+}, H^{+}, Cl^{-}, SO_4^{2-}, strongly influences the chemical and physical environment for nitrogen transformation, and degradation of xenobiotics in soils of some geographic areas . Furthermore, the long-term application of the same management practices shifts the potential equilibria among macro elements. Though chemical equilibrium is not generally attainable in field soils, soil chemical systems oscillate near equilibrium states and always tend to equilibrium. Therefore, shifts in potential equilibriums lead to shifts in the environmental conditions for root activity and for chemical movement/transformation in soils. The macro element equilibria chemistry module in the 2DSOIL model describes a system of interphase chemical interactions that include dissolution-precipitation of gypsum and calcite, Ca-Mg-Na cation exchange, formation of ion pairs in solution, and dissolution of gaseous CO_2. The mathematical model was described elsewhere (Pachepsky and Platonova, 1988; Pachepsky. 1990).

11.1 Model of chemical interactions

Basic assumptions. The chemistry of nine ions in the soil solution are simulated (Ca^{2+}, Mg^{2+}, Na^{+}, H^{+}, Cl^{-}, SO_4^{2-}, CO_3^{2-}, HCO_3^{-}, OH^{-}), as well as the ion pairs formed by these ions ($CaCO_3^{0}$, $MgCO_3^{0}$, $NaCO_3^{-}$, $CaSO_4^{0}$, $MgSO_4^{0}$, $NaSO_4^{-}$, $CaHCO_3^{+}$, $MgHCO_3^{+}$, $NaHCO_3^{0}$, $CaOH^{+}$, and $MgOH^{+}$). The ion-exchange phase contains Ca^{2+}, Mg^{2+}, and Na^{+}. The sum of these three ions is considered to be the cation exchange capacity (CEC), and this sum depends only on position in the soil profile, not on the chemical content. A solid salt phase, gypsum or calcite, may be also be present. The carbonate-hydrogen system is controlled by the partial pressure of CO_2 in the soil air, which also depends on position in the soil profile. The following processes are taken into consideration: 1) association of ions in the soil solutions; 2) transfers of CO_2 to and from the soil air; 3) dissociation of carbonic acid and water; 4) ion exchanges between *Na-Ca* and *Na-Mg*; 5) solution-precipitation of gypsum and calcite; and 6) electrostatic redistribution of ions, which leads to the formation of an exclusion volume free of anions.

The following symbols are used. The letter m indicates the concentration of an ion or an ion pair in the soil solution in mol L^{-1}. Thus, m_{Ca} is the concentration of free (i.e., not bound in ion pairs) Ca^{2+}; $m_{CaHCO_3^+}$ is the concentration of the ion pair $CaHCO_3^+$, and so on. The total analytical concentrations of ions in solution, including their concentration in ion pairs, are symbolized with m': m'_{Ca}, m'_{Mg}, etc. The concentration (mol L^{-1} of soil) of cations in the soil adsorption complex is symbolized by s_{Ca}, s_{Mg}, and s_{Na}. The concentrations of gypsum and calcite, M_{Gyps} and M_{Calc}, are measured in mol L^{-1} of soil for $CaSO_4$ and $CaCO_3$, respectively. The total masses of ions in the liquid, solid, salt, and cation-exchange phases are symbolized by M_{Ca}, M_{Mg}, M_{SO_4}, and M_{Cl}, mol L^{-1} of soil. The partial pressure of CO_2 in the soil air is symbolized by P_{CO_2}, atm, the cation-exchange capacity by CEC, eq L^{-1}, and the ionic strength of the soil solution by i. The soil moisture content is denoted by θ, cm^3 of soil solution per cm^3 of soil; θ_1 is the volumetric moisture content minus the exclusion volume. Other symbols are given as used in the text.

11.1.1 Equilibrium relationships.

The major relationships and values for the various constants are given below. The model consists of several groups of equations that are responsible for different processes.

Mass conservation in the system:

$$
\begin{aligned}
&M_{Ca}=\theta_1 m_{Ca}+s_{Ca}+M_{Gyps}+M_{Calc};\\
&M_{Mg}=\theta_1 m_{Mg}+s_{Mg};\\
&M_{Na}=\theta_1 m_{Na}+s_{Na};\\
&M_{Cl}=\theta_1 m_{Cl};\\
&M_{SO_4}=\theta_1 m_{SO_4}+M_{Gyps};
\end{aligned}
\qquad \mathbf{(11.1)}
$$

Mass conservation in the solution:

$$
\begin{aligned}
&m'_{Ca}=m_{Ca}+m_{CaCO_3^0}+m_{CaHCO_3^+}+m_{CaSO_4^0}+m_{CaOH^+};\\
&m'_{Mg}=m_{Mg}+m_{MgCO_3^0}+m_{MgCO_3^+}+m_{MgSO_4^0}+m_{MgOH^+};\\
&m'_{Na}=m_{Na}+m_{NaCO_3^-}+m_{NaHCO_3^0}+m_{NaSO_4^-};\\
&m'_{Cl}=m_{Cl};\ m'_{H}=m_{H};\ m'_{OH}=m_{OH}+m_{CaOH^+}+m_{MgOH^+};\\
&m'_{SO_4}=m_{SO_4}+m_{CaSO_4^0}+m_{MgSO_4^0}+m_{NaSO_4^-};\\
&m'_{CO_3}=m_{CO_3}+m_{CaCO_3^0}+m_{MgCO_3^0}+m_{NaCO_3^-};\\
&m'_{HCO_3}=m_{HCO_3}+m_{CaHCO_3^-}+m_{MgHCO_3^-}+m_{NaHCO_3^0};
\end{aligned}
\tag{11.2}
$$

Activity of ions in solution:

$$
\begin{aligned}
&a_{Ca}=\gamma_1{}^4 m_{Ca};\ a_{Mg}=\gamma_1{}^4 m_{Mg};\ a_{Na}=\gamma_1 m_{Na};\\
&a_{Cl}=\gamma_1 m_{Cl};\ a_{SO_4}=\gamma_1{}^4 m_{SO_4};\ a_{H}=\gamma_1 m_{H};\\
&a_{OH}=\gamma_1 m_{OH};\ a_{HCO_3}=\gamma_1 m_{HCO_3};\ a_{CO_3}=\gamma_1{}^4 m_{CO_3};
\end{aligned}
\tag{11.3}
$$

Activity coefficient of a monovalent ion:

$$
\gamma_1=10^{-\left(\frac{R_6\sqrt{I_e}}{1+R_7\sqrt{I_e}}-R_8 I_e\right)}
\tag{11.4}
$$

Effective ionic strength:

$$
\begin{aligned}
I_e=\frac{1}{2}[&(m_{Ca}+m_{Mg}+m_{CO_3}+m_{SO_4})4+m_{Na}+m_{Cl}\\
&+m_H+m_{OH}+m_{CaHCO_3^+}+m_{MgHCO_3^+}+m_{NaCO_3^-}+m_{NaSO_4^-}]
\end{aligned}
\tag{11.5}
$$

Activity of ion pairs:

$$\begin{aligned}
&a_{CaCO_3^0}=m_{CaCO_3^0}\ ;\\
&a_{MgCO_3^0}=m_{MgCO_3^0}\ ;\\
&a_{CaHCO_3^+}=m_{CaHCO_3^+}\gamma_1\cdot 10^{-R_{11}I_e}\ ;\\
&a_{MgHCO_3^+}=m_{MgHCO_3^+}\gamma_1\cdot 10^{-R_{12}I_e}\ ;\\
&a_{CaSO_4^0}=m_{CaSO_4^0}\gamma_1\cdot 10^{-R_{13}I_e}\ ;\\
&a_{MgSO_4^0}=m_{MgSO_4}\ ;\\
&a_{NaSO_4^-}=m_{NaSO_4^-}\gamma_1\cdot 10^{-R_{14}I_e}\ ;\\
&a_{NaCO_3^-}=m_{NaCO_3^-}\gamma_1\cdot 10^{-R_{15}I_e}\ ;\\
&a_{NaHCO_3^0}=m_{NaHCO_3^0}\ ;\\
&a_{CaOH^+}=\gamma_1 m_{CaOH^+}\ ;\\
&a_{MgOH^+}=\gamma_1 m_{MgOH^+}\ ;
\end{aligned} \qquad \mathbf{(11.6)}$$

