3.3.1 Governing Equations

The governing equation for advective-dispersive solute transport through variably-saturated porous media, based on the laws of conservation of mass and flux, can be written in the form:

$$2\frac{\partial C}{\partial t} + D_b\frac{\partial S}{\partial t} = \nabla\cdot(2\mathbf{D}\cdot\nabla C) - \mathbf{V}\cdot\nabla C - \theta(2C + D_b S) + QC_{in} - QC \qquad (3\text{-}19)$$

where

2	= moisture content (L^3/L^3)
D_b	= bulk density of the porous medium (M/L^3)
C	= concentration of the dissolved species (M/L^3)
S	= species concentration in the adsorbed phase (M/M)
t	= time (T)
$\mathbf{V}$	= Darcy velocity (i.e., specific discharge) (L/T)
$\nabla\cdot$	= del operator indicating divergence
∇	= del operator indicating gradient
$\mathbf{D}$	= dispersion coefficient tensor (L^2/T)
θ	= material decay constant (T)
Q	= water source/sink rate (M/T)
C_{in}	= dissolved species concentration of the source/sink fluid (M/L^3)

Note that for a fluid sink, such as a production well, $C_{in} = C$.

The dispersion coefficient tensor, **D**, which defines the spreading of the dissolved species as it is advected through the system, is defined as:

$$2\mathbf{D} = \alpha_T|\mathbf{V}|\delta + (\alpha_L - \alpha_T)\mathbf{V}\mathbf{V}/|\mathbf{V}| + 2a_m J\delta \qquad (3\text{-}20)$$

where

$\|\mathbf{V}\|$	= magnitude of the Darcy velocity vector (L/T)
δ	= Kronecker delta tensor
α_L	= longitudinal dispersivity (L)
α_T	= transverse dispersivity (L)
a_m	= molecular diffusion coefficient (L^2/T)
J	= tortuosity coefficient (--)

The dispersivity parameters quantify the magnitude of longitudinal and lateral spreading of the dissolved species as it is advected through the system. This spreading, called hydrodynamic dispersion, is due to the combined influence of 1) water movement through the complex

pathways, and 2) associated mixing patterns (Figure 3.13) that occur over spatial scales not accounted for by the flow field approximated in the advective term of Equation 3-19. These complex pathways may vary in scale from pore spaces and microfractures to larger scale features such as joints and fracture zones. Since dispersion is a function of features of various scales, the appropriate value of dispersivity must take into

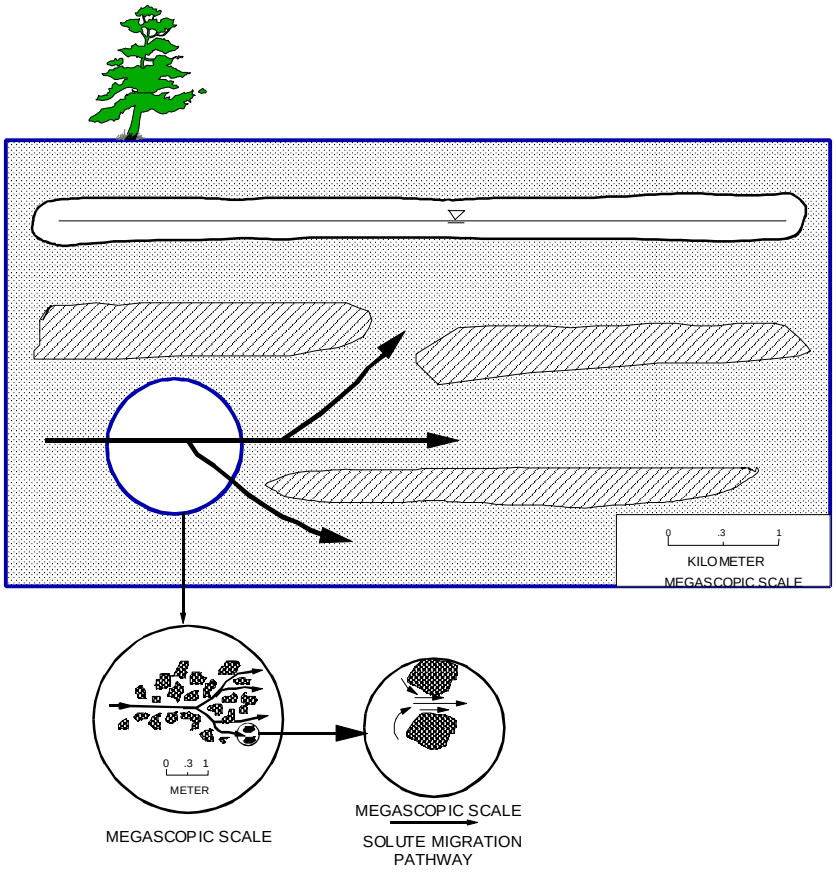
0 .3 1
KILOMETER
MEGASCOPIC SCALE
0 .3 1
METER
MEGASCOPIC SCALE
MEGASCOPIC SCALE
SOLUTE MIGRATION
PATHWAY

Figure 3.13. Diagram showing the effect of scale on hydrodynamic dispersion processes.

consideration the distance the species travels. The molecular diffusion coefficient in Equation 3-20 quantifies the spreading due to molecular diffusion.

In order to solve Equation 3-19 for a single dependent variable, the constitutive relationship between the species concentrations in the dissolved and adsorbed phases must be defined. The 3DLEWASTE code allows the user to choose from three relationships: 1) a linear isotherm, 2) Freundlich isotherm, or 3) Langmuir isotherm. The isotherms, as determined in laboratory partitioning experiments, can be plotted in log-log form to derive:

$$\log S = n \log C + \log K \qquad (3\text{-}21)$$

or

$$S = KC^n \qquad (3\text{-}22)$$

where n is slope of the plot of log S versus log C and K is the S-axis intercept (Freeze and Cherry, 1979). Equation 3-22 defines the Freundlich isotherm, which is often used to describe the partitioning between the dissolved and absorbed
phases. When the isotherm has a slope n=1, the isotherm is linear and the relationship can be defined as:

$$\frac{dS}{dC} = K_d \qquad (3\text{-}23)$$

where K_d is called the distribution coefficient (L^3/M). Linear isotherms are often used to describe the adsorption of hydrophobic organic compounds to organic matter in soils. The distribution coefficient is described as a function of the organic carbon content of the soil as:

$$K_d = f_{oc}K_{oc} \qquad (3\text{-}24)$$

where f_{oc} is the fractional organic carbon content and K_{oc} is the normalized distribution coefficient. There are many published lists of values for K_{oc} (e.g., Lyman et al., 1982; U.S. EPA, 1986; Verschueren, 1983). Data are available primarily for pesticides and, to a lesser degree, aromatic and polycyclic aromatic compounds. If data on K_{oc} are not available for a particular chemical, a value can be estimated from empirical relationships between K_{oc} and some other property of the chemical such as the water solubility, S, the octanol-water partition coefficient, K_{ow}, or the bioconcentration factor for aquatic life, BCF. Lyman et al. (1982) tabulate 12 such regression equations obtained from data sets of different classes of chemicals. One commonly-used relationship (Karickhoff et al., 1979) takes the form:

$$K_{oc} \approx 0.41 K_{ow} \quad (3\text{-}25)$$

The Langmuir isotherm takes the form:

$$S = \frac{S_{max} KC}{1 + KC} \tag{3-26}$$

where S_{max} is the maximum concentration allowed in the medium.

The effective decay constant, θ, is a degradation constant that can be used to quantify the effects of radioactive decay, or the composite effects of hydrolysis and biodegradation. When used to quantify the effects of hydrolysis and biodegradation, the effective decay coefficient (for a linear isotherm) takes the form:

$$\theta = \frac{\theta_1 \theta + \theta_2 K_d D_b}{\theta + K_d D_b} + \theta_b \tag{3-27}$$

where θ_1 is the first-order hydrolysis rate constant for the dissolved species, θ_2 is the first-order hydrolysis rate constant for the sorbed species, and θ_b is the first-order biodegradation rate constant. The dissolved species first-order hydrolysis rate can be written in terms of the acid-catalyzed (K_a), base-catalyzed (K_b), and neutral (K_n) hydrolysis rate constants as:

$$\theta_1 = K_a[H^+] + K_n + K_b[OH^-] \tag{3-28}$$

where $[H^+]$ is the hydrogen ion concentration and $[OH^-]$ is the hydroxyl ion concentration. The sorbed phase first-order hydrolysis rate is considered to be a function of the acid and neutral hydrolysis rates and is usually written in the form:

$$\theta_2 = \eta K_a[H^+] + K_n \tag{3-29}$$

where η is the acid-catalyst hydrolysis rate enhancement factor for the sorbed phase with a typical value of 10.0. Note that for a nonlinear isotherm the formulation in 3DLEWASTE is valid only if $\theta_1 = \theta_2$.

The governing equation for advective-dispersive solute transport in a porous medium, as presented in Equation 3-19, describes the transport from an Eulerian or fixed framework. The numerical algorithm may begin to oscillate and fail to converge to a solution of this equation when the advective term starts to dominate over the dispersive term and the equation takes on a hyperbolic nature. Dominance of the advective term over the dispersive term is reflected in the non-dimensional Peclet number, which is defined as the ratio of the product of the velocity magnitude and distance advected to the dispersion coefficient. In finite element analysis the critical Peclet number is the local Peclet number of an element, where the local Peclet number is defined as:

$$P = L/\alpha_L \tag{3-30}$$

where L is the element length.

One method of circumventing the numerical problems (i.e., oscillation and failure to converge) associated with Peclet numbers greater than 2 is to address the system through a moving (i.e., Lagrangian) coordinate system. In the Lagrangian formulation for solute transport in a porous medium, the temporal term is defined as a material derivative of the form:

$$\left(\theta + \rho_b \frac{dS}{dC}\right)\frac{DC}{Dt} = \theta \frac{\partial C}{\partial t} + \rho_b \frac{\partial S}{\partial t} + \mathbf{V}\cdot\nabla C \tag{3-31}$$

where D denotes the material derivative.

The advective term, $\mathbf{V}\cdot\nabla C$, written in index notation becomes:

$$\mathbf{V}\cdot\nabla C = \frac{dx_i}{dt}\frac{\partial C}{\partial x_i} \tag{3-32}$$

where the repeated indices indicate summation. Substituting Equation 3-31 into Equation 3-19, the governing equation for a Lagrangian framework becomes:

$$\left(\theta + \rho_b \frac{dS}{dC}\right)\frac{DC}{Dt} = \nabla\cdot(\theta\mathbf{D}\cdot\nabla C) - (\theta + \rho_b S)Q C_{in} - QC \tag{3-33a}$$

for a linear isotherm. The average linear velocity, $\mathbf{V}^*$, for a linear isotherm becomes:

$$\mathbf{V}^* = \mathbf{V}/\left(\theta + \rho_b \frac{dS}{dC}\right) \tag{3-33b}$$

For a non-linear isotherm, the Lagrangian equation becomes:

$$\theta\frac{DC}{Dt} + \rho_b \frac{dS}{dC}\frac{\partial C}{\partial t} = \nabla\cdot(\theta\mathbf{D}\cdot\nabla C) - (\theta + \rho_b S)Q C_{in} - QC \tag{3-34a}$$

where

$$\mathbf{v}' = \mathbf{v}/2 \qquad (3\text{-}34b)$$

Full implementation of the Lagrangian approach implies the solution of Equation 3-33 using a moving coordinate system. Another method of circumventing the instability problem is to utilize a hybrid Eulerian-Lagrangian approach. Such an approach is implemented in 3DLEWASTE. In the hybrid approach, the advective term of the material derivative is evaluated in a Lagrangian manner by a backwards particle tracking scheme (Figure 3.14). The particle tracking scheme generates a particle starting location and an associated concentration, C^*. This concentration, C^*, is the starting concentration of each particle which reaches