Stability of ion pairs:

$$\begin{aligned}
&R_{21}a_{CaCO_3^0}= a_{Ca}a_{CO_3};\ R_{22}a_{MgCO_3^0}= a_{Mg}a_{CO_3};\\
&R_{23}a_{NaCO_3^-}= a_{Na}a_{CO_3};\ R_{24}a_{CaSO_4^0}= a_{Ca}a_{SO_4};\\
&R_{25}a_{MgSO_4^0}= a_{Mg}a_{SO_4};\ R_{26}a_{NaSO_4}= a_{Na}a_{SO_4};\\
&R_{27}a_{CaHCO_3^+}= a_{Ca}a_{HCO_3};\ R_{30}a_{CaOH^+}= a_{Ca}a_{OH^+};\\
&R_{28}a_{MgHCO_3^+}= a_{Mg}a_{HCO_3};R_{31}a_{MgOH^+}= a_{Mg}a_{OH};\\
&R_{29}a_{NaHCO_3^0}= a_{Na}a_{HCO_3};
\end{aligned} \qquad \mathbf{(11.7)}$$

Components of the carbonate system:

$$\begin{aligned}
&R_0P_{CO_2}= m_{H_2CO_3};\ R_1m_{H_2CO_3}= a_H\ a_{HCO_3};\\
&R_2a_{HCO_3}= a_H\ a_{CO_3};\ R_3= a_H\ a_{OH}
\end{aligned} \qquad \mathbf{(11.8)}$$

Solubility:

$$a_{Ca}\, a_{SO_4} \le R_4$$
$$a_{Ca}\, a_{CO_3} \le R_5 \tag{11.9}$$

Electroneutrality:

$$2(m'_{Ca}+m'_{Mg})+m'_{Na}+m'_{H}= 2(m'_{SO_4}+m'_{CO_3})$$
$$+m'_{OH}+m'_{Cl}+m'_{HCO_3};\ 2(s_{Ca}+s_{Mg})+s_{Na}=EKO \tag{11.10}$$

Exchangeable cations:

$$\frac{s_{Na}}{s_{Ca}}=\kappa_1\frac{a_{Na}}{\sqrt{a_{Mg}}};\ \frac{s_{Na}}{s_{Mg}}=\kappa_2\frac{a_{Na}}{\sqrt{a_{Mg}}} \tag{11.11}$$

Values of constants:

$PR_0=10^{2.47}$	$R_6=0.510$	$R_{14}=0.42$	$PR_{25}=2.36$
$PR_1=10^{6.35}$	$R_7=1.532$	$R_{15}=0.21$	$PR_{26}=0.42$
$PR_2=10^{10.32}$	$R_8=0.033$	$PR_{21}=3.20$	$PR_{27}=0.76$
$PR_3=10^{14.00}$	$R_{11}=0.870$	$PR_{22}=3.40$	$PR_{28}=0.78$
$PR_4=10^{4.62}$	$R_{12}=0.150$	$PR_{23}=0.36$	$PR_{29}=-0.25$
$PR_5=10^{8.31}$	$R_{13}=0.330$	$PR_{24}=2.31$	$PR_{30}=-1.40$
$PR_{31}=10^{-2.60}$			

The relationships in Eq. 11.1 to 11.11 allow one to use concentrations of Ca^{2+}, Mg^{2+}, Na^{+}, Cl^{+}, and SO_4^{2-} in a volume of soil and the values for θ_1, P_{CO2}, and CEC to find the distribution of ions among the soil solution, the ion-exchange phase, and the solid salt phases of the soil. All of the relationships in the model have been tested against measured data (Lindsay, 1979; Pachepsky, 1990).

The use of thermodynamic equations is advantageous as the majority of model parameters do not depend on the amounts of ions and salts in soils. Only selectivity coefficients of cation exchange are a function of soil composition (Bolt, 1982).

11.1.2 The computer code of the chemical equilibrium model.

This code, LIBRA (Platonova and Pachepsky, 1988), calculates activities of ions in soil solutions and determines the concentration of ion pairs, estimates the degree of saturation with respect to gypsum and calcite of soil solutions and their solubility, calculates the relative abundance of carbonate- and bicarbonate-ions in soil solutions, evaluates the effect of applying gypsum to the soil on the compositions of the phases. LIBRA can be used to plan experiments to study cation-exchange equilibria in soils, evaluate the effect of soil moisture on the compositions of the phases, and find the composition of the soil solutions using data on the composition of water extracts. The model can also be used to predict changes in the composition of soil phases as a function of quality of input water.

The values of selectivity coefficients of cation exchange K_1 and K_2 are not, generally speaking, constant. The most important parameter that determines their values in soils of the arid zone is the effective ionic strength of the solution I_e, although at high organic-matter contents the proportion of Na^+ in the sum of exchange cations is also highly significant.

The **MacroChem** module is based on the LIBRA code. This module is used to calculate redistribution of ions between soil phases at nodal points after every step of water and solute movement. This module, as implemented in 2DSOIL, operates at present with five solutes. These are ions of Ca^{2+}, Mg^{2+}, Na^+, SO_4^{2-}, Cl^-. Concentrations of these solutes are included in the list of public variables. The **MacroChem** module also calculates pH of the soil solution, contents of exchangeable cations, solid gypsum and calcite, ion pairs in solution, and concentrations of bicarbonate and carbonate ions. These values are currently included in the private information of the module. If these values will be required in calculations for plant development or soil processes, they can readily be transferred to the public domain.

11.2 Input files '*Param_E.dat*' and '*Nodal_E.dat*'

The number of parameters in the LIBRA model is not large because thermodynamic equations are used. The parameters are read from the **'Param_E.dat'** data file (Table 11.1). The input data include factors for adjusting units. The factors *ExchUnitCa*, *ExchUnitMg*, and *ExchUnitNa* are equal to the amounts of exchangeable cations in mol·kg^{-1} soil divided by those amounts in units used in the **'Param_E.dat'** data file. The factors *SolidUnitGypsum* and *SolidUnitCalcite* are equal to the moles of $CaSO_4$ and $CaCO_3$ in solid salts per kg^{-1} soil, divided by these amounts in units used in the **'Param_E.dat'** data file. The factors *ConcUnitCa, ConcUnitMg, ConcUnitNa, ConcUnitSO4*, and *ConcUnitCl* are equal to the amounts of ions in mol·L^{-1} divided by the amounts in units used in the **'Param_E.dat'** data file. Example 11.1 following Table 11.1 contains the factors mentioned above for the case when the amounts of exchangeable cations have been measured in meq/kg of soil, the gypsum and calcite contents in g of solid salt per g of soil, and the concentrations in the solution in meq per L.

The initial distribution of exchangeable cations and solid salts is read from the file **'Param_E.dat'**. Table 11.2 shows the contents of this file. In Example 11.2 following the table, exchangeable cations are in meq/kg of soil and solid salt contents are in g salt per g dry soil.

Table 11.1. Format for the file **'Param_E.dat'**.

Record	Variable	Description
1,3	-	Comment lines.
4	*ExchUnitCa*	Factor for changing exchangeable Ca^{2+} units.
4	*ExchUnitMg*	Same as above for exchangeable Mg^{2+}.
4	*ExchUnitNa*	Same as above for exchangeable Na^{+}.
5	-	Comment line.
6	*SolidUnitGypsum*	Factor for changing gypsum content units.
6	*SolidUnitCalcite*	Same as above for calcite.
7	-	Comment line.
8	*ConcUnitCa*	Factor for changing units of Ca^{2+} concentration.
8	*ConcUnitMg*	Same as above for Mg^{2+}.
8	*ConcUnitNa*	Same as above for Na^{+}.
8	*ConcUnitSO4*	Same as above for SO_4^{2-}.
8	*ConcUnitCl*	Same as above for Cl^{-}.
9,10	-	Comment lines.
11	*BulkDn(1)*	Bulk density of soil material in subdomain #1, g cm^{-3}.
11	*BulkDn(2)*	Same as above for soil material in subdomain #2.
.	....	.....
11	*BulkDn(NMat)*	Same as above for soil material in subdomain *NMat*.
12	-	Comment line.
13	*SelCoefCaNa(1)*	Selectivity coefficient of cation exchange Ca - Na on soil material 1 for the Gaines-Thomas isotherm equation, $(mol/L)^{-1/2}$.
13	*SelCoefCaNa(2)*	Same as above for soil material in subdomain #2.
.	... .	.....
13	*SelCoefCaNa(NMat)*	Same as above for soil material in subdomain *NMat*.
14	-	Comment line.
15	*SelCoefMgNa(1)*	Selectivity coefficient of cation exchange Mg-Na on soil material 1 for the Gaines-Thomas isotherm equation,$(mol/L)^{-1/2}$.
15	*SelCoefMgNa(2)*	Same as above for soil material in subdomain #2.
.	....	.....
15	*SelCoefMgNa(NMat)*	Same as above for soil material in subdomain *NMat*.

```
*** Example 11.1: MACROCHEM PARAMETERS: file 'Param_E.in'
Conversion factors to recalculate original units into mol/kg soil
ExchUnitCa      ExchUnit Mg     ExchUnitNa (from eq/kg)
  0.5           0.5             1.0
SolidunitGypsum   SolidUnitCalcite (from kg/kg soil)
  5.814           10.0
ConcUnitCa ConcUnitMg ConcUnitNa ConcUnitSO4 ConcUnitCl(from meq/l)
  5.0E-04    5.0E-04    1.0E-03    5.0E-04     1.0E-03
Soil material parameters in subdomains
BulkDn Mat # 1   (Bulk density, g/cc)
   1.4
SelCoefCaNa Mat # 1
   0.6
SelCoefMgNa Mat # 1
   0.7
END OF FILE 'PARAM_E.DAT'
```

Table 11.2. Format for the file **'Nodal_E.dat'**.

Record	Variable	Description
1,2	-	Comment line.
3	*n*	Nodal number.
3	*ExchCa(n)*	Initial value of the exchangeable Ca content at node *n*.
3	*ExchMg(n)*	Same as above for Mg.
3	*ExchNa(n)*	Same as above for Na.
3	*GypsumNod(n)*	Initial value of solid gypsum content at node *n*.
3	*CalciteNod(n)*	Same as above for calcite.
3	*PCO2Nod(n)*	Carbon dioxide partial pressure in the soil air, atm. Leave blank if gas movement is included in current simulation.

Record 3 information is required for each node.

```
*** Example 11.2: MACROCHEM MODULE SOLID PHASE DATA: FILE NODAL_E
n     ExchCa   ExchMg   ExchNa  GypsumNOd  CalciteNod  PCO2Nod
1     0.07     0.05     0.02    0.05       0.05        0.06
.      ...      ...      ..      .          .          ....
11    0.05     0.04   . 0.02    0.08       0.05        0.032
```

Chapter 12: Nitrogen Transformation in Soil: *Soilnitrogen* Module

Yakov Pachepsky and Dennis Timlin

The area of nitrogen transformations in soils is important in agricultural modeling and many models have been developed. We have chosen to use the model SOILN that was developed by Johnsson et al. (1987). Recent comparisons of the performance of this model with others have shown that it simulates soil nitrogen transformation with similar accuracy or better than comparable models (de Willingen, 1991; Jabro et al., 1993).

12.1 Model of nitrogen transformation

An illustration of the nitrogen pools and associated fluxes in the module **SOILNITROGEN** is shown in Fig. 12.1. Three organic pools are distinguished as:

- a fast cycling organic pool that includes plant residues and represents the organic residue-microbial biomass complex,
- a slow cycling organic pool that includes humus and represents stabilized decomposition products, and
- an organic fertilizer pool that is used for organic amendments if their chemical composition differs significantly from the composition of a plant residue pool.

State variables of the model are:

N_h - elemental nitrogen (N) content in humus, mg L^{-3},

C_h - elemental carbon (C) content in humus, mg L^{-3},

N_L - elemental nitrogen content in the plant residues, mg L^{-3},

C_L - elemental carbon content in the plant residues, mg L^{-3},

N_m - elemental nitrogen content in the organic fertilizer, mg L^{-3},

C_m - elemental carbon content in the organic fertilizer, mg L^{-3},

N_{NH4} - elemental mineral ammonium content in soil, mg L^{-3}

c_{NO3} concentration of nitrate ions in the soil solution, mg L^{-3}

All mineral ammonium is assumed to be immobile with respect to leaching whereas nitrate ions

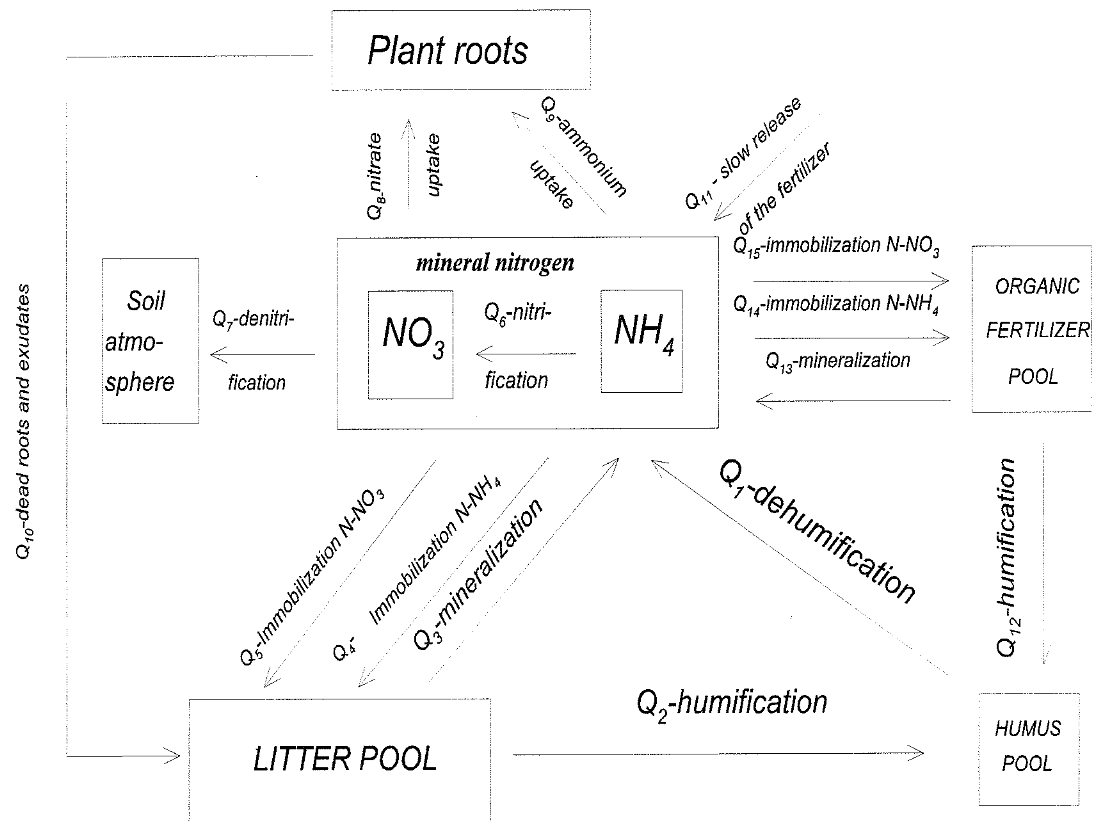

Figure 12.1 Illustration of nitrogen pools and fluxes in the model **SOILN**

are present only in the soil solution. The following is a description of how the fluxes. Q_1 - Q_{15} shown in Fig. 12.1, are calculated.

1) The mineralization of N from stable soil organic matter (*Q_1*). The rate of nitrogen release from soil organic matter is proportional to amount of nitrogen in the organic matter:

$$Q_1 = k_h \; e_\theta \; e_T \; N_h \tag{12.1}$$

The rate constant is a product of the potential mineralization rate constant k_h and the rate correction factors e_θ and e_T. The potential mineralization rate constant is valid at optimal water content and temperature. The correction factor for water, e_θ, adjusts for deviations of soil water content from optimal; the temperature correction, e_T, adjusts for deviations of the soil temperature from optimal. The same rate constant in equation 12.1 is also used to calculate the rate, P_1, of carbon release from organic matter as:

$$P_1 = k_h \; e_\theta \; e_T \; C_h \tag{12.2}$$

2) Immobilization in the stable humus pool of N and C from plant residues (Q_2) and organic fertilizer (Q_{12}). The amount of nitrogen immobilized in the stable humus pool during the decomposition of plant residue is proportional to the amount of carbon transferred to the stable humus pool according to the C/N ratio of microorganisms, r_0:

$$Q_2 = \frac{P_2}{r_0} \tag{12.3}$$

Here P_2 is the rate of carbon transfer from plant residues to humus. The rate, P_2, is proportional to the amount of carbon in plant residues and is calculated as:

$$P_2 = k_L \; e_\theta \; e_T \, f_e \, f_h \; C_L \tag{12.4}$$

The rate constant is a product of the rate constant for optimal conditions k_L, the correction factors for water and temperature, e_θ and e_T, the proportion of carbon retained in soil after respiration f_e (microbial synthesis efficiency constant), and the proportion of carbon transferred to humus f_h.