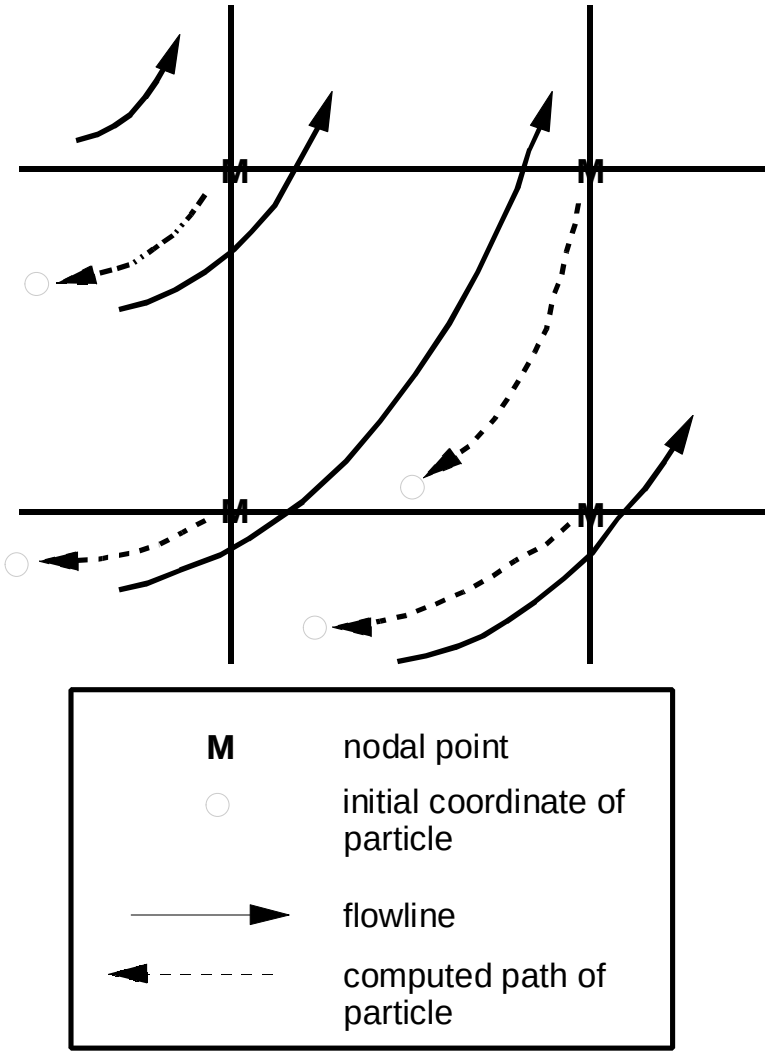

Figure 3.14.Backward particle tracking to determine the starting point of an advected particle.

a nodal point at the end of that particular time step. The material term of Equation 3-33 is then approximated by:

$$\frac{DC}{Dt} \approx \frac{C - C^{(}}{)t} \qquad (3\text{-}35)$$

The diffusion-type equation is then solved using a fixed coordinate system. Note that for a steady-state simulation, where)t64, the logic is implemented by multiplying the transient storage terms by zero and evaluating the advection term in a fixed coordinate system.

3.3.2 Boundary Conditions and Transient Source/Sink Terms

Unique solutions to advective-dispersive solute transport problems are generated by solving the governing equation (Equation 3-19) in conjunction with 1) a set of boundary conditions, defined at the physical edges of the modeled system, and where appropriate, 2) source/sink terms applied within the system (see Figure 3.4).

Boundary conditions and source/sink terms available in the 3DLEWASTE model include:

- Prescribed-concentration (Dirichlet) boundaries
- Specified-flux (Cauchy) boundaries
- Specified-dispersive-flux (Neumann) boundaries
- Variable boundaries
- Point sources
- Distributed sources

Prescribed-concentration or *Dirichlet* boundaries are defined by prescribing dissolved species concentrations at specified boundary nodes as:

$$C = C_d(x_b, y_b, z_b, t) \quad \text{on } B_d \tag{3-36}$$

where C_d is the specified solute concentration, B_d is the portion of the system boundary subject to a Dirichlet boundary condition, and (x_b,y_b,z_b) is the spatial coordinate on the boundary. Dirichlet boundaries are typically used to test computer programs by allowing comparisons with analytical solutions. Unlike the analogous constant-head boundaries of flow models, constant-concentration boundaries are generally poor approximations of contaminant source terms. Bodies of fresh water located upgradient from contaminant sources can be approximated using constant concentration nodes. When used to define sources, specified concentrations may be constant or allowed to vary with time, reflecting physical processes such as degradation of the source due to radioactive decay, hydrolysis, biodegradation, or physical removal. Concentration versus time profiles can be defined to account for seasonal or other time-variant changes in dissolved species levels.

The *specified-flux (Cauchy)* boundary represents the portions of the system boundary where infiltration can be quantified. The specified-flux boundary has many representations including: 1) infiltration due to leachate migration from a landfill or surface impoundment, 2) application of pesticides or fertilizer to fields, and 3) the dilution effects of rainfall or irrigation on previously

applied constituents. The specified-flux boundary condition can be written:

$$n \cdot (\mathbf{V}C - 2\mathbf{D} \cdot \nabla C) = q_c(x_b, y_b, z_b, t) \quad \text{on } B_c \tag{3-37}$$

where n is an outward unit vector normal to the boundary, $-2\mathbf{D}\cdot\nabla C$ is the dispersive flux caused by the concentration gradient ∇C, $\mathbf{V}C$ is the advective flux, q_c is the specified flux rate ($M/T/L^2$), and B_c is the portion of the system boundary subject to a specified-flux boundary condition. The specified boundary is simulated by assigning mass flux rates along specified element sides. Flux rate versus time profiles can be defined to account for seasonal or other time-variant changes in flux rates.

In addition to the user-supplied mass flux rates, 3DLEWASTE automatically accounts for the influence of the water entering the system along the boundary. The infiltration of fresh water is simulated by applying the specified-flux boundary condition and setting the mass flux rate to zero. The automatically generated term accounting for water flow normal to the boundary will simulate the dilution due to infiltration.

Also available in 3DLEWASTE is a *specified-dispersive-flux* or *Neumann* boundary condition of the form:

$$n \cdot (-2\mathbf{D} \cdot \nabla C) = q_n(x_b, y_b, z_b, t) \text{ on } B_n \tag{3-38}$$

where q_n ($M/T/L^2$) is the portion of the boundary flux attributable to the concentration and B_n is the portion of the system boundary subject to a specified-dispersive-flux boundary condition. Note that exit boundaries can be declared using this boundary condition and letting q_n=0. This physically simulates mass being advected out of the system.

For solute transport, the *variable composite* boundary condition represents a combined specified-flux/dispersive-flux boundary which allows for time-variant infiltration/water-loss rates. The boundary condition during infiltration is:

$$n \cdot (\mathbf{V}C - 2\mathbf{D} \cdot \nabla C) = n \cdot \mathbf{V}C_v(x_b, y_b, z_b, t) \text{ on } B_v \text{ if } n \cdot \mathbf{V} \neq 0 \tag{3-39a}$$

where $n\cdot\mathbf{V}$ is the Darcy velocity or discharge normal to the boundary, C_v is the concentration of the dissolved species in the water entering at the boundary, and B_v is the portion of the boundary subject to a variable boundary condition. When water is exiting at the boundary, the boundary condition defaults to the dispersive flux condition:

$$n \cdot (-2\mathbf{D} \cdot \nabla C) = 0 \quad \text{on } B_v \text{ if } n \cdot \mathbf{V} > 0 \tag{3-39b}$$

and mass is advected out of the system. Like the specified-flux boundary condition, the variable boundary can represent: 1) infiltration due to leachate migration from a landfill or surface impoundment, 2) application of pesticides or fertilizer to fields, and 3) the dilution effects of rainfall or irrigation on previously applied constituents. When the boundary being modeled may be either an exit or an infiltration boundary, such as a precipitation/ evapotranspiration boundary or a seepage face, the variable boundary condition is the proper choice. The variable boundary condition can also be used in a manner similar to the dispersive-flux condition to simulate strictly exit nodes.

Internal source/sink terms, as represented by the term QC_{in} in Equation 3-19 are also accounted for in 3DLEWASTE. As with the boundary conditions, the source/sink terms can be constant or allowed to vary with time. Both the fluid flux rate, Q, and the injected fluid species concentration, C_{in}, are allowed to vary with time. Two source/sink options are available in the code. The first is a point source/sink option and the second, a distributed source/sink option. The first option is generally used to represent production or injection wells. The fluid fluxes in wells are represented as volumetric water fluxes, q_1 (L^3/T), applied at a nodal point or to better represent a screened interval, a column of nodal points (see Figure 3.6). If vertically adjacent nodes are used to represent the screened interval of a well, the volumetric flux must be distributed among the nodes. The most appropriate method of doing this is discussed in Section 3.1.2. Note that the applied fluid fluxes must match those used in the associated flow simulation.

The distributed source option is a source intensity that is integrated over the volume of an element. For a distributed source element, the user defines a fluid source intensity, q_2 ($L^3/T/L^3$), or fluid flux rate per unit volume for each distributed source element. This option allows a user modelling a large area to approximate the influence of a well field within an element.

Time-variant boundary conditions and source/sink flux or flux intensity rates are defined by a series of paired time and value points. This paired data is used to assemble a look-up table from which appropriate values are obtained using linear interpolation at specified times of analysis. Constant values can be specified by assigning the same value to a set of two time/data point pairs, making sure that the simulation time is fully spanned.

3.3.3 Initial Conditions

The solution of the governing equation for solute transport in a porous medium also requires the initialization of concentration values such that:

$$C = C_i(x,y,z,t = 0) \quad \text{in } R \tag{3-40}$$

where C_i is the initial concentration distribution and R is the region of interest. The initial conditions are used to define the starting water quality and soil concentration levels for

determining the fate of the dissolved constituents. Besides providing a frame of reference for transient analyses, the initial conditions are used to set the storage parameters for Freundlich and Langmuir isotherms at the beginning of nonlinear simulations. For transient problems, an appropriate set of initial concentration values may either be input directly or derived from a steady-state simulation. For more information on these options see Section 4.2.10.

3.3.4 Steady-State

When looking for a bounding solution to determine the maximum possible concentration levels that may be reached in a solute transport problem, a steady-state option may be employed. In the steady-state case, the time derivatives in Equation 3-19 are discarded and the equation, including the advective term, is solved in an Eulerian or fixed-coordinate framework. Note that any solute source prescribed as a boundary condition or source term becomes modeled as an infinite source. For many systems this upper bound may be highly conservative. The steady-state option is of no use if the source is solely defined by initial conditions.

3.4 NUMERICAL APPROXIMATION IN 3DLEWASTE

The 3DLEWASTE model was developed to simulate advective-dispersive solute transport in variably-saturated porous media. In the model, the hybrid Eulerian-Lagrangian governing equation (Equation 3-33) is approximated using the Galerkin finite element technique. The time integral term in Equation 3-33 is approximated using backwards differencing in time. The nonlinearity of the system is treated using Picard iteration and the generated set of linearized equations is solved using a block iterative method.

3.4.1 Galerkin Formulation

In 3DLEWASTE, the diffusion equation is approximated using the Galerkin finite element method where the dependent variable, concentration, is approximated by a trial function of the form:

$$C \simeq N_j(x_i,t)C_j(t) \quad j = 1,2,\ldots,n \tag{3-41}$$

where $N_j(x_i,t)$ are the three-dimensional shape functions and $C_j(t)$ are nodal values of concentration at time t for the n nodes of which the finite element grid is comprised (see Figure 3.9). Substituting the trial functions into Equation 3-33 and applying the Galerkin criterion, a set of weighted residual minimization equations of the form:

$$\int_{R_s} W_i \left[(\theta + \rho_b K_d) \frac{\partial C}{\partial t} - \nabla \cdot (\theta \mathbf{D} \nabla C) + (\theta + \rho_b K_d) C \theta Q C_{in} - Q C \right] dR = 0 \tag{3-42}$$

are generated for the linear isotherm case, where W_i are the weighting functions. For the Galerkin method, the weighting functions are the same as the shape functions and therefore, Equation 3-42 can be written in the form:

$$\int_{R_s} N_i \left[(2 + D_b K_d) \frac{DC}{Dt} - \nabla \cdot (\mathbf{D} \nabla C) + (2 + D_b K_d) C + QC_{in} - QC \right] dR = 0 \qquad (3\text{-}43)$$

Integration by parts can be applied to the dispersive term to eliminate all second order terms in Equation 3-43, leaving an equation of the form:

$$\int_{R_s} N_i (2 + D_b K_d) N_j \frac{DC_j}{Dt} dR + \int_{R_s} \nabla N_i \cdot \mathbf{D} \nabla N_j dR C_j - \int_{B_s} n \cdot \mathbf{D} \nabla N_j dB C_j$$
$$+ (2 + D_b K_d) N_i N_j dR C_j + \int_{R_s} \frac{\partial 2}{\partial t} N_i N_j dR C_j - \int_{R_s} QC_{in} N_i dR + \int_{R_s} Q N_i N_j dR C_j = \qquad (3\text{-}44)$$

where B_s is the entire region boundary. The integrals given in Equation 3-44, which are taken over the entire region being modeled, can be replaced by the summation of integrals taken over the volumes and surfaces of individual elements of the finite element grid. This finite element approximation generates a set of n nodal equations of the form:

$$A_{ij} \frac{dC_j}{dt} + (B_{ij} + E_{ij}) C_j = R_{ij} \qquad \begin{matrix} i = 1,2,...n \\ j = 1,2,...n \end{matrix} \qquad (3\text{-}45a)$$

where

$$A_{ij} = \sum_{k=1}^{m} \int_{R_e} (2 + D_b K_d) N_i^e N_j^e dR \qquad (3\text{-}45b)$$

$$B_{ij} = \sum_{k=1}^{m} \int_{R_e} \nabla N_i^e \cdot \mathbf{D} \nabla N_i^e dR \qquad (3\text{-}45c)$$

$$E_{ij} = \sum_{k=1}^{m} \int_{R_e} N_i^e \left[\theta(2\%D_b K_d)\%Q\right] N_j^e dR \qquad (3\text{-}45d)$$

and

$$R_{ij} = \sum_{k=1}^{m} \left[\int_{R_e} QC_{in} N_i^e dR \% \int_{B_e} n\hat{\imath}2\mathbf{D}C_j \nabla N_j^e dB \right] \qquad (3\text{-}45e)$$

where m is the number of elements into which the system is discretized and N^e are the elemental shape functions. Note that for a steady-state simulation, the full Eulerian approach is used. The Lagrangian term DC/Dt is replaced by $\partial C/\partial t$ and the Eulerian term:

$$\sum_{k=1}^{M} \int_{R_e} N_i^e \mathbf{V}\hat{\imath}\nabla N_j^e dR \qquad (3\text{-}46)$$

is added to B_{ij}.