The amounts of nitrogen and carbon from organic fertilizer immobilized in humus during the decomposition of organic fertilizer is calculated as:

$$Q_{12}=\frac{P_{12}}{r_0} \qquad \textbf{(12.5)}$$

$$P_{12}=k_m\ e_\theta\ e_T\ f_e\ f_h\ C_m \qquad \textbf{(12.6)}$$

Here P_{12} is the rate of carbon transfer from organic fertilizer to organic matter. The rate constant in (12.6) includes the potential rate constant for the decomposition of organic fertilizer, k_m and correction factors for soil water content and temperature.

3) The mineralization of N and C from plant residues (Q_3) and organic fertilizer (Q_{13}). The rate of nitrogen release from plant residues is proportional to the rate of the carbon release:

$$Q_3=\frac{N_L}{C_L}P_3 \qquad \textbf{(12.7)}$$

Here P_3 is the rate of carbon release from plant residues. This rate is proportional to the carbon content in plant residues:

$$P_3=k_L\ e_\theta\ e_T\ C_L \qquad \textbf{(12.8)}$$

where the potential rate constant k_L, and correction factors e_θ and e_T are the same as in (12.4). The decomposition of organic fertilizer is handled in the same manner as the decomposition of plant residues. The mineralization rate of N from organic fertilizer is calculated as:

$$Q_{13}=\frac{N_m}{C_m}P_{13} \qquad \textbf{(12.9)}$$

Here P_{13}, the rate of carbon release from the organic fertilizer, is:

$$P_{13}=k_m\ e_\theta\ e_T\ C_m \qquad \textbf{(12.10)}$$

where the potential rate constant, k_m, is the same as in (12.6).

4) Immobilization of ammonium (Q_4 and Q_{14}) and nitrate (Q_5 and Q_{15}) in organic fertilizer and the litter pool. During decomposition of organic fertilizer and litter, some nitrogen may be immobilized if the C:N ratio of the fertilizer or litter is very high. The potential rate of nitrogen transfer to the plant residues pool, $Q_{4,5}^{pot}$, is proportional to the rate of carbon transformation by microorganisms adjusted for their microbial synthesis efficiency f_e and the C/N ratio, r_0, of microorganisms:

$$Q_{4,5}^{pot}=\frac{f_e\ P_3}{r_0} \qquad \textbf{(12.11)}$$

The potential rate of nitrogen transfer to the organic fertilizer pool is defined as:

$$Q_{14,15}^{pot}=\frac{f_e P_{13}}{r_0} \qquad \textbf{(12.12)}$$

It is assumed that ammonium is preferentially immobilized over nitrate nitrogen.

When net immobilization occurs, there may not be enough mineral nitrogen to support rates Q_4^{pot}, Q_5^{pot}, Q_{14}^{pot}, and Q_{15}^{pot}. If there is sufficient mineral nitrogen, the actual immobilization fluxes are equal to the potential values. If the amount of mineral nitrogen is insufficient, the daily immobilization rate is assumed to be equal to a prescribed fraction, f_a, of the mineral nitrogen available for immobilization. The corresponding total immobilization flux is further distributed among fluxes Q_4, Q_5, Q_{14}, and Q_{15}. It is initially distributed among plant residues and the organic fertilizer pool in proportion to $Q_{4,5}^{pot}$ and $Q_{14,15}^{pot}$, and later between ammonium and nitrates with preference to ammonium.

The fluxes of carbon, P_4, P_5, P_{14}, and P_{15}, are functions of fluxes of immobilized nitrogen as:

$$P_4=Q_4*r_0,\quad P_5=Q_5*r_0,\quad P_{14}=Q_{14}*r_0,\quad P_{15}=Q_{15}*r_0 \qquad \textbf{(12.13)}$$

5) Conversion of ammonium to nitrate (nitrification), Flux Q_6. It is assumed that there is an equilibrium ratio, n_q, of mineral nitrate and ammonium which can not be exceeded during to nitrification.

$$Q_6 = \begin{cases} k_n \, e_\theta \, e_T \, (N_{NH_4} - \dfrac{\theta c_{NO_3}}{n_q}), & if \quad \dfrac{\theta c_{NO_3}}{N_{NH_4}} < n_q \\ 0, & if \quad \dfrac{\theta c_{NO_3}}{N_{NH_4}} \geq n_q \end{cases} \qquad \textbf{(12.14)}$$

Here k_n is the potential nitrification rate in the absence of nitrate in the substrate.

6) Denitrification (Q_7). This flux is controlled by water content, temperature and nitrate concentration:

$$Q_7 = k_d \, e_d \, e_T \, \frac{c_{NO_3}}{c_{NO_3} + c_s} \qquad \textbf{(12.15)}$$

Here k_d is the potential denitrification rate, e_T is the correction factor reflecting temperature, c_s is the Michaelis-Menten constant, and e_d is water content correction factor. These correction factors are not those calculated for immobilization and mineralization.

7) Plant uptake of nitrate (Q_8) ammonium (Q_9). Nitrogen uptake is generally plant-specific and depends on how the plant develops. Therefore, these fluxes must be calculated in the root activity model or in a separate uptake module. The nitrate-nitrogen taken up by the plant must be accumulated in the variable *cSink* which is passed to the solute transport code.

8) Nitrogen (Q_{10}) and carbon (P_{10}) from dead roots and plant exudates. Carbon and nitrogen transfers from these sources are also calculated in an external module. At the present time

2DSOIL does not account for carbon and nitrogen from these sources. Neither Q_8 and Q_9 nor Q_{10} have any effect in the **SoilNitrogen** module.

9) The gradual release of nitrogen from inorganic fertilizer into soil solution (Q_{11}). This flux is calculated in the management module that applies the fertilizer. Mass conservation equations complete the system of equations of the model:

$$\begin{aligned}
&\frac{dC_h}{dt}=-P_1+P_2+P_{12}; && \frac{dN_h}{dt}=-Q_1+Q_2+Q_{12};\\
&\frac{dC_L}{dt}=-P_2-P_3+P_4+P_5; && \frac{dN_L}{dt}=-Q_2-Q_3+Q_4+Q_5;\\
&\frac{dC_m}{dt}=-P_{12}-P_{13}+P_{14}+P_{15}; && \frac{dN_m}{dt}=-Q_{12}-Q_{13}+Q_{14}+Q_{15};\\
& && \frac{dN_{HN_4}}{dt}=Q_1+Q_3+Q_{13}-Q_4-Q_{14}-Q_6;\\
& && \frac{d(\theta c_{NO_3})}{dt}=Q_6-Q_7-Q_5-Q_{15}
\end{aligned} \qquad \textbf{(12.16)}$$

The correction factors, e_θ, e_T, and e_d, are calculated by a separate submodule which is discussed in Section 12.3. The initial values of the state variables N_h, C_h, N_L, C_L, N_m, C_m, N_{NH4}, and c_{NO3} have to be given for each node as described in the following section. They can be modified by management operations like harvest, plowing, fertilizer application, etc. We assume that management is simulated by separate modules. Any atmospheric deposition of N is handled by the **SetSurface** module.

12.2 Input files '*Param_N.dat*' and '*Nodal_N.dat*'

The parameters of the **SoilNitrogen** module are given in the file **'Param_N.dat'**. The parameters must be provided for the soil material in each subdomain. The units are mg, L and day. A description of the file content is in the Table 12.1 and the following example, 12.1, contains a listing of a sample file. The initial values of the state variables of the model related to the soil solid phase are in the file '**Nodal_N.dat**' . The initial values of nitrate concentrations are read in by the **SoluteMover** module along with the other solutes. The first solute must be nitrate. A description of the file content is in the Table 12.2 and the following example is a listing of a sample file.