3.4.2 Solution Techniques

To solve the series of linearized ordinary differential equations represented by Equation 3-45a, the time differential is replaced by a finite difference formulation, resulting in working equations for 3DLEWASTE of the form:

$$\frac{A_{ij}}{\Delta t}\left(C_j^{k+1} - C_j^{(k)}\right) + \left(B_{ij}^{k+1} + E_{ij}^{k+1}\right) C_j^{k+1} = R_i^{k+1} \qquad (3\text{-}47)$$

where k+1 represents the current time step, k the previous time step, and Δt the length of the current time step. Note that since the transient solution scheme allows only for a backwards difference approximation the associated flow runs should also be solved using backwards-in-time approximation.

For each time step, the solution method involves an inner iterative scheme (see Figure 3.10) which controls the block iterative method of solving the linear equations. For simulations where the nonlinear Freundlich or Langmuir isotherms are used, the solution method also involves an outer iterative scheme where the iterations control convergence of the nonlinear terms in the linearized set of equations. For each nonlinear iteration, the linearized set of equations is solved using storage terms updated using concentration values from the previous nonlinear (outer) iteration. Storage terms for the first iteration in a time step are based on concentration values from the previous time step, or for the first time step, from the initial conditions. If the outer iterative scheme becomes unstable it may be helpful to damp the iterative changes in the concentration. One method of damping the iterative changes is through the use of an under-relaxation factor. Implementation of the under-relaxation factor for the outer iterations in 3DLEWASTE is as follows:

$$C_i^{r+1} = (1 - u_o)C_i^r + u_o C_i^{r+1} \qquad (3\text{-}48)$$

where u_o is the outer under-relaxation factor and r is the iteration number. If damping is needed, values between 0.5 and 0.9 should suffice. Acceleration or over-relaxation ($1.0<u_o<2.0$) is generally not recommended for the nonlinear iterations as it may make the solution become unstable.

The linear or linearized set of simultaneous equations is solved using a block iterative scheme. The user defines a set of subregions (or blocks) by prescribing the nodes contained in each subregion. Subregions are discussed in Section 3.2.2.

The block iterative logic contains a relaxation factor which can be used to under- or over-relax the solution and help damp or accelerate the rate of convergence. Implementation of the inner relaxation scheme is as follows:

$$C_i^{s+1} = (1 - o)C_i^s + oC_i^{s+1} \qquad (3\text{-}49)$$

where s denotes the inner iteration number and o is the relaxation factor. In general, the use

of acceleration by over-relaxation (1.0<o<1.9) is appropriate
for solutions of a diffusion-type equation, as generated in the hybrid formulation. For steady-state simulations where the advective-dispersive equation is utilized, under-relaxation (0.5<o<1.0) may be needed.

SECTION 4

DATA INPUT REQUIREMENTS

4.1 3DFEMWATER INPUT SEQUENCE

This section describes how to construct a data input file for 3DFEMWATER, the variably-saturated flow code. Background information about the code that will aid in building an input file, such as construction of a grid or selection of boundary condition types, is provided in Section 3.1. In addition, help in selecting values for some of the input parameters is given in Section 5.1.

Note that maximum control parameters are associated with a number of the input variables. These control parameters are used in the code to specify array dimensions. For some problems, the default values set for these parameters may be too small. If so, they can be easily changed. The maximum control parameters and their default values are listed in Appendix C. Note also that the logical units used by 3DFEMWATER are defined in Appendix B.

A complete input file consists of information supplied in 18 data sets. The contents and format of each data set are listed below. When constructing an input sequence, it is important to note that data sets 2 through 17 must be preceded by a record which contains a description of the data set. This can be seen in the example input sequences provided in Section 6.1. Most of the input is entered in free-format, which means that the spacing of the input data in a record does not need to follow a set pattern. Note that a record can consist of multiple lines, with a line defined as up to 80 columns.

The user may choose to run the model using any set of units as long as they are consistently maintained in all the input. Units of mass (M), length (L), and time (T) are indicated in the input descriptions.

4.1.1 Data Set 1: Title of the Simulation Run

One record with FORMAT(I5,A70,2X,I2,2I1) per problem. This record contains the following variables:

1. NPROB = Problem number (columns 1-5).

2. TITLE = Array for the title of the problem. It may contain up to 70 characters (columns 6 - 75).

3. IGEOM = Integer indicating if (1) the geometry, boundary and pointer arrays are to be printed and if (2) the boundary and pointer arrays are to be computed or read via logical units (column 78). If IGEOM is an even number, geometry, boundary and pointer arrays will not be printed. If IGEOM is an odd number, they will be printed. If IGEOM is less than or equal to 1, boundary arrays will be computed and written on logical unit LUBAR, but if IGEOM is greater than 1, boundary arrays will be read via logical unit LUBAR. If IGEOM is less than or equal to 3, pointer arrays will be computed and written on logical unit LUPAR, but if IGEOM is greater than 3, pointer arrays will be read via logical unit LUPAR. In summary:

   IGEOM = Even No. Print the geometry, boundary, and pointer arrays.
   IGEOM = Odd No. Do not print the arrays.
   IGEOM $\leq$ 1 Compute and write boundary and pointer arrays.
   1 < IGEOM $\leq$ 3 Read boundary arrays, compute and write pointer arrays (not used under normal conditions).
   IGEOM > 3 Read boundary and pointer arrays.

4. IBUG = Integer indicating if diagnostic output is desired to help determine problems encountered while executing the code (column 79);
   0 = no,
   1 = yes.

5. ICHNG = Integer control number indicating if the cyclic change of rainfall-seepage nodes is to be printed (column 80);
   0 = no,
   1 = yes.

4.1.2 Data Set 2: Basic Integer Parameters

One record with FREE-FORMAT per problem. It contains the following variables:

1. NNP = Number of nodal points.

2. NEL = Number of elements.

3. NMAT = Number of material types.

4. NCM = Number of elements with material property correction.

5. NTI = Number of time steps or time increments (see notes at the end of Data Set 2).

6. KSS = Steady-state control;
   0 = steady-state solution,
   1 = transient-state solution (see note at the end of Data Set 2).

7. NMPPM = Number of material properties per material; this parameter should be set equal to 6 in the present version of the code (see Data Set 5).

8. KGRAV = Gravity term control;
   0 = no gravity term,
   1 = gravity term included.

9. ILUMP = Mass lumping control;
   0 = no,
   1 = yes.

10. IMID = Mid-difference control;
    0 = no,
    1 = yes.

11. NITER = Number of iterations allowed for solving the non-linear equation.

12. NCYL = Number of cycles permitted for iterating rainfall-seepage boundary conditions per time step.

13. NDTCHG = Number of times the time-step size will be reset to the initial time-step size; NDTCHG should be $\geq$ 1 (see Section 5.1.2.10).

14. NPITER = Number of iterations for a pointwise solution.

**** NOTE: NTI can be computed by NTI = I1 + 1 + I2 + 1, where I1 is the largest integer not exceeding Log(DELMAX/DELT)/Log(1+CHNG), I2 is the largest integer not exceeding (RTIME-DELT*((1+CHNG) **(I1+1)-1)/CHNG)/DELMAX, RTIME is the real simulation time, and DELMAX, DELT,and CHNG are defined in data set 3.

**** NOTE: A steady-state option may be used to provide either the final state of a system under study or the initial condition for a transient-state calculation. In the former case, KSS = 0 and NTI = 0 in this data set. In the latter case, KSS = 0 and NTI > 0. If KSS > 0, there will be no steady-state calculation.

4.1.3 Data Set 3: Basic Real Parameters

One record with FREE-FORMAT per problem. It contains the following variables:

1. DELT = Initial time step size, (T).

2. CHNG = Fractional change in the time-step size in each subsequent time increment, (dimensionless decimal-point value).

3. DELMAX = Maximum value of DELT, (T).

4. TMAX = Maximum simulation time, (T).

5. TOLA = Steady-state convergence criterion, (L).

6. TOLB = Transient-state convergence criterion, (L).

7. RHO = Density of water, (M/L^3).

8. GRAV = Acceleration of gravity, (L/T^2); (e.g., 32.17 ft/s^2 or 9.81 m/s^2).

9. VISC = Dynamic viscosity of water, (M/L/T).

10. W = Time derivative weighting factor;
    0.5 = Crank-Nicolson central and/or mid-difference,
    1.0 = backward difference.

11. OME = Iteration parameter for solving the nonlinear matrix equation;
    0.0 < OME < 1.0 = under-relaxation,
    1.0 = exact relaxation,
    1.0 < OME < 2.0 = over-relaxation.

12. OMI = Relaxation parameter for solving the linearized matrix equation pointwise;
    0.0 < OMI < 1.0 = under relaxation,
    1.0 = exact relaxation,
    1.0 < OMI < 2.0 = over relaxation.

4.1.4 Data Set 4: Printer and Disk Storage Control and Times for Step Size Resetting

Three records are needed per problem. The first two records are formatted input with FORMAT(2I1). The third record is a FREE-FORMAT input. The number of lines for the first two records depends on the value of NTI, the number of time increments. The number of lines for the third record depends on the value of NDTCHG, the number of times to reset the time-step size.

Record 1 - FORMAT(2I1): This record contain the following variables:

1. KPR0 = Printer control for steady-state and initial conditions;
   0 = print nothing,
   1 = print the values for the variables FLOW, FRATE, and TFLOW,
   2 = print values above plus pressure head H,
   3 = print values above plus total head,
   4 = print values above plus moisture content,
   5 = print values above plus Darcy velocity.

2. KPR(I) = Printer control for the I-th (I = 1, 2, …, NTI) time step;
   0 = print nothing,
   1 = print the values for the variables FLOW, FRATE, and TFLOW,
   2 = print values above plus pressure head H,
   3 = print values above plus total head,
   4 = print values above plus moisture content,
   5 = print values above plus Darcy velocity.

Record 2 - FORMAT(2I1): This record can be used to store 3DFEMWATER output in a binary file for use in plotting or as input to 3DLEWASTE. It contains the following variables:

1. KDSK0 = Auxiliary storage control for the steady-state or initial condition;
   0 = no storage,
   1 = store on logical unit LUSTO.

2. KDSK(I) = Auxiliary storage control for the I-th (I = 1, 2, …, NTI) time step;
   0 = no storage,
   1 = store on logical unit LUSTO.

Record 3 - FREE-FORMAT: This record contains the following variables:

1. TDTCH(I) = Time when the I-th (I = 1, 2, …, NDTCHG) time-step-size resetting is needed.

4.1.5 Data Set 5: Material Properties

Either hydraulic conductivity or permeability can be input in this data set. The flag KCP in data set 6A is used to indicate which of the two is being used. A total of NMAT records are needed per problem, one for each material.