Table 12.1. Format of the file **'Param_n.dat'.**

Record	Variable	Description
1-2	-	Comment lines
3	Integer *m*	Soil material number
3	*kh*	Potential mineralization rate fro the stable humus pool, day^{-1}
3	*kL*	Potential plant residue decomposition rate, day^{-1}
3	*km*	Potential rate of the organic fertilizer decomposition, day^{-1}
3	*kn*	Potential rate of nitrification, day^{-1}
3	*kd*	Potential rate of denitrification, mg L^{-1} day^{-1}
Record 3 must be repeated for the soil material in each subdomain *m, m=1,NMat*		
4,5	-	Comment lines
6	*m*	Soil material number
6	*fe*	Microbial synthesis efficiency
6	*fh*	Humification fraction
6	*r0*	C/N ratio of the decomposer biomass and humification products
6	*rL*	C/N ratio of plant residues
6	*rm*	C/N ratio of the organic fertilizer
6	*fa*	Fraction of the mineral nitrogen available for immobilization
6	*nq*	Ratio of the mineral nitrate amount to the mineral ammonium amount characteristic to the particular soil material
6	*cs*	Michaelis-Menten constant of denitrification, mg L^{-1}
Record 6 must be repeated for each soil material in each subdomain *m, m=1,NMat*		

```
*** Example 12.1: SoilNit parameters: file 'Param_N.dat'
m Potential rate constants:  kh      kL       km     kn     kd
1                            7E-05  3.5E-02 7E-02 2E-01 5E-02
  Ratios and fractions
m  fe   fh   r0   rL   rm   fa    nq   cs
1  0.6  0.2  10   25   10   0.08  8    1.E-05
END OF FILE 'PARAM_N.DAT'
```

Table 12.2. Format of the file **'Nodal_N.dat'**.

Record	Variable	Description
1,2	-	Comment line.
3	*n*	Nodal number.
3	*Ch(n)*	Initial value of the carbon content in humus at node *n*.
3	*Nh(n)*	Same as above for the nitrogen.
3	*CL(n)*	Initial value of the carbon content in plant residues at node *n*.
3	*NL(n)*	Same as above for the nitrogen.
3	*Cm(n)*	Initial value of the carbon content in the organic fertilizer at node *n*.
3	*Nm(n)*	Same as above for the nitrogen.
3	*NNH4(n)*	Initial value of the nitrogen content in the mineral ammonium at node *n*

Record 3 information is required for each node.
All values in mg L^{-1}

```
*** Example 12.2: SoilNit module initial solid phase data: FILE NODAL_N.DAT
n      Nh        Ch        NL        CL        Nm        Cm        NNH4
1     1.5E-03   1.5E-02 5.0E-05   1.0E-03   0.0       0.0       5.0E-07
.       ...       ...       ..       .          .         ....
11    0.3E-03   0.3E-04 0.0       0.0                           2.0E-09
End of file 'Nodal_N.DAT'
```

12.3 Rate correction factors for temperature and soil water content

The factors, e_θ and e_T, adjust the potential immobilization and mineralization rate constants for soil water content and temperature. The factor, e_d, adjusts the denitrification rate for soil water content. These factors are calculated in the module **SetAbio** as:

$$e_\theta = \begin{cases} e_s + (1-e_s)\left(\dfrac{\theta_s - \theta}{\theta_s - \theta_h}\right)^m, & \theta_s \geq \theta > \theta_h \\ 1, & \theta_h \geq \theta > \theta_l \\ \left(\dfrac{\theta - \theta_w}{\theta_l - \theta_w}\right)^m & \theta_l \geq \theta > \theta_w \end{cases}$$

$$\theta_h = \theta_s - \Delta\theta_h, \quad \theta_l = \theta_w + \Delta\theta_l$$

$$e_T = Q^{\frac{T-t_b}{10}} \qquad \textbf{(12.17)}$$

$$e_d = \begin{cases} \left(\dfrac{\theta - \theta_d}{\theta_s - \theta_d}\right)^d, & \theta > \theta_d \\ 0, & \theta \leq \theta_d \end{cases}$$

$$\theta_d = \theta_s - \Delta\theta_d$$

Here

θ = volumetric water content,

θ_s = volumetric soil water content at saturation,

θ_w = minimum volumetric soil water content for process activity

θ_h = high volumetric water content for which the process is optimal

θ_l = low volumetric water content for which the process is optimal

$\Delta\theta_h$ = width of the water content interval where activity decreases as water content increases

$\Delta\theta_l$ = width of the water content interval where activity increases as water content increases

e_s = relative effect of moisture when the soil is saturated

T = soil temperature, °C

t_b = base temperature at which e_T is 1

Q = factor change in rate with a 10 degree C change in temperature

θ_d = threshold water content below which no denitrification occurs

$\Delta\theta_h$ = range of water contents where denitrification occurs

These data are given in the data file '**SetAbio.dat**' as shown in Table 12.3 and listing in Example 12.3.

Table 12.3. Format of the file **'SetAbio.dat')**.

Record	Variable	Description
1-2	-	Comment lines
3	*m*	Number of the soil material
3	*ThSat(m)*	Volumetric soil water content at saturation for soil material *m*
3	*ThW(m)*	Minimum volumetric soil water content for process activity for soil material *m*
Record 4 must be repeated for each soil material *m, m=1,NMat*		
4-5	-	Comment lines
6	*dThH*	The highest volumetric water content for which the process is optimal
6	*dThL*	The lowest volumetric water content for which the process is optimal
6	*es*	Relative effect of moisture when the soil is saturated
6	*Th_m*	Exponent in dependencies of e_θ on θ
7-8	-	Comment lines
9	*tb*	Base temperature at which $e_T = 1$
9	*QT*	Factor change in rate with a 10 degree change in temperature
10-11	-	Comment lines
12	*ThD*	Threshold water content below which no denitrification occurs
12	*Th_d*	Exponent in dependencies of e_d on θ

```
*** Example 12.3: Parameters of abiotic response: file 'SetAbio.dat'
Material Saturated water content ThSat   Wilting point ThW
1                              0.453                0.157
2                              0.387                0.137
Dehumification, mineralization, nitrification dependencies on moisture
dThH    dThL    es    Th_m
0.10    0.08    0.6   1.0
Dependencies of temperature
tb      QT
20       3
Denitrification dependencies on water content
dThD    Th_d
0.10    2.0
END OF FILE 'SetAbio.DAT'
```

Chapter 13: Input and Output of Data

Yakov Pachepsky and Dennis Timlin

13.1 Data input

Each module of 2DSOIL reads data from files managed by that module. There is no input subroutine that reads all data and passes that data to the appropriate module. The structures of the files are described in the appropriate sections of this manual. Table 13.1 gives the module names and associated data files for this release of 2DSOIL. If the module is not used, then its input files need not be present. The program will produce an error message and give the location of the error if problems reading any input file is encountered (see Section 13.4).

Table 13.1. Data files of modules and submodules of 2DSOIL.02.

Module	Data files	Manual Section
Syncronizer	Time.dat	2
Get_Grid_and_Boundary	Grid_bnd.dat	3
ShootImitator	Param_P.dat	10
WaterMover	Param_W.dat, Nodal_W.dat	6
SetMat01	Closefrm.dat	6
SetMat02	Hydprop.dat	6
SoluteMover	Param_S.dat, Nodal_S.dat	7
HeatMover	Param_T.dat, Nodal_T.dat	8
GasMover	Param_G.dat, Nodal_G.dat	9
Water_Uptake01	Param_R.dat, Nodal_R.dat	10
Water_Uptake02	Param_U.dat, Nodal_U.dat	10
SoilNitrogen	Param_n.dat, Nodal_n.dat, SetAbio.dat	
MacroChem	Param_E.dat, Nodal_E.dat	11

Module	Data files	Manual Section
SetTDB	VarBW.dat, VarBS.dat, VarBT.dat, VarBG.dat	4
SetSurf01	SetSurf.dat	5
SetSurf02	Weather.dat, Furnod.dat[2]	5
Output	Output.dat	12

[1]The actual set of necessary files depends on the list of modules and on the presence of time-dependent boundaries.
[2]File 'Furnod.dat' is needed only if flooding irrigation is simulated.

13.2 *DataGen*, A Simple Grid Generator

A simple grid generator, **DATAGEN**, has been developed for 2DSOIL. The program will only generate rectangular grids, and the user has to manually draw the grid to determine some parameters. If a grid with a ridge and furrow structure is desired, the user must add the ridge part manually. The rectangular portion of the grid is referred to below as RC. The data file of **DATGEN** is called **'Datgen.dat'** and the structure is shown in Table 13.1. A listing of an example file is in Example 13.1 following Table 13.1.

An interactive mouse-based DOS program called 2DPREP and a MS-Windows based program for data input are also available from the authors. These simple programs are useful for creating grids and data files. They can be obtained from the FTP site listed at the beginning of this manual.

Table 13.1. Format of the file **Datagen.dat.**

Record	Variable	Description
1	-	Comment line.
2	IJ	Number of nodes in the horizontal (x) direction
2	*e00*	Number of the first element of the RC part of the grid.
2	*n00*	Nodal number of the first node of the RC of the grid.
2	*NumNP*	Total number on nodal points.
2	*NumEl*	Total number of elements.
3	-	Comment line.
4	*x(1)*	Horizontal coordinate of the first vertical grid line in the RC part.
4	*x(2)*	Same as above for the second vertical line.
.	.	.
4	*x(IJ)*	Same as above for the last vertical line.
5	-	Comment line.
6	*y(1)*	Vertical coordinate of the upper horizontal line in the RC part.
6	*y(2)*	Same as above for the second line.
.	.	.
7	*y((NumNP-n00)/IJ+1*	Same as above for the bottom line of the RC part.
8	-	Comment line.
9	*p(1)*	Initial capillary pressure at nodes of upper grid line in the RC part.
9	*p(2)*	Same as above for the second line.
.	.	.
9	*p((NumNP-n00+1)/NumVL)*	Same as above for the bottom line of the RC part.

```
Example 13.1: Listing of the file 'Datagen.dat'
**** Example of the Datgen data files
IJ   E00  n00    NumNP  NumEl
22    67   61        357      320
x(j): 1    2     3     4     5     6    7      8      9    10    11   12    13    14    15
16   17    18    19    20    21     22
      0.0 10.0 15.0 20.0 24.0 30.0 35.0 40.0 45.0 50.0 55.0 60.0 65.0 70.0 75.0
80.0 85.0 90.0 92.0 95.0 98.0 100.0
y(i): 1->(NumNP-n00)/IJ+1
      130.0 125.0 120.0 115.0 110.0 105.0 102.0 100.0 97.0 95 90 85 75 60 45 30 0
hBottom
-30.
```

DATAGEN builds files called '**Grid_bnd**,' '**Output**,' '**Nodal_W**,' and '**Nodal_R**.' These files correspond to the same 2DSOIL files that have the extension '.dat'. The files will contain sequences of question marks that mark locations for data to be added manually. Portions of the grid that are outside of the rectangular boundary must be added manually. This outside portion may correspond to the ridge in Figure 3.1, for example. The program **DATAGEN.FOR** is supplied with 2DSOIL.

13.3 Conversion of units for chemical application

When fertilizer applications are carried out, it is necessary to convert the units from an areal basis of kg ha $^{-1}$ to concentration on a volume basis, mg L^{-1}. The simulation domain, which is seen as a grid, has a polygonal structure with dimensions vertically into the soil and horizontally across the rows. It is also considered to be 1cm in width. The grid itself, therefore, can be considered to have volume. The first step in the conversion process is to scale the kg ha $^{-1}$ chemical application rate to the surface area of the grid and find the total mass, in grams, of chemical to be applied to the grid. The total mass of chemical to be applied to the grid is obtained by multiplying the chemical application rate by the surface area of the grid. The surface area of the grid is simply the width (in meters) of the grid multiplied by 0.01 m.

The total number of grams of chemical to be applied must next be distributed among the nodes that will receive the chemical. Concentration at a node is obtained by using the area of the elements that are associated with the nodes. This is illustrated in the following example and Figure 13.1. Assume you want to apply 150 kg/ha of nitrogen, and the grid is 30 cm wide (if the grid has a ridge and furrow, use the width below the ridge). The total application, in grams N, is:

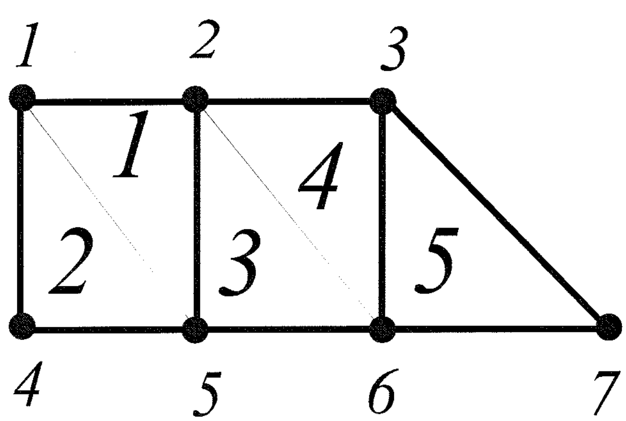

Figure 13.1 Illustration of method to determine nodal concentrations from area applications

$$\frac{150\times(0.01\times0.30)}{10}=0.045$$

The factor, 10, scales kg ha^{-1} to g. Suppose this will be applied to three nodes at the surface of a ridge in Figure 13.1 (nodes 1, 2, and 3). Note that the grid is input as rectangular elements except at the edges of the ridges (element 5). The rectangular elements are shown as bold lines. The finite-element program actually subdivides each rectangular element into two triangles. The nodal concentrations must be determined using the area of these triangles. The first element, 1, in Figure 13.1, has two nodes (1 and 2) that contribute to the chemical concentration out of the total of three nodes. Therefore, the contribution of the area of this triangle is 2/3 of it's total area. Triangle 2 has one node (1) so it contributes only 1/3 of its area, triangle 3 contributes 1 node, triangle 4 contributes 2 nodes and triangle 5 contributes 1 node. The total area for application is calculated as:

$$Total\ area\ =\ \frac{2}{3}A1+\frac{1}{3}A2+\frac{1}{3}A3+\frac{2}{3}A4+\frac{1}{3}A5.$$

Here 'A' refers to the area of the respective triangle. If the areas were all 6.25 cm^2, for example, then the total area would be 14.58 cm^2 . The concentration for each node is calculated as:

$$\frac{0.045}{14.58}=3.086\times10^{-3}\ g\ cm^{-3}\ of\ soil$$

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Since nitrogen is in the form of nitrate in 2DSOIL, this number must be multiplied by 14/62 to obtain NO_3 concentration. Finally, if this number is used to initialize the solute concentrations in the file **Nodal_S.dat**, it must be divided by water content to obtain g L^{-1}. Water contents can be obtained by running the model through one time step and inspecting the file **Theta2D.out**.

13.4 <u>Output of simulation results</u>

A single module, **Output**, is used to send output to disk files; only public soil state variables are output. There is an option to print with two formats. The first format outputs values of the variables together with the nodal coordinates for nodal variables or the coordinates of the center of the element in the case of elemental data in a three column format. This format is suitable for graphic packages to draw contour maps of two-dimensional distributions. The second format outputs nodal and element variable values in strings that correspond to sequences of nodes along the transverse lines of the grid. This format is more convenient for looking through and quickly evaluating results, but it is not convenient for importing into graphic packages, and requires special data preparation (see below).

The first format produces files with the extension '.grp'; the second format output files with the extension '.out.' (Table 13.2). If a module is not used, then the corresponding public variable will not be printed.

Table 13.2. Output files of 2DSOIL.03.

Variable	Filename	Variable	Filename	Variable	Filename
hNew	h____2d.*	Q	Q____2d.*	Sink	Sink_2d.*
ThNew	Theta2d.*	Conc	Conc_2d.*	cSink	cSink2d.*
Vx	Vx___2d.*	Tmpr	Tmpr_2d.*	gSink	gSink2d.*
Vz	Vz___2d.*	g	g____2d.*	RTWT	RTWT_2d.*
RUTDN	RUTDN2D.*				

The wildcard '*' may be replaced with 'out' or 'grp'.

The module **Output** reads a data file called **'Output.dat'** that contains parameters to specify how and when the data are to be written to files. The structure of this file is given in Table 13.3 which is followed by Example 13.3, a listing of an example file. The parameters include the format switch and printout times. The initial distribution will be printed automatically after the first time step, so the first printout time must be greater then initial time. If the second format is used, the node numbers and elements must be given in the same sequence that they will print out (see Example 13.3 for an illustration). These data do not have to be supplied if the first format is used. The program currently allows a maximum of 80 print times. This value can be changed in the array dimension of the variable *tPrint*.