Record I (I = 1, 2, …, NMAT) - FREE-FORMAT: Each record contains following variables:

1. PROP(1,I) = Saturated xx-hydraulic conductivity or permeability of the medium I, (L/T or L^2).

2. PROP(2,I) = Saturated yy-hydraulic conductivity or permeability of the medium I, (L/T or L^2).

3. PROP(3,I) = Saturated zz-hydraulic conductivity or permeability of the medium I, (L/T or L^2).

4. PROP(4,I) = Saturated xy-hydraulic conductivity or permeability of the medium I, (L/T or L^2).

5. PROP(5,I) = Saturated xz-hydraulic conductivity or permeability of the medium I, (L/T or L^2).

6. PROP(6,I) = Saturated yz-hydraulic conductivity or permeability of the medium I, (L/T or L^2).

4.1.6 Data Set 6: Soil Property Parameters

6A. Soil Property Control Integers

One record per problem. This record is FREE-FORMATTED and contains the following variables:

1. KSP = Soil property input control;
   0 = analytical input,
   1 = tabular data input.

2. NSPPM = Number of points in the tabular soil property functions when KSP = 1. The number of parameters needed to specify the analytical soil functions per material when KSP = 0. (For analytical soil functions, NSPPM = 5 in the current version of the code.)

3. KCP = Permeability input control;
   0 = input saturated hydraulic conductivity,
   1 = input saturated permeability.

6B. Analytical Soil Parameters

This subdata set is needed if and only if KSP = 0. NMAT records are needed, one for each material type.

Record I (I = 1, 2, …, NMAT) - FREE-FORMAT: Each record contains the following variables:

1. THPROP(1,I) = Residual moisture (water) content for material I, (--).

2. THPROP(2,I) = Saturated moisture (water) content for material I, (--).

3. THPROP(3,I) = Air entry pressure head for material I, (L).

4. THPROP(4,I) = Van Genuchten empirical coefficient alpha for material I, (1/L).

5. THPROP(5,I) = Van Genuchten empirical coefficient beta for material I, (--).

6C. Soil Properties in Tabular Form

This subdata set is needed if and only if KSP = 1. Four sets of records are needed -- one each for pressure, water-content, relative conductivity (or relative permeability), and water capacity, respectively. Each set contains NMAT records, one for each material type. Thus the total number of records for this subdata set is 4*NMAT. The number of lines in each record is determined by the input parameter NSPPM, defined in data set 6A.

Record I (I = 1, 2, …, NMAT) - FREE-FORMAT: Each record contains the following variables:

1. HPROP(1,I) = Tabular value of pressure head for the first data point of material I, (L).

2. HPROP(2,I) = Tabular value of pressure head for the second data point of material I, (L).

.

.

NSPPM. HPROP(NSPPM,I) = Tabular value of pressure head for the NSPPM-th data point of material I, (L).

Record (NMAT + I) (I = 1, 2, …, NMAT) - FREE-FORMAT: Each record contains the following variables:

1. THPROP(1,I) = Tabular value of moisture-content for the first data point in material I, (--).

2. THPROP(2,I) = Tabular value of moisture-content for the second data point in material I, (--).

.
.

NSPPM. THPROP(NSPPM,I) = Tabular value of moisture-content for the NSPPM-th data point in material I, (--).

Record (2*NMAT + I) (I = 1, 2, …, NMAT) - FREE-FORMAT: Each record contains the following variables:

1. AKPROP(1,I) = Tabular value of relative conductivity for the first data point in material I, (--).

2. AKPROP(2,I) = Tabular value of relative conductivity for second data point in material I, (--).

.
.

NSPPM. AKPROP(NSPPM,I) = Tabular value of relative conductivity for the NSPPM-th data point in material I, (--).

Record (3*NMAT + I) (I = 1, 2, …, NMAT) - FREE-FORMAT: Each record contains the following variables:

1. CAPROP(1,I) = Tabular value of moisture-content capacity for the first data point in material I, (1/L).

2. CAPROP(2,I) = Tabular value of moisture-content capacity for the second data point in material I, (1/L).

.
.

NSPPM. CAPROP(NSPPM,I) = Tabular value of moisture content capacity for the NSPPM-th data point in material I, (1/L).

4.1.7 Data Set 7: Nodal Point Coordinates

Coordinates for NNP nodes, specified in data set 2, are needed. Usually a total of NNP records are required. However, if a group of subsequent nodes appears in regular pattern, an automatic generation input option can be used.

Each record is FREE-FORMATTED and contains the following variables:

1. NI = Node number of the first node in the sequence.

2. NSEQ = NSEQ subsequent nodes will be automatically generated.

3. NAD = Increment of node number for each of the NSEQ subsequent nodes.
4. XNI = X-coordinate of node NI, (L).

5. YNI = Y-coordinate of node NI, (L).

6. ZNI = Z-coordinate of node NI, (L).

7. XAD = Increment of x-coordinate for each of the NSEQ subsequent nodes, (L).

8. YAD = Increment of y-coordinate for each of the NSEQ subsequent nodes, (L).

9. ZAD = Increment of z-coordinate for each of the NSEQ subsequent nodes, (L).

**** NOTE: A record with nine zeroes must be used to signal the end of this data set.

4.1.8 Data Set 8: Subregional Data

8A. Subregion Control Integer

One FREE-FORMATTED record is needed for this subdata set. It contains the following variable:

1. NREGN = Number of subregions.

8B. Number of Nodes in Each Subregion

Normally, NREGN records are required. However, if the sequence of node numbers follows a regular pattern between sequential subregions, the automatic generation input option can be used.

Each record is FREE-FORMATTED and contains the following five variables:

1. NK = Subregion number of the first subregion in a sequence.

2. NSEQ = Number of subsequent subregions which will be automatically generated.

3. NKAD = Increment of NK in each of the NSEQ subsequent subregions.

4. NODES = Number of nodes in the subregion NK.

5. NOAD = Increment of NODES in each of the NSEQ subsequent subregions.

**** NOTE: A record with five zeroes must be used to end the input of this subdata set.

8C. Mapping between Global Nodes and Subregion Nodes

This subdata set should be repeated NREGN times, once for each subregion. For each subregion, normally, the number of records equals the number of nodal points in the subregion. Automatic generation can be used, however, if the sequence of subregional node numbers follows a regular pattern.

Each record is FREE-FORMATTED and contains the following five variables:

1. LI = Local node number of the first node in a sequence.

2. NSEQ = Number of subsequent local nodes which will be generated automatically.

3. LIAD = Increment of LI for each of the NSEQ subsequent nodes.

4. NI = Global node number of local node LI.

5. NIAD = Increment of NI for each of the NSEQ subsequent nodes.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

**** NOTE: Local node numbers have values between one and the total number of nodes in a subregion (i.e., 1,2,...,NODES). Global node numbers are associated with the entire grid and are entered using data set 7.

4.1.9 Data Set 9: Element Incidences

Element incidences for NEL elements, specified in data set 2, are needed. Usually, a total of NEL records are needed. However, if a sequence of element numbers follows a regular pattern, the automatic generation input option can be used.

Each record is FREE-FORMATTED and contains the following variables:

1. MI = Global element number of the first element in a sequence.
2. NSEQ = Number of subsequent elements which will be automatically generated.
3. MIAD = Increment of MI for each of the NSEQ subsequent elements.
4. IE(MI,1) = Global node number of the first node of element MI.
5. IE(MI,2) = Global node number of the second node of element MI.
6. IE(MI,3) = Global node number of the third node of element MI.
7. IE(MI,4) = Global node number of the fourth node of element MI.
8. IE(MI,5) = Global node number of the fifth node of element MI.
9. IE(MI,6) = Global node number of the sixth node of element MI.
10. IE(MI,7) = Global node number of the seventh node of element MI.
11. IE(MI,8) = Global node number of the eighth node of element MI.
12. IEMAD = Increment of IE(MI,1) through IE(MI,8) for each of the NSEQ elements.

**** NOTE: IE(MI,1) - IE(MI,8) are numbered according to the convention shown in Figure 4.1. The first four nodes start from the front, lower, left corner and progress around the bottom element surface in a counterclockwise direction. The other four nodes begin from the front, upper, left corner and progress around the top element surface in a counterclockwise direction.

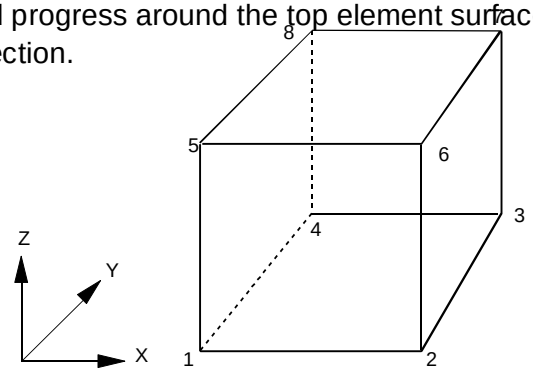

Figure 4.1. Node numbering convention for the elements.

4.1.10 Data Set 10: Material Type Correction

This data set is required only if NCM, defined in data set 2, is greater than zero. Normally, NCM records are required. However, if a group of element numbers follow a regular pattern, the automatic generation input option may be used.

Each record is FREE-FORMATTED and contains the following variables:

1. MI = Global element number of the first element in the sequence.

2. NSEQ = Number of subsequent elements which will be generated automatically.

3. MAD = Increment of element number for each of the NSEQ subsequent elements.

4. MITYP = Type of material for element MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent elements.

**** NOTE: A record with five zeroes must be used to signal the end of this data set.

4.1.11 Data Set 11: Card Input for Initial or Pre-Initial Conditions

NNP records (i.e., one record for each node) are normally needed. However, if a sequence of node numbers follows a regular pattern, automatic generation can be used.

Each record is FREE-FORMATTED and contains the following variables:

1. NI = Global node number of the first node in the sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NAD = Increment of node number for each of the NSEQ nodes.

4. HNI = Initial or pre-initial pressure head of node NI, (L).

5. HAD = Increment of initial or pre-initial head for each of the NSEQ nodes, (L).

6. HRD = Geometrical increment of HNI for each of the NSEQ subsequent nodes; (i.e, HNI**HRD).

**** NOTE: A record with six zeroes must be used to signal the end of this data set.

**** NOTE: The initial condition for a transient calculation may be obtained in two different ways: 1) it can be read directly from data set 11, or 2) the code can perform a steady-state simulation using time-invariant boundary conditions before automatically beginning the transient computations. For the first case, both KSS and NTI in data set 2 should be greater than zero. In the latter case, KSS = 0 and NTI > 0 and data set 11 is used to input the pre-initial condition, which is required as the starting condition for the steady-state iteration. In order to obtain a steady-state solution, both KSS and NTI are set equal to zero and data set 11 supplies the starting condition for the steady-state solution.

4.1.12 Data Set 12: Integer Parameters for Source and Boundary Conditions

One record per problem is needed. This record is FREE-FORMATTED and contains the following variables:

1. NSEL = Number of distributed source/sink elements.

2. NSPR = Number of distributed source/sink profiles (i.e., time histories).

3. NSDP = Number of data points in each of the NSPR source/sink profiles.

4. KSAI = Option for the distributed source/sink profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

5. NWNP = Number of well or point source/sink nodes.

6. NWPR = Number of well or point source/sink profiles (i.e., time histories).

7. NWDP = Number of data points in each of the NWPR profiles.

8. KWAI = Option for the well source/sink profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

9. NDNP = Number of fixed-head (Dirichlet) nodes (NDNP should be $\geq$ 1).

10. NDPR = Number of fixed-head profiles (i.e., time histories) (NDPR should be $\geq$ 1).

11. NDDP = Number of data points in each fixed-head profile (NDDP should be $\geq$ 2).

12. KDAI = Option for the fixed-head boundary value profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

13. NVES = Number of variable composite (rainfall/evaporation-seepage) boundary element sides.

14. NVNP = Number of variable composite boundary nodal points.

15. NRPR = Number of variable composite profiles (i.e., time histories).

16. NRDP = Number of data points in each of the NRPR profiles.

17. KRAI = Option for the variable composite profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

18. NCES = Number of specified-flux (Cauchy) boundary element sides.

19. NCNP = Number of specified-flux nodal points.

20. NCPR = Number of specified-flux profiles (i.e., time histories).

21. NCDP = Number of data points in each of the NCPR profiles.

22. KCAI = Option for the specified-flux profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

23. NNES = Number of specified-pressure-head gradient (Neumann) boundary element sides.

24. NNNP = Number of specified-pressure-head gradient nodal points.

25. NNPR = Number of specified-pressure-head gradient flux profiles (i.e., time histories).

26. NNDP = Number of data points in each of the NNPR profiles.

27. KNAI = Option for the specified-pressure-head gradient profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

4.1.13 Data Set 13: Distributed and Point Sources/Sinks

This data set is used to supply data for both distributed sources/sinks and well (point) sources/sinks.

13A. Distributed Sources/Sinks

The following three subdata sets are needed if and only if NSEL in data set 12 is greater than zero. The first subdata set is used to specify the distributed source/sink profiles. The second subdata set is used to read the global element numbers of the distributed source/sink elements. The third subdata set is used to assign a source/sink profile to each distributed source/sink element.

(a) Source/Sink Profiles

There will be NSPR (see data set 12) records in this subdata set. The number of lines in each record depends on the value of NSDP, defined in data set 12.

Record I (I = 1, 2, ..., NSPR) - FREE-FORMAT: Each record contains the following variables:

1. TSOSF(1,I) = Time of the first data point in the I-th profile, (T).

2. SOSF(1,I) = Source/sink value (as flux rate per unit volume of element) of the first data point in the I-th profile, ($L^3/T/L^2/L$); positive for a source and negative for a sink.

3. TSOSF(2,I) = Time of the second data point in the I-th profile, (T).

4. SOSF(2,I) = Source/sink value of the second data point in the I-th profile, ($L^3/T/L^2/L$); positive for a source and negative for a sink.

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Up to NSDP data points.

(b) Global Element Number of All Distributed Source/Sink Elements

One record is needed for this subdata set. The number of lines in this record depends on NSEL, defined in data set 12. The record is FREE-FORMATTED and contains the following variables:

1. MSEL(1) = Global element number of the first distributed source/sink element.

2. MSEL(2) = Global element number of the second distributed source/sink element.

.
.

Up to NSEL numbers.

(c) Source/Sink Profile Type Assigned to Each Element

Usually NSEL records are needed. However, automatic generation can be used. Each record is FREE-FORMATTED and contains the following variables:

1. MI = Compressed element number of the first element in the sequence.

2. NSEQ = Number of elements which will be generated automatically.

3. MAD = Increment of element number for each of the NSEQ subsequent elements.

4. MITYP = Source/sink profile type associated with element MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent elements.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

**** NOTE: Compressed element numbers have values between one and the total number of distributed source/sink elements. Compressed element one corresponds to the first element listed in 13A(b), compressed element two corresponds to the second global element, etc.

13B. Point (Well) Source/Sink

The following three subdata sets are needed if and only if NWNP in data set 12 is greater than zero. The first subdata set is used to specify the point source/sink profiles. The second subdata set is used to read the global node numbers of the point source/sink nodes. The third subdata set is used to assign a source/sink profile to each point source/sink node.

(a) Source/Sink Profiles

There will be NWPR (see data set 12) records in this subdata set. The number of lines in each record depends on NWDP, defined in data set 12.

Record I (I = 1, 2, …, NWPR) - FREE-FORMAT: Each record contains the following variables:

1. TWSSF(1,I) = Time of the first data point in the I-th profile, (T).

2. WSSF(1,I) = Source/sink flow rate of the first data point in the I-th profile, (L^3/T); positive for a source and negative for a sink.

3. TWSSF(2,I) = Time of the second data point in the I-th profile, (T).

4. WSSF(2,I) = Source/sink flow rate of the second data point in the I-th profile, (L^3/T); positive for a source and negative for a sink.

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Up to NWDP data points.

(b) Global Node Number of All Point (Well) Source/Sink Nodes

One record is needed for this subdata set. The number of lines in this record depends on NWNP, defined in data set 12. The record is FREE-FORMATTED and contains the following variables:

1. NPW(1) = Global node number of the first point source/sink node.

2. NPW(2) = Global node number of the second point source/sink node.

.
.

Up to NWNP numbers.

(c) Source/Sink Profile Type for Each Node

Usually NWNP records are needed. However, automatic generation can be used. Each record is FREE-FORMATTED and contains the following variables:

1. NI = Compressed point source/sink node number of the first node in the sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NAD = Increment of NI for each of the NSEQ subsequent nodes.

4. NITYP = Source/sink profile type associated with node NI.

5. NTYPAD = Increment of NITYP for each of the NSEQ subsequent nodes.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

4.1.14 Data Set 14: Variable Composite (Rainfall/Evaporation-Seepage) Boundary Condition

The following six subdata sets are required if and only if NVES in data set 12 is greater than zero. The first subdata set is used to specify the rainfall/evaporation profiles. The second subdata set is used to assign the type of rainfall/evaporation profile to each of the variable composite boundary element sides. The third subdata set is used to specify the variable composite boundary element sides. The fourth subdata set is used to read the global nodal numbers of all the variable composite boundary nodes. The fifth subdata set is used to read the ponding depth for each of the nodes. The sixth subdata set is used to read the allowed minimum pressure for each of the nodes.

14A. Rainfall/Evaporation-Seepage Profiles

There will be NRPR records (see data set 12) in this subdata set. The number of lines in each record depends on NRDP, defined in data set 12.

Record I (I = 1, 2, …, NRPR) - FREE-FORMAT: Each record contains the following variables:

1. TRF(1,I) = Time of the first data point in the I-th profile, (T).

2. RF(1,I) = Rainfall/evaporation rate of the first data point in the I-th profile, (L/T).

3. TRF(2,I) = Time of the second data point in the I-th profile, (T).

4. RF(2,I) = Rainfall/evaporation rate of the second data point in the I-th profile, (L/T).

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Up to NRDP data points.

14B. Rainfall/Evaporation-Seepage Profile Type Assigned to Each Boundary Element Side

At most, NVES (see data set 12) records are needed. However, automatic generation

can be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed variable boundary element side number of the first element side in a sequence.

2. NSEQ = Number of subsequent variable boundary element sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ subsequent variable boundary element sides.

4. MITYP = Type of rainfall/evaporation-seepage profile assigned to side MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent sides.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

14C. Specification of Variable Composite Boundary Element Sides

Normally, NVES records are required, one each for a variable boundary element side. However, if a sequence of variable composite boundary element side numbers follows a regular pattern, automatic generation may be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed variable boundary element side number of the first element side in a sequence.

2. NSEQ = Number of subsequent variable boundary element sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ subsequent variable boundary element sides.

4. I1 = Global node number of the first node of element side MI.

5. I2 = Global node number of the second node of element side MI.

6. I3 = Global node number of the third node of element side MI.

7. I4 = Global node number of the fourth node of element side MI.

8. I1AD = Increment of I1 for each of the NSEQ subsequent variable boundary element sides.

9. I2AD = Increment of I2 for each of the NSEQ subsequent variable boundary element sides.

10. I3AD = Increment of I3 for each of the NSEQ subsequent variable boundary element sides.

11. I4AD = Increment of I4 for each of the NSEQ subsequent variable boundary element sides.

**** NOTE: A record with 11 zeroes must be used to signal the end of this subdata set.

14D. Global Node Number of All Variable Composite Boundary Nodes

At most, NVNP records (see data set 12) are needed for this subdata set, one for each variable boundary node.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following five variables:

1. NI = Compressed variable boundary node number of the first node in the sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NIAD = Increment of NI for each of the NSEQ nodes.

4. NODE = Global node number of node NI.

5. NODEAD = Increment of NODE for each of the NSEQ nodes.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

14E. Ponding Depth Allowed for Each Variable Composite Boundary Node

Normally, NVNP records (see data set 12) are needed. However, if a sequence of node numbers follows a regular pattern of ponding depth, automatic generation is used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed variable boundary node number of the first node in a sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NIAD = Increment of NI for each of the NSEQ subsequent nodes.

4. HCONNI = Ponding depth of node NI, (L).

5. HCONAD = Increment of HCONNI for each of the NSEQ nodes, (L).

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

14F. Minimum Pressure Head Allowed for Each Variable Composite Boundary Node

Normally, NVNP records are needed. However, if a sequence of node numbers follows a regular pattern of minimum pressure head, automatic generation is used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed variable boundary node number of the first node in a sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NIAD = Increment of NI for each of the NSEQ subsequent nodes.

4. HMINNI = Minimum pressure head allowed for node NI, (L).

5. HMINAD = Increment of HMINNI for each of the NSEQ nodes, (L).

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

4.1.15 Data Set 15: Fixed-Head (Dirichlet) Boundary Condition

This data set is required if and only if NDNP in data set 12 is greater than zero. It consists of three subdata sets. The first subdata set is used to specify the fixed-head

profiles. The second subdata set is used to read the global node numbers of the fixed-head boundary nodes. The third subdata set is used to assign a head profile to each Dirichlet boundary node.

15A. Fixed-Head Profiles

There will be NDPR (see data set 12) records in this subdata set. The number of lines in each record depends on NDDP, the number of data points in each profile.

Record I (I = 1, 2, ..., NDPR) - FREE-FORMAT: Each record contains the following variables:

1. THDBF(1,I) = Time of the first data point in the I-th profile, (T).

2. HDBF(1,I) = Total head of the first data point in the I-th profile, (L).

3. THDBF(2,I) = Time of the second data point in the I-th profile, (T).

4. HDBF(2,I) = Total head of the second data point in the I-th profile, (L).

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Up to NDDP data points.

15B. Global Node Number of All the Dirichlet Nodes

One FREE-FORMATTED record is needed for this subdata set. The number of lines in this record depends on NDNP, defined in data set 12.

1. NPDB(1) = Global node number of the first compressed Dirichlet node.

2. NPDB(2) = Global node number of the second compressed Dirichlet node.

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Up to NDNP numbers.

15C. Type of Head Profile Assigned to Each Fixed-Head Node

Normally one record per Dirichlet node (i.e., a total of NDNP records) is needed. However, if the Dirichlet node numbers follow a regular pattern, automatic generation may be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed Dirichlet node number of the first node in the sequence.

2. NSEQ = Number of subsequent Dirichlet nodes which will be generated automatically.

3. NIAD = Increment of NI for each of the NSEQ nodes.

4. NITYP = Type of total head profile assigned to node NI and NSEQ subsequent nodes.

5. NTYPAD = Increment of NITYP for each of the NSEQ subsequent nodes.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

4.1.16 Data Set 16: Specified-Flux (Cauchy) Boundary Condition

This data set is required if and only if NCES in data set 12 is greater than zero. Four subdata sets are required. The first subdata set is used to read the specified-flux profiles. The second subdata set is used to read the type of specified-flux profile assigned to each of the specified-flux boundary element sides. The third subdata set is used to read the specified-flux boundary element sides. The fourth subdata set is used to read the global nodes associated with the specified-flux boundaries.

16A. Specified-Flux Profiles

There will be NCPR records (see data set 12) in this subdata set. The number of lines in each record depends on NCDP, defined in data set 12.

Record I (I = 1, 2, ..., NCPR) - FREE-FORMAT: Each record contains the following variables:

1. TQCBF(1,I) = Time of the first data point in the I-th profile, (T).

2. QCBF(1,I) = Normal specified-flux of the first data point in the I-th profile, ($L^3/T/L^2$); positive out from the region, negative into the region.

3. TQCBF(2,I) = Time of the second data point in the I-th profile, (T).

4. QCBF(2,I) = Normal specified-flux of the second data point in the I-th profile, ($L^3/T/L^2$); positive out from the region, negative into the region.

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Up to NCDP data points.

16B. Type of Specified-Flux Profile Assigned to Each Boundary Element Side

At most, NCES records (see data set 12) are needed. However, automatic generation can be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-flux boundary element side number of the first side in the sequence.

2. NSEQ = Number of sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ sides.

4. MITYP = Type of specified-flux profile assigned to side MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ sides.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

16C. Specified-Flux Boundary Element Sides

Normally, NCES records are required, one for each specified-flux boundary element side. However, if a group of specified-flux boundary element side numbers follows a regular pattern, automatic generation can be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-flux boundary element side number of the first element side in a sequence.

2. NSEQ = Number of subsequent specified-flux element sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ subsequent sides.

4. I1 = Global node number of the first node of element side MI.

5. I2 = Global node number of the second node of element side MI.

6. I3 = Global node number of the third node of element side MI.

7. I4 = Global node number of the fourth node of element side MI.

8. I1AD = Increment of I1 for each of the NSEQ subsequent element sides.

9. I2AD = Increment of I2 for each of the NSEQ subsequent element sides.

10. I3AD = Increment of I3 for each of the NSEQ subsequent element sides.

11. I4AD = Increment of I4 for each of the NSEQ subsequent element sides.

**** NOTE: A record with 11 zeroes must be used to end this subdata set.

16D. Global Node Number of All Compressed Specified-Flux Nodes

One FREE-FORMATTED record is needed for this subdata set. The number of lines in this record depends on NCNP, defined in data set 12.

1. NPCB(1) = Global node number of the first compressed specified-flux node.

2. NPCB(2) = Global node number of the second compressed specified-flux node.

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Up to NCNP numbers.

4.1.17 Data Set 17: Specified-Pressure-Head Gradient (Neumann) Boundary Condition

This data set is required if and only if NNNP in data set 12 is greater than zero. It consists of four subdata sets. The first subdata set is used to specify the specified-pressure-head gradient flux profiles. The second subdata set is used to assign a profile to each boundary element side. The third subdata set is used to read the global element sides of the specified-pressure-head gradient boundary elements. The fourth subdata set is used to read the global node numbers associated with the specified-pressure-head gradient boundaries.

17A. Prescribed Pressure-Head Gradient Flux Profiles

There will be NNPR records (see data set 12) in this subdata set. The number of lines in each record depends on NNDP, defined in data set 12.

Record I (I = 1, 2, ..., NNPR) - FREE-FORMAT: Each record contains the following variables:

1. TQNBF(1,I) = Time of the first data point in the I-th profile, (T).

2. QNBF(1,I) = Normal specified-pressure-head gradient flux of the first data point in the I-th profile, ($L^3/T/L^2$); positive out from the region, negative into the region.

3. TQNBF(2,I) = Time of the second data point in the I-th profile, (T).

4. QNBF(2,I) = Normal specified-pressure-head gradient flux of the second data point in the I-th profile, ($L^3/T/L^2$); positive out from the region, negative into the region.

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Up to NNDP data points.

17B. Type of Specified-Pressure-Head Gradient Flux Profile Assigned to Each Boundary Element Side

At most, NNES records are needed (see data set 12). However, automatic generation can be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-pressure-head gradient element side number of the first side in the sequence.

2. NSEQ = Number of subsequent sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ sides.

4. MITYP = Type of specified-pressure-head gradient flux profile assigned to side MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ sides.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

17C. Specified-Pressure-Head Gradient Boundary Element Sides

Normally, NNES records are required, one for each specified-pressure-head gradient boundary element side. However, if a group of specified-pressure-head gradient boundary element side numbers follow a regular pattern, automatic generation may be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-pressure-head gradient boundary element side number of the first side in sequence.

2. NSEQ = Number of subsequent sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ subsequent sides.

4. I1 = Global node number of the first node of element side MI.

5. I2 = Global node number of the second node of element side MI.

6. I3 = Global node number of the third node of element side MI.

7. I4 = Global node number of the fourth node of element side MI.

8. I1AD = Increment of I1 for each of the NSEQ subsequent element sides.

9. I2AD = Increment of I2 for each of the NSEQ subsequent element sides.

10. I3AD = Increment of I3 for each of the NSEQ subsequent element sides.

11. I4AD = Increment of I4 for each of the NSEQ subsequent element sides.

**** NOTE: A record with 11 zeroes must be used to end this subdata set.

17D. Global Node Number of All Compressed Specified-Pressure-Head Gradient Nodes

One FREE-FORMATTED record is needed for this subdata set. The number of lines in this record depends on NNNP, defined in data set 12.

1. NPNB(1) = Global node number of the first compressed specified-pressure-head gradient node.

2. NPNB(2) = Global node number of the second compressed specified-pressure-head gradient node.

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Up to NNNP numbers.

4.1.18 Data Set 18: End of Job

If another problem is to be run, then input begins again with input data set 1. If termination of the job is desired, a blank line must be inserted at the end of the data set.

4.2 3DLEWASTE INPUT SEQUENCE

This section describes how to construct a data input file for 3DLEWASTE, the transport code. Background information about the code that will aid in building an input file, such as the types of adsorption isotherms allowed, is provided in Section 3.3. In addition, help in selecting values for some of the input parameters is given in Section 5.2.

Note that maximum control parameters are associated with a number of the input variables. These control parameters are used in the code to specify array dimensions. For some problems, the default values set for these parameters may be too small. If so, they can be easily changed. The maximum control parameters and their default values are listed in Appendix C. Note also that the logical units used by 3DLEWASTE are defined in Appendix B.

A complete input file consists of information supplied in 18 data sets. The contents and format of each data set are listed below. When constructing an input sequence, it is important to note that data sets 2 through 17 must be preceded by a record which contains a description of the data set. This can be seen in the example input sequences provided in Section 6.2. Most of the input is entered in free-format, which means that the spacing of the input data in a record does not need to follow a set pattern. Note that a record can consist of multiple lines, with a line defined as up to 80 columns.

The user may choose to run the model using any set of units as long as they are consistently maintained in all the input. Units of mass (M), length (L), and time (T) are indicated in the input descriptions.

4.2.1 Data Set 1: Title of the Simulation Run

One record with FORMAT(I5,A70,3X,2I1) per problem. This record contains the following variables:

1. NPROB = Problem number (columns 1-5).

2. TITLE = Array for the title of the problem. It may contain up to 70 characters (columns 6 - 75).

3. IGEOM = Integer indicating if (1) the geometry, boundary and pointer arrays are to be printed and if (2) the boundary and pointer arrays are to be computed or read via logical units (column 79). If IGEOM is an even number, geometry, boundary and pointer arrays will not be printed. If IGEOM is an odd number, they will be printed. If IGEOM is less than or equal to 1, boundary arrays will be computed and written on logical unit LUBAR, but if IGEOM is greater than 1, boundary arrays will be read via logical unit LUBAR. If IGEOM is less than or equal to 3, pointer arrays will be computed and written on logical unit LUPAR, but

if IGEOM is greater than 3, pointer arrays will be read via logical unit LUPAR. In summary:

IGEOM = Even No.	Print the geometry, boundary, and pointer arrays.
IGEOM = Odd No.	Do not print the arrays.
IGEOM $\leq$ 1	Compute and write boundary and pointer arrays.
1 < IGEOM $\leq$ 3	Read boundary arrays, compute and write pointer arrays.
IGEOM > 3	Read boundary and pointer arrays.

4. IBUG = Integer indicating if diagnostic output is desired (column 80);
   0 = no,
   1 = yes.

4.2.2 Data Set 2: Basic Integer Parameters

One record with FREE-FORMAT per problem. It contains the following variables:

1. NNP = Number of nodal points.

2. NEL = Number of elements.

3. NMAT = Number of material types.

4. NCM = Number of elements with material property correction.

5. NTI = Number of time steps or time increments (see notes at the end of Data Set 2).

6. KSS = Steady-state control;
   0 = steady-state solution,
   1 = transient-state solution (see note at the end of Data Set 2).

7. NMPPM = Number of material properties per material; this parameter should be set equal to 8 in the present version of the code (see Data Set 5).

8. KVI = Velocity input control;
   -1 = velocity and moisture content read from data set 17,
   1 = steady-state velocity and moisture content input read from FEMWATER binary file,
   2 = transient velocity and moisture content input read from FEMWATER binary file.

9. ILUMP = Mass lumping control;

0 = no,
1 = yes.

10. IWET = Weighting function control;
    0 = Galerkin weighting,
    1 = upstream weighting.

11. IOPTIM = Optimization control;
    1 = upstream weighting optimization factor is to be computed,
    0 = factor is to be set equal to 1.0.

12. NITER = Number of iterations allowed for solving the non-linear equation.

13. NDTCHG = Number of times the time-step size will be reset to the initial time-step size; NDTCHG should be $\geq$ 1 (see Section 5.2.2.9).

14. NPITER = Number of iterations for a block or pointwise solution.

15. KSORP = Sorption model control;
    1 = linear isotherm,
    2 = Freundlich isotherm,
    3 = Langmuir isotherm.

**** NOTE: NTI can be computed by NTI = I1 + 1 + I2 + 1, where I1 is the largest integer not exceeding Log(DELMAX/DELT)/Log(1+CHNG), I2 is the largest integer not exceeding (RTIME-DELT*((1+CHNG)** (I1+1)-1)/CHNG)/DELMAX, RTIME is the real simulation time, and DELMAX, DELT, and CHNG are defined in data set 3.

**** NOTE: A steady-state option may be used to provide either the final state of a system under study or the initial condition for a transient-state calculation. In the former case, KSS = 0 and NTI = 0 in this data set. In the latter case, KSS = 0 and NTI > 0. If KSS > 0, there will be no steady-state calculation.

4.2.3 Data Set 3: Basic Real Parameters

One record with FREE-FORMAT per problem. It contains the following variables:

1. DELT = Initial time step size, (T).

2. CHNG = Fractional change in the time-step size in each subsequent time increment, (dimensionless decimal-point value).

3. DELMAX = Maximum value of DELT, (T).

4. TMAX = Maximum simulation time, (T).

5. OME = Iteration parameter for solving the nonlinear matrix equation;
   0.0 < OME < 1.0 = under-relaxation,
   1.0 = exact relaxation,
   1.0 < OME < 2.0 = over-relaxation.

6. OMI = Relaxation parameter for solving the linearized matrix equation pointwise;
   0.0 < OMI < 1.0 = under relaxation,
   1.0 = exact relaxation,
   1.0 < OMI < 2.0 = over relaxation.

7. TOLB = Transient-state convergence criterion, (L).

8. TOLA = Steady-state convergence criterion, (L).

4.2.4 Data Set 4: Printer and Disk Storage Control and Times for Step Size Resetting

Three records are needed per problem. The first two records are formatted input with FORMAT(2I1). The third record is a FREE-FORMAT input. The number of lines for the first two records depends on the value of NTI, the number of time increments. The number of lines for the third record depends on the value of NDTCHG, the number of times to reset the time-step size.

Record 1 - FORMAT(2I1): This record contain the following variables:

1. KPR0 = Printer control for steady-state and initial conditions;
   0 = print nothing,
   1 = print values for the variables FLOW, FRATE, and TFLOW,
   2 = print values above plus concentration,
   3 = print values above plus material fluxes.

2. KPR(I) = Printer control for the I-th (I = 1, 2, …, NTI) time step; 0 = print nothing,
   1 = print values for the variables FLOW, FRATE, and TFLOW,
   2 = print values above plus concentration,
   3 = print values above plus material fluxes.

Record 2 - FORMAT(2I1): This record can be used to store 3DLEWASTE output in a binary file for use in plotting results. It contains the following variables:

1. KDSK0 = Auxiliary storage control for the steady-state or initial condition;
   0 = no storage,
   1 = store on logical unit LUSTO.

2. KDSK(I) = Auxiliary storage control for the I-th (I = 1, 2, …, NTI) time step;
   0 = no storage,
   1 = store on logical unit LUSTO.

Record 3 - FREE-FORMAT: This record contains the following variables:

1. TDTCH(I) = Time when the I-th (I = 1, 2, …, NDTCHG) time-step-size resetting is needed.

4.2.5 Data Set 5: Material Properties

A total of NMAT records are required for this data set, one for each material.

Record I (I = 1, 2, …, NMAT) - FREE-FORMAT: Each record contains the following variables:

1. PROP(1,I) = Distribution coefficient (L^3/M) or Freundlich K or Langmuir K for medium I, depending on the value of KSORP in data set 2.

2. PROP(2,I) = Bulk density for medium I, (M/L^3).

3. PROP(3,I) = Longitudinal dispersivity for medium I, (L).

4. PROP(4,I) = Transverse dispersivity for medium I, (L).

5. PROP(5,I) = Molecular diffusion coefficient for medium I, (L^2/T).

6. PROP(6,I) = Tortuosity for medium I, (Dimensionless).

7. PROP(7,I) = Decay constant in medium I, (1/L).

8. PROP(8,I) = Freundlich N or Langmuir SMAX for medium I.

4.2.6 Data Set 6: Nodal Point Coordinates

Coordinates for NNP nodes are needed only if KVI $\leq$ 0, where NNP and KVI are defined in data set 2. Usually a total of NNP records are required. However, if a group of subsequent node numbers follows a regular pattern, an automatic generation input option can be used.

Each record contains the following variables and is FREE-FORMATTED.

1. NI = Node number of the first node in the sequence.

2. NSEQ = Number of subsequent nodes which will be automatically generated.

3. NAD = Increment of node number for each of the NSEQ subsequent nodes.
4. XNI = X-coordinate of node NI, (L).

5. YNI = Y-coordinate of node NI, (L).

6. ZNI = Z-coordinate of node NI, (L).

7. XAD = Increment of x-coordinate for each of the NSEQ subsequent nodes, (L).

8. YAD = Increment of y-coordinate for each of the NSEQ subsequent nodes, (L).

9. ZAD = Increment of z-coordinate for each of the NSEQ subsequent nodes, (L).

**** NOTE: A record with nine zeroes must be used to signal the end of this data set.

4.2.7 Data Set 7: Element Incidences

Element incidences for NEL elements, specified in data set 2, are needed if KVI $\leq$ 0. Usually, a total of NEL records are needed. However, if a group of element numbers follows a regular pattern, the automatic generation input option can be used.

Each record is FREE-FORMATTED and contains the following variables:

1. MI = Global element number of the first element in a sequence.

2. NSEQ = Number of subsequent elements which will be automatically generated.

3. MIAD = Increment of MI for each of the NSEQ subsequent elements.

4. IE(MI,1) = Global node number of the first node of element MI.

5. IE(MI,2) = Global node number of the second node of element MI.

6. IE(MI,3) = Global node number of the third node of element MI.

7. IE(MI,4) = Global node number of the fourth node of element MI.

8. IE(MI,5) = Global node number of the fifth node of element MI.

9. IE(MI,6) = Global node number of the sixth node of element MI.

10. IE(MI,7) = Global node number of the seventh node of element MI.

11. IE(MI,8) = Global node number of the eighth node of element MI.

12. IEMAD = Increment of IE(MI,1) through IE(MI,8) for each of the NSEQ elements.

**** NOTE: IE(MI,1) - IE(MI,8) are numbered according to the convention shown in Figure 4.2. The first four nodes start from the front, lower, left corner and progress around the bottom element surface in a counterclockwise direction. The other four nodes begin from the front, upper, left corner and progress around the top element surface in a counterclockwise direction.

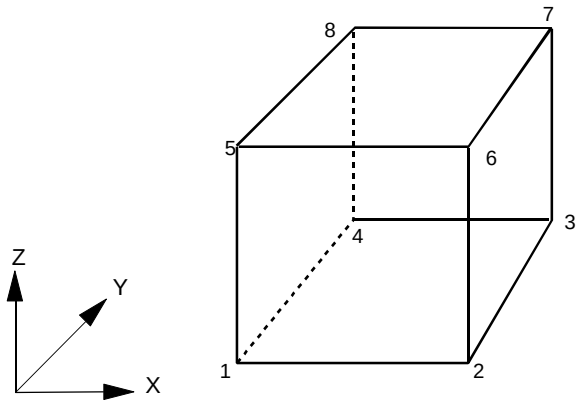

Figure 4.2. Node numbering convention for the elements.

4.2.8 Data Set 8: Subregional Data

This data set is needed only if KVI $\leq$ 0, where KVI is defined in data set 2.

8A. Subregion Control Integer

One FREE-FORMATTED record is needed for this subdata set. It contains the following variable:

1. NREGN = Number of subregions.

8B. Number of Nodes in Each Subregion

Normally, NREGN records are required. However, if the sequence of node numbers follows a regular pattern between sequential subregions, the automatic generation input option can be used.

Each record is FREE-FORMATTED and contains the following five variables:

1. NK = Subregion number of the first subregion in a sequence.

2. NSEQ = Number of subsequent subregions which will be automatically generated.

3. NKAD = Increment of NK in each of the NSEQ subsequent subregions.

4. NODES = Number of nodes in the subregion NK.

5. NOAD = Increment of NODES in each of the NSEQ subsequent subregions.

**** NOTE: A record with five zeroes must be used to end the input of this subdata set.

8C. Mapping between Global Nodes and Subregion Nodes

This subdata set should be repeated NREGN times, once for each subregion. For each subregion, normally, the number of records equals the number of nodal points in the subregion. Automatic generation can be used, however, if the subregional node numbers follow a regular pattern.

Each record contains five variables and is FREE-FORMATTED.

1. LI = Local node number of the first node in a sequence.

2. NSEQ = Number of subsequent local nodes which will be generated automatically.

3. LIAD = Increment of LI for each of the NSEQ subsequent nodes.

4. NI = Global node number of local node LI.

5. NIAD = Increment of NI for each of the NSEQ subsequent nodes.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

**** NOTE: Local node numbers have values between one and the total number of nodes in a subregion (i.e., 1,2,...,NODES). Global node numbers are associated with the entire grid and are entered using data set 6.

4.2.9 Data Set 9: Material Type Correction

This data set is required only if NCM > 0 and KVI $\leq$ 0, where NCM and KVI are defined in data set 2. Normally, NCM records are required. However, if a group of element numbers follows a regular pattern, automatic generation may be used.

Each record is FREE-FORMATTED and contains the following variables:

1. MI = Global element number of the first element in the sequence.

2. NSEQ = Number of subsequent elements which will be generated automatically.

3. MAD = Increment of element number for each of the NSEQ subsequent elements.

4. MITYP = Type of material for element MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent elements.

**** NOTE: A record with five zeroes must be used to signal the end of this data set.

4.2.10 Data Set 10: Card Input for Initial or Pre-Initial Conditions

NNP records (i.e., one record for each node) are normally needed. However, if a group of node numbers follow a regular pattern, automatic generation can be used.

Each record is FREE-FORMATTED and contains the following variables:

1. NI = Global node number of the first node in the sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NAD = Increment of node number for each of the NSEQ nodes.

4. CNI = Initial or pre-initial concentration of node NI, (M/L^3).

5. CAD = Increment of CNI for each of the NSEQ nodes, (M/L^3).

6. CRD = Geometrical increment of CNI for each of the NSEQ subsequent nodes (i.e, CNI**CRD).

**** NOTE: A record with six zeroes must be used to signal the end of this data set.

**** NOTE: The initial condition for a transient calculation may be obtained in two different ways: 1) it can be read directly from data set 10, or 2) the code can perform a steady-state simulation using time-invariant boundary conditions before beginning the transient computations. For the first case, both KSS and NTI in data set 2 should be greater than zero. In the latter case, KSS = 0 and NTI > 0 and data set 10 is used to input the pre-initial condition, which is required as the starting condition for the steady-state iteration. In order to obtain a steady-state solution, both KSS and NTI are set equal to zero and data set 11 supplies the starting condition for the

steady-state solution.

4.2.11 Data Set 11: Integer Parameters for Sources and Boundary Conditions

One record per problem is needed. This record is FREE-FORMATTED and contains the following variables:

1. NSEL = Number of distributed source/sink elements.

2. NSPR = Number of distributed source/sink profiles (i.e., time histories) (NSPR should be $\geq$ 1).

3. NSDP = Number of data points in each of the NSPR source/sink profiles (NSDP should be $\geq$ 2).

4. KSAI = Option for the distributed source/sink profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

5. NWNP = Number of well or point source/sink nodes.

6. NWPR = Number of well or point source/sink profiles (i.e., time histories).

7. NWDP = Number of data points in each of the NWPR profiles.

8. KWAI = Option for the well source/sink profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

9. NDNP = Number of prescribed-concentration (Dirichlet) nodes (NDNP should be $\geq$ 1).

10. NDPR = Number of prescribed-concentration profiles (i.e., time histories) (NDPR should be $\geq$ 1).

11. NDDP = Number of data points in each prescribed-concentration profile (NDDP should be $\geq$ 2).

12. KDAI = Option for the prescribed-concentration boundary profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

13. NVES = Number of variable composite boundary element sides.

14. NVNP = Number of variable composite boundary nodal points.

15. NRPR = Number of variable composite profiles (i.e., time histories).

16. NRDP = Number of data points in each of the NRPR profiles.

17. KRAI = Option for the variable composite profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

18. NCES = Number of specified-flux (Cauchy) boundary element sides.

19. NCNP = Number of specified-flux boundary nodal points.

20. NCPR = Number of specified-flux profiles (i.e., time histories).

21. NCDP = Number of data points in each of the NCPR profiles.

22. KCAI = Option for the specified-flux profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

23. NNES = Number of specified-dispersive-flux (Neumann) boundary element sides.

24. NNNP = Number of specified-dispersive-flux boundary nodal points.

25. NNPR = Number of specified-dispersive-flux profiles (i.e., time histories).

26. NNDP = Number of data points in each of the NNPR profiles.

27. KNAI = Option for the specified-dispersive-flux profiles to be input analytically. This variable should be set equal to zero in the current version of the code.

4.2.12 Data Set 12: Distributed and Point Sources/Sinks

This data set is used to supply data for both distributed sources/sinks, and point (well) sources/sinks.

12A. Distributed Sources/Sinks

The following three subdata sets are needed if and only if NSEL in data set 11 is greater than zero. The first subdata set is used to specify the distributed source/sink profiles. The second subdata set is used to read the global element numbers of the distributed source/sink elements. The third subdata set is used to assign a source/sink profile to each distributed source/sink element.

(a) Sources/Sink Profiles

NSPR records (see data set 11) are needed. Each record contains NSDP data points, defined in data set 11. Three numbers, representing the time, source flow rate, and source concentration, respectively, are associated with each data point.

Record I (I = 1, 2, …, NSPR) - FREE FORMAT: Each record contains the following variables:

1. TSOSF(J,I) = Time of J-th data point in I-th profile, (T).

2. SOSF(J,I,1) = Source/sink flow rate of the J-th data point in the I-th profile, ($L^3/T/L^3$); positive for source and negative for sink.

3. SOSF(J,I,2) = Source/sink concentration of the J-th data point in the I-th profile, (M/L^3).

.
.

Up to NSDP data points.

(b) Global Element Number of All Distributed Source/Sink Elements

One record is needed for this subdata set. The number of lines in the record depends on NSEL, defined in data set 11. The record is FREE-FORMATTED and contains the following variables:

1. LES(1) = Global element number of the first distributed source/sink element.

2. LES(2) = Global element number of the second distributed source/sink element.

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.
.

Up to NSEL numbers.

(c) Source/Sink Profile Type Assigned to Each Element

Usually NSEL records are needed. However, automatic generation can be used. Each record is FREE-FORMATTED and contains the following variables:

1. MI = Compressed element number of the first element in the sequence.

2. NSEQ = Number of subsequent elements which will be automatically generated.

3. MAD = Increment of element number for each of the NSEQ elements.

4. MITYP = Source/sink profile associated with element MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent elements.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

**** NOTE: Compressed element numbers have values between one and the total number of distributed source/sink elements. Compressed element one corresponds to the first element listed in 12A(b), compressed element two corresponds to the second global element, etc.

12B. Point (Well) Source/Sink

The following three subdata sets are needed if and only if NWNP in data set 11 is greater than zero. The first subdata set is used to specify the point source/sink profiles. The second subdata set reads the source/sink global node numbers, and the third assigns a source/sink profile type to each node.

(a) Source/Sink Profiles

NWPR records (see data set 11) are needed. Each record contains NWDP data points, defined in data set 11. Three numbers, representing the time, source flow rate, and source concentration, respectively, are associated with each data point.

Record I (I = 1, 2, …, NWPR) - FREE FORMAT: Each record contains the following variables:

1. TWSSF(J,I) = Time of J-th data point in I-th profile, (T).

2. WSSF(J,I,1) = Source/sink flow rate of the J-th data point in the I-th profile, (L^3/T); positive for source and negative for sink.

3. WSSF(J,I,2) = Source/sink concentration of the J-th data point in the I-th profile, (M/L^3).

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Up to NWDP numbers.

(b) Global Node Number of All Point (Well) Source/Sink Nodes

One record is needed for this subdata set. The number of lines in this record depends on NWNP, defined in data set 11. The record is FREE-FORMATTED and contains the following variables:

1. NPW(1) = Global node number of the first point source/sink node.

2. NPW(2) = Global node number of the second point source/sink node.

.
.

Up to NWNP numbers.

(c) Source/Sink Profile Type for Each Node

Usually one record per node (i.e., NWNP records) are needed. However, automatic generation can be used. Each record is FREE-FORMATTED and contains the following variables:

1. NI = Compressed point source/sink node number of the first node in a sequence.

2. NSEQ = Number of subsequent nodes which will be automatically generated.

3. NIAD = Increment of NI for each of the NSEQ nodes.

4. NITYP = Source/sink profile associated with node NI.

5. NTYPAD = Increment of NITYP for each of the NSEQ subsequent nodes.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

4.2.13 Data Set 13: Variable Composite Boundary Condition

The following four subdata sets are required if and only if NVES in data set 11 is greater than zero. The first subdata set is used to specify the concentration profiles. The second subdata set is used to assign a concentration profile type to each of the variable composite boundary element sides. The third subdata set is used to specify the variable composite boundary element sides. The fourth subdata set is used to read the global nodal number of all the variable composite boundary nodes.

13A. Concentration Profiles

There will be NRPR records (see data set 11) in this subdata set. The number of lines in each record depends on NRDP, defined in data set 11.

Record I (I = 1, 2, ..., NRPR) - FREE-FORMAT: Each record contains the following variables:

1. TCRSF(1,I) = Time of the first data point in the I-th profile, (T).

2. CRSF(1,I) = Concentration of the first data point in the I-th profile, (M/L^3).

3. TCRSF(2,I) = Time of the second data point in the I-th profile, (T).

4. CRSF(2,I) = Concentration of the second data point in the I-th profile, (M/L^3).

.

.

Up to NRDP data points.

13B. Concentration Profile Type Assigned to Each Boundary Element Side

Usually one record per variable composite boundary element side is needed. However, automatic generation can be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed variable boundary element side of the first side in a sequence.

2. NSEQ = Number of subsequent sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ subsequent sides.

4. MITYP = Type of concentration profile assigned to side MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent sides.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

13C. Specification of Variable Composite Boundary Element Sides

Normally, NVES records are required, one each for a variable boundary element side. However, if a group of variable composite boundary element sides appears in a regular pattern, automatic generation may be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed variable composite boundary element side number of the first side in a sequence.

2. NSEQ = Number of subsequent element sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ element sides.

4. I1 = Global node number of the first node of element side MI.

5. I2 = Global node number of the second node of element side MI.

6. I3 = Global node number of the third node of element side MI.

7. I4 = Global node number of the fourth node of element side MI.

8. I1AD = Increment of I1 for each of the NSEQ subsequent element sides.

9. I2AD = Increment of I2 for each of the NSEQ subsequent element sides.

10. I3AD = Increment of I3 for each of the NSEQ subsequent element sides.

11. I4AD = Increment of I4 for each of the NSEQ subsequent element sides.

**** NOTE: A record with 11 zeroes must be used to signal the end of this subdata set.

13D. Global Nodal Number of All Variable Composite Boundary Nodes

At most, NVNP records (see data set 11) are needed for this subdata set.
Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed variable boundary node number of the first node in the sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NIAD = Increment for NI for each of the NSEQ nodes.

4. NODE = Global nodal number of the node NI.

5. NODEAD = Increment of NODE for each of the NSEQ subsequent nodes.

**** NOTE: A record with five zeroes must be used to signal end of this subdata set.

4.2.14 Data Set 14: Prescribed-Concentration (Dirichlet) Boundary Condition

This data set is required if and only if NDNP in data set 11 is greater than zero. It consists of three subdata sets. The first subdata set is used to specify the prescribed-concentration profiles, the second is used to read the prescribed-concentration boundary nodes, and the third is used to assign a concentration profile type to each of the Dirichlet nodes.

14A. Prescribed-Concentration Profiles

There will be NDPR records (see data set 11) in this subdata set. The number of lines in each record depends on NDDP, defined in data set 11.

Record I (I = 1, 2, ..., NDPR) - FREE-FORMAT: Each record contains the following variables:

1. TCDBF(1,I) = Time of first data point in I-th profile, (T).

2. CDBF(1,I) = Concentration of first data point in I-th profile, (M/L^3).

3. TCDBF(2,I) = Time of second data point in I-th profile, (T).

4. CDBF(2,I) = Concentration of second data point in I-th profile, (M/L^3).

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Up to NDDP data points.

14B. Global Node Number of All the Prescribed-Concentration Nodes

One FREE-FORMATTED record is needed for this subdata set. The number of lines in this record depends on NDNP, defined in data set 11.

1. NPDB(1) = Global node number of the first compressed prescribed-concentration node.

2. NPDB(2) = Global node number of the second compressed prescribed-concentration node.

.

.

Up to NDNP numbers.

14C. Type of Concentration Profile Assigned to Each Dirichlet Node

Normally one record per Dirichlet node (i.e., a total of NDNP records) is needed. However, if the Dirichlet node numbers follow a regular pattern, automatic generation may be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed Dirichlet node number of the first node in the sequence.

2. NSEQ = Number of subsequent Dirichlet nodes which will be automatically generated.

3. NIAD = Increment of NI for each of the NSEQ nodes.

4. NITYP = Dirichlet concentration profile type assigned to node NI and NSEQ subsequent nodes.

5. NTYPAD = Increment of NITYP for each of the NSEQ subsequent nodes.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

4.2.15 Data Set 15: Specified-Flux (Cauchy) Boundary Condition

Four subdata sets are required if and only if NCES in data set 11 is greater than zero. The first subdata set is used to read the specified-flux profiles. The second subdata set is used to assign the type of specified-flux profile to each of the specified-flux boundary element sides. The third subdata set is used to read the specified-flux boundary element sides. The fourth subdata set is used to read the global nodal numbers associated with the specified-flux boundaries.

15A. Specified-Flux Profiles

There will be NCPR records (see data set 11) in this subdata set. The number of lines in each record depends on NCDP, defined in data set 11.

Record I (I = 1, 2, ..., NCPR) - FREE-FORMAT: Each record contains the following variables:

1. TQCBF(1,I) = Time of the first data point in the I-th profile, (T).

2. QCBF(1,I) = Normal specified-flux of the first data point in the I-th profile,

($M/T/L^2$); positive out of the region, negative into the region.

3. TQCBF(2,I) = Time of the second data point in the I-th profile, (T).

4. QCBF(2,I) = Normal specified-flux of the second data point in the I-th profile, ($M/T/L^2$); positive out of the region, negative into the region.

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Up to NCDP data points.

15B. Type of Specified-Flux Profile Assigned to Each Boundary Element Side

At most, NCES records (see data set 11) are needed. However, automatic generation can be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-flux boundary element side number of the first side in the sequence.

2. NSEQ = Number of subsequent sides which will be generated automatically.

3. MIAD = Increment of MI for each of NSEQ subsequent sides.

4. MITYP = Type of specified-flux profile assigned to side MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent sides.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

15C. Specified-Flux Boundary Element Sides

Normally, NCES records are required, one for each specified-flux boundary element side. However, if a group of specified-flux boundary element side numbers follows a regular pattern, automatic generation may be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-flux boundary element side number of the first element side in a sequence.

2. NSEQ = Number of subsequent element sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ subsequent sides.

4. I1 = Global node number of the first node of element side MI.

5. I2 = Global node number of the second node of element side MI.

6. I3 = Global node number of the third node of element side MI.

7. I4 = Global node number of the fourth node of element side MI.

8. I1AD = Increment of I1 for each of the NSEQ subsequent element sides.

9. I2AD = Increment of I2 for each of the NSEQ subsequent element sides.

10. I3AD = Increment of I3 for each of the NSEQ subsequent element sides.

11. I4AD = Increment of I4 for each of the NSEQ subsequent element sides.

**** NOTE: A record with 11 zeroes must be used to signal the end of this subdata set.

15D. Global Node Number of All Compressed Specified-Flux Boundary Nodes

Usually NCNP records (see data set 11) are needed for this subdata set. However, automatic generation can be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed specified-flux boundary node number of the first node in a sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NIAD = Increment for NI for each of the NSEQ nodes.

4. NODE = Global nodal number of the node NI.

5. NODEAD = Increment of the global nodal number for each of the NSEQ subsequent nodes.

**** NOTE: A record with five zeroes must be used to signal end of this subdata set.

4.2.16 Data Set 16: Specified-Dispersive-Flux (Neumann) Boundary Condition

The following four subdata sets are required if and only if NNES in data set 11 is greater than zero. The first subdata set is used to read the specified-dispersive-flux profiles. The second subdata set is used to assign a specified-dispersive-flux profile type to each boundary element sides. The third subdata set is used to read the specified-dispersive-flux boundary element side. The fourth subdata set is used to read the global nodal numbers associated with the specified-dispersive-flux boundaries.

16A. Prescribed Specified-Dispersive-Flux Profiles

There will be NNPR records (see data set 11) in this subdata set. The number of lines in each record depends on NNDP, defined in data set 11.

Record I (I = 1, 2, ..., NNPR) - FREE-FORMAT: Each record contains the following variables:

1. TQNBF(1,I) = Time of the first data point in the I-th profile, (T).

2. QNBF(1,I) = Normal specified-dispersive flux of the first data point in the I-th profile, ($M/T/L^2$); positive out of the region, negative into the region.

3. TQNBF(2,I) = Time of the second data point in the I-th profile, (T).

4. QNBF(2,I) = Normal specified-dispersive flux of the second data point in the I-th profile, ($M/T/L^2$); positive out of the region, negative into the region.

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.

Up to NNDP data points.

16B. Type of Specified-Dispersive-Flux Profile Assigned to Each Boundary Element Side

At most, NNES records (see data set 11) are needed. However, automatic generation can be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-dispersive-flux boundary element side of the first

side in a sequence.

2. NSEQ = Number of subsequent sides which will be generated automatically.

3. MIAD = Increment of MI for each of NSEQ subsequent sides.

4. MITYP = Type of specified-dispersive-flux profile assigned to side MI.

5. MTYPAD = Increment of MITYP for each of the NSEQ subsequent sides.

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

16C. Specified-Dispersive-Flux Boundary Element Sides

Normally, NNES records are required, one for each specified-dispersive-flux boundary element side. However, if a group of specified-dispersive-flux element side numbers follows a regular pattern, automatic generation may be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. MI = Compressed specified-dispersive-flux boundary element side number of the first element side in a sequence.

2. NSEQ = Number of subsequent sides which will be generated automatically.

3. MIAD = Increment of MI for each of the NSEQ subsequent sides.

4. I1 = Global node number of the first node of element side MI.

5. I2 = Global node number of the second node of element side MI.

6. I3 = Global node number of the third node of element side MI.

7. I4 = Global node number of the fourth node of element side MI.

8. I1AD = Increment of I1 for each of the NSEQ subsequent element sides.

9. I2AD = Increment of I2 for each of the NSEQ subsequent element sides.

10. I3AD = Increment of I3 for each of the NSEQ subsequent element sides.

11. I4AD = Increment of I4 for each of the NSEQ subsequent element sides.

**** NOTE: A record with 11 zeroes must be used to signal the end of this subdata set.

16D. Global Node Number of All Compressed Specified-Dispersive-Flux Boundary Nodes

Usually NNNP records (see data set 11) are needed for this subdata set. However, automatic generation can be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. NI = Compressed specified-dispersive-flux boundary node number of the first node in a sequence.

2. NSEQ = Number of subsequent nodes which will be generated automatically.

3. NIAD = Increment of NI for each of the NSEQ nodes.

4. NODE = Global nodal number of the node NI.

5. NODEAD = Increment of the global nodal number for each of the NSEQ subsequent nodes.

**** NOTE: A record with five zeroes must be used to signal end of this subdata set.

4.2.17 Data Set 17: Hydrological Variables

This data set is needed if and only if KVI in data set 2 is less than or equal to zero. When KVI $\leq$ 0, two subdata sets are needed: one for the velocity field and the other for the moisture content.

17A. Velocity Field

Usually NNP records (see data set 2) are needed. However, if the velocity values follow a regular pattern, automatic generation can be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. NI = Node number of the first node in a sequence.

2. NSEQ = Number of subsequent nodes which will be automatically

generated.

3. NIAD = Increment of NI for each of the NSEQ subsequent nodes.

4. VXNI = X-velocity component at node NI, (L/T).

5. VYNI = Y-velocity component at node NI, (L/T).

6. VZNI = Z-velocity component at node NI, (L/T).

7. VXAD = Increment of VXNI for each of the NSEQ subsequent nodes, (L/T).

8. VYAD = Increment of VYNI for each of the NSEQ subsequent nodes, (L/T).

9. VZAD = Increment of VZNI for each of the NSEQ subsequent nodes, (L/T).

**** NOTE: A record with nine zeroes must be used to signal the end of this subdata set.

17B. Moisture Content Field

Usually, NEL records (see data set 2) are needed. However, if the moisture content values follow a regular pattern, automatic generation can be used.

Record I (I = 1, 2, ...,) - FREE-FORMAT: Each record contains the following variables:

1. MI = Element number of the first element in a sequence.

2. NSEQ = Number of subsequent elements which will be automatically generated.

3. MIAD = Increment of MI for each of NSEQ subsequent elements.

4. THNI = Moisture content of element MI, (decimal point).

5. THNIAD = Increment of THNI for the NSEQ subsequent elements, (decimal point).

**** NOTE: A record with five zeroes must be used to signal the end of this subdata set.

4.2.18 Data Set 18: End of Job

If another problem is to be run, then input begins again with input data set 1. If termination of the job is desired, a blank line must be inserted at the end of the data set.

SECTION 5

PARAMETER SELECTION

This section provides guidance in selecting values for some of the parameters required as input to the 3DFEMWATER/3DLEWASTE codes. This guidance is not intended in any way to be used as a substitute for data collection. The most accurate model results are obtained from simulations which are based on site-specific information. In some cases, however, it is not feasible to measure certain parameters