Table 13.3. Format of the file **'Output.dat.'**

Record	Variable	Description
1-2	-	Comment lines.
3	*NumPrint*	Number of specified print-times (maximum is 80).
3	*iForm*	Switch to select the printout format, =1 if first format is selected, =2 if second format is selected, =3 if both formats are to be used.
	The definition of formats is in Sect. 13.2.	
4	-	Comment line.
5	*Tprint(1)*	First specified print-time
5	*Tprint(2)*	Second specified print-time.
.	.	.
.	.	.
5	*Tprint(NumPrint)*	Last specified print-time.
If *iForm*=1 then the file is ended here.		
6	-	Comment line.
7	*NumLinNod*	Total number of transverse grid lines.
7	*NumLinCell*	Total number of horizontal layers of elements (soil cells).
8	-	Comment line.
9	*NumPoint(i)*	Total number of values to be printed in the *i*-th printout line.
9	*NumNod(i,1)*	Number of the node that corresponds to the first value of the *i*-th printout line.
9	*NumNod(i,2)*	Number of the node that corresponds to the second value of the *i*-th printout line.
.	.	.
9	*NumNod(i,NumPoint(i))*	Number of the node that corresponds to the last value of the *i*-th printout line.
Record 9 is provided for all lines of printout *i=1,2,..,NumLinNod*		
10	-	Comment line.
11	*NumCell(e)*	Total number of values to be printed in the *e*-th printout line.
11	*NumElem(e,1)*	Number of the element that corresponds to the first value of the *e*-th printout line.
11	*NumElem(e,2)*	Number of the element that corresponds to the second value the *e*-th printout line.
.	.	.
11	*NumElem(e,NumPoint(e))*	Number of the element that corresponds to the last value of the *e*-th printout line.
Record 11 is provided for all lines of printout *e=1,2,..,NumLinCell*		

```
*** Example 13.2: OUTPUT CONTROL INFORMATION - file 'Output.dat'
NumPrint    iForm
   3          3
TPrint(1),TPrint(2),...,TPrint(NumPrin
   1         10             30
NumLinNod    NumLinCell
   5          4
NumPoint          NodNum to print
   2             1   2
   4             3   4   5   6
   4             7   8   9  10
   4            11  12  13  14
   4            15  16  17  18
NumCell         NumElements to print
   2             1   2
   3             3   4   5
   3             6   7   8
   3             9  10  11
```

13.5 Error messages

If a run time fatal error occurs during the data input, the number of the error message appears in the window and in the separate **'2DSOIL.log'** file. The latter contains also the number of the line with erroneous data. A list of errors is in the following Table 13.5.

Table 13.5. Error messages

Number	Meaning
1	No 'Time.dat' file found.
2	Error in record 1 of 'Time.dat' file.
3	Error in record 2 of 'Time.dat' file.
4	Error in record 3 of 'Time.dat' file.
5	Error in record 4 of 'Time.dat' file.
6	Error in record 5 of 'Time.dat' file.
7	Error in record 6 of 'Time.dat' file.
8	Error in record 7 of 'Time.dat' file.
20	No 'Grid_bnd.dat' file found.
21	Error in record 1 of 'Grid_bnd.dat' file.
22	Error in record 2 of 'Grid_bnd.dat' file.

Table 13.5. Error messages

Number	Meaning
23	Error in record 3 of 'Grid_bnd.dat' file.
24	Error in record 4 of 'Grid_bnd.dat' file.
25	Error in record 5 of 'Grid_bnd.dat' file.
26	Error in record 6 of 'Grid_bnd.dat' file.
27	Error in record 7 of 'Grid_bnd.dat' file.
28	Error in record 8 of 'Grid_bnd.dat' file.
29	Error in record 9 of 'Grid_bnd.dat' file.
30	Error in record 10 of 'Grid_bnd.dat' file.
31	Error in record 11 of 'Grid_bnd.dat' file.
32	Error in record 12 of 'Grid_bnd.dat' file.
33	Error in record 13 of 'Grid_bnd.dat' file.
34	Error in record 14 of 'Grid_bnd.dat' file.
35	Error in record 15 of 'Grid_bnd.dat' file.
36	Error in record 16 of 'Grid_bnd.dat' file.
37	Error in record 17 of 'Grid_bnd.dat' file.
38	Error in record 18 of 'Grid_bnd.dat' file.
40	No 'HydProp.dat' file found.
41	Error in the 'HydProp.file'.
42	Error in record 2 of 'HydProp.dat' file.
43	Error in record 3 of 'HydProp.dat' file.
44	Error in record 4 of 'HydProp.dat' file.
45	Error in record 5 of 'HydProp.dat' file.
46	Error in record 6 of 'HydProp.dat' file.
47	Error in record 7 of 'HydProp.dat' file.
48	Error in record 8 of 'HydProp.dat' file.
49	Error in record 9 of 'HydProp.dat' file.
50	No 'Param_W.dat' file found.
51	Error in record 1 of 'Param_W.dat' file.

Table 13.5. Error messages

Number	Meaning
52	Error in record 2 of 'Param_W.dat' file.
53	Error in record 3 of 'Param_W.dat' file.
55	No 'Nodal_W.dat' file found.
56	Error in record 1 of 'Nodal_W.dat' file.
57	Error in record 2 of 'Nodal_W.dat' file.
58	Error in record 3 of 'Nodal_W.dat' file.
60	No 'Closefrm.dat' file found.
61	Error in record 1 of 'Closefrm.dat' file.
62	Error in record 2 of 'Closefrm.dat' file.
63	Error in record 3 of 'Closefrm.dat' file.
70	No 'Param_S.dat' file found.
71	Error in record 1 of 'Param_S.dat' file.
72	Error in record 2 of 'Param_S.dat' file.
73	Error in record 3 of 'Param_S.dat' file.
74	Error in record 4 of 'Param_S.dat' file.
75	Error in record 5 of 'Param_S.dat' file.
76	Error in record 6 of 'Param_S.dat' file.
77	Error in record 7 of 'Param_S.dat' file.
78	Error in record 8 of 'Param_S.dat' file.
79	Error in record 9 of 'Param_S.dat' file.
80	Error in record 10 of 'Param_S.dat' file.
81	Error in record 11 of 'Param_S.dat' file.
82	Error in record 12 of 'Param_S.dat' file.
83	Error in record 13 of 'Param_S.dat' file.
84	Error in record 14 of 'Param_S.dat' file.
85	Error in record 15 of 'Param_S.dat' file.
86	Error in record 16 of 'Param_S.dat' file.
95	No 'Nodal_S.dat' file found.

Table 13.5. Error messages

Number	Meaning
96	Error in record 1 of 'Nodal_S.dat' file.
97	Error in record 2 of 'Nodal_S.dat' file.
98	Error in record 3 of 'Nodal_S.dat' file.
100	No 'Param_T.dat' file found.
101	Error in record 1 of 'Param_T.dat' file.
102	Error in record 2 of 'Param_T.dat' file.
103	Error in record 3 of 'Param_T.dat' file.
104	Error in record 4 of 'Param_T.dat' file.
105	Error in record 5 of 'Param_T.dat' file.
106	Error in record 6 of 'Param_T.dat' file.
125	No 'Nodal_T.dat' file found.
126	Error in record 1 of 'Nodal_T.dat' file.
127	Error in record 2 of 'Nodal_T.dat' file.
128	Error in record 3 of 'Nodal_T.dat' file.
130	No 'Param_G.dat' file found.
131	Error in record 1 of 'Param_G.dat' file.
132	Error in record 2 of 'Param_G.dat' file.
133	Error in record 3 of 'Param_G.dat' file.
134	Error in record 4 of 'Param_G.dat' file.
135	Error in record 5 of 'Param_G.dat' file.
136	Error in record 6 of 'Param_G.dat' file.
137	Error in record 7 of 'Param_G.dat' file.
138	Error in record 8 of 'Param_G.dat' file.
139	Error in record 9 of 'Param_G.dat' file.
140	Error in record 10 of 'Param_G.dat' file.
141	Error in record 11 of 'Param_G.dat' file.
142	Error in record 12 of 'Param_G.dat' file.
143	Error in record 13 of 'Param_G.dat' file.

Table 13.5. Error messages

Number	Meaning
144	Error in record 14 of 'Param_G.dat' file.
145	Error in record 15 of 'Param_G.dat' file.
146	Error in record 16 of 'Param_G.dat' file.
147	Error in record 17 of 'Param_G.dat' file.
148	Error in record 18 of 'Param_G.dat' file.
149	Error in record 19 of 'Param_G.dat' file.
150	Error in record 20 of 'Param_G.dat' file.
151	Error in record 21 of 'Param_G.dat' file.
155	No 'Nodal_G.dat' file found.
156	Error in record 1 of 'Nodal_G.dat' file.
157	Error in record 2 of 'Nodal_G.dat' file.
158	Error in record 3 of 'Nodal_G.dat' file.
160	No 'Weather.dat' file found.
161	Error in record 1 of 'Weather.dat' file.
162	Error in record 2 of 'Weather.dat' file.
163	Error in record 3 of 'Weather.dat' file.
164	Error in record 4 of 'Weather.dat' file.
165	Error in record 5 of 'Weather.dat' file.
166	Error in record 6 of 'Weather.dat' file.
167	Error in record 7 of 'Weather.dat' file.
168	Error in record 8 of 'Weather.dat' file.
169	Error in record 9 of 'Weather.dat' file.
170	Error in record 10 of 'Weather.dat' file.
171	Error in record 11 of 'Weather.dat' file.
172	Error in record 12 of 'Weather.dat' file.
173	Error in record 13 of 'Weather.dat' file.
174	Error in record 14 of 'Weather.dat' file.
180	No 'Furnod.dat' file found.

Table 13.5. Error messages

Number	Meaning
181	Error in record 1 of 'Furnod.dat' file.
182	Error in record 2 of 'Furnod.dat' file.
183	Error in record 3 of 'Furnod.dat' file.
184	Error in record 4 of 'Furnod.dat' file.
185	Error in record 5 of 'Furnod.dat' file.
186	Error in record 6 of 'Furnod.dat' file.
187	Error in record 7 of 'Furnod.dat' file.
190	No 'Setsurf.dat' file found.
191	Error in record 1 of 'Setsurf.dat' file.
192	Error in record 2 of 'Setsurf.dat' file.
193	Error in record 3 of 'Setsurf.dat' file.
194	Error in record 4 of 'Setsurf.dat' file.
220	No 'Param_R.dat' file found.
221	Error in record 1 of 'Param_R.dat' file.
222	Error in record 2 of 'Param_R.dat' file.
223	Error in record 3 of 'Param_R.dat' file.
224	Error in record 4 of 'Param_R.dat' file.
225	Error in record 5 of 'Param_R.dat' file.
226	Error in record 6 of 'Param_R.dat' file.
227	Error in record 7 of 'Param_R.dat' file.
228	Error in record 8 of 'Param_R.dat' file.
229	Error in record 9 of 'Param_R.dat' file.
235	No 'Nodal_R.dat' file found.
236	Error in record 1 of 'Nodal_R.dat' file.
237	Error in record 2 of 'Nodal_R.dat' file.
238	Error in record 3 of 'Nodal_R.dat' file.
240	No 'Param_U.dat' file found.
241	Error in record 1 of 'Param_U.dat' file.

Table 13.5. Error messages

Number	Meaning
242	Error in record 2 of 'Param_U.dat' file.
243	Error in record 3 of 'Param_U.dat' file.
244	Error in record 4 of 'Param_U.dat' file.
245	Error in record 5 of 'Param_U.dat' file.
246	Error in record 6 of 'Param_U.dat' file.
250	No 'Nodal_U.dat' file found.
251	Error in record 1 of 'Nodal_U.dat' file.
252	Error in record 2 of 'Nodal_U.dat' file.
253	Error in record 3 of 'Nodal_U.dat' file.
255	No 'Param_P.dat' file found.
256	Error in record 1 of 'Param_P.dat' file.
257	Error in record 2 of 'Param_P.dat' file.
258	Error in record 3 of 'Param_P.dat' file.
260	No 'Output.dat' file found.
261	Error in record 1 of 'Output.dat' file.
262	Error in record 2 of 'Output.dat' file.
263	Error in record 3 of 'Output.dat' file.
264	Error in record 4 of 'Output.dat' file.
265	Error in record 5 of 'Output.dat' file.
266	Error in record 6 of 'Output.dat' file.
267	Error in record 7 of 'Output.dat' file.
268	Error in record 8 of 'Output.dat' file.
269	Error in record 9 of 'Output.dat' file.
270	Error in record 10 of 'Output.dat' file.
271	Error in record 11 of 'Output.dat' file.
272	No 'Param_E.dat' file found.
273	Error in record 1 of 'Param_E.dat' file.
274	Error in record 2 of 'Param_E.dat' file.

Table 13.5. Error messages

Number	Meaning
275	Error in record 3 of 'Param_E.dat' file.
276	Error in record 4 of 'Param_E.dat' file.
277	Error in record 5 of 'Param_E.dat' file.
278	Error in record 6 of 'Param_E.dat' file.
279	Error in record 7 of 'Param_E.dat' file.
280	Error in record 8 of 'Param_E.dat' file.
281	Error in record 9 of 'Param_E.dat' file.
282	Error in record 10 of 'Param_E.dat' file.
283	Error in record 11 of 'Param_E.dat' file.
284	Error in record 12 of 'Param_E.dat' file.
285	Error in record 13 of 'Param_E.dat' file.
286	Error in record 14 of 'Param_E.dat' file.
287	Error in record 15 of 'Param_E.dat' file.
290	No 'Nodal_E.dat' file found.
291	Error in record 1 of 'Nodal_E.dat' file.
292	Error in record 2 of 'Nodal_E.dat' file.
293	Error in record 3 of 'Nodal_E.dat' file.
300	No 'VarBW.dat' file found.
301	Error in record 1 of 'VarBW.dat' file.
302	Error in record 2 of 'VarBW.dat' file.
303	Error in record 3 of 'VarBW.dat' file.
304	Error in record 4 of 'VarBW.dat' file.
325	No 'VarBS.dat' file found.
326	Error in record 1 of 'VarBS.dat' file.
327	Error in record 2 of 'VarBS.dat' file.
328	Error in record 3 of 'VarBS.dat' file.
329	Error in record 4 of 'VarBS.dat' file.
350	No 'VarBT.dat' file found.

Table 13.5. Error messages

Number	Meaning
351	Error in record 1 of 'VarBT.dat' file.
352	Error in record 2 of 'VarBT.dat' file.
353	Error in record 3 of 'VarBT.dat' file.
354	Error in record 4 of 'VarBT.dat' file.
375	No 'VarBG.dat' file found.
376	Error in record 1 of 'VarBG.dat' file.
377	Error in record 2 of 'VarBG.dat' file.
378	Error in record 3 of 'VarBG.dat' file.
379	Error in record 4 of 'VarBG.dat' file.
400	No ‘Param_n.dat’ file found
401	Error in record 1 of 'Param_n.dat' file.
402	Error in record 2 of 'Param_n.dat' file.
403	Error in record 3 of 'Param_n.dat' file.
404	Error in record 4 of 'Param_n.dat' file.
405	Error in record 5 of 'Param_n.dat' file.
406	Error in record 6 of 'Param_n.dat' file.
407	Error in record 7 of 'Param_n.dat' file.
408	Error in record 8 of 'Param_n.dat' file.
409	Error in record 9 of 'Param_n.dat' file.
410	Error in record 10 of 'Param_n.dat' file.
412	Error in record 11 of 'Param_n.dat' file.
413	Error in record 12 of 'Param_n.dat' file.
414	Error in record 13 of 'Param_n.dat' file.
415	Error in record 14 of 'Param_n.dat' file.
420	No 'SetAbio.dat' file found
421	Error in record 1 of 'SetAbio,dat' file .
422	Error in record 2 of 'SetAbio.dat' .
423	Error in record 3 of 'SetAbio.dat' .

Table 13.5. Error messages

Number	Meaning
424	Error in record 4 of 'SetAbio.dat' .
425	Error in record 5 of 'SetAbio.dat' .
426	Error in record 6 of 'SetAbio.dat' .
427	Error in record 7 of 'SetAbio.dat' .
427	Error in record 8 of 'SetAbio.dat' .
429	Error in record 9 of 'SetAbio.dat' .
450	No 'Nodal_n.dat' file found
451	Error in record 1 of 'Nodal_n.dat' file.
452	Error in record 2 of 'Nodal_n.dat' file.
453	Error in record 3 of 'Nodal_n.dat' file.
454	Error in record 4 of 'Nodal_n.dat' file.
455	Error in record 5 of 'Nodal_n.dat' file.
456	Error in record 6 of 'Nodal_n.dat' file.
457	Error in record 7 of 'Nodal_n.dat' file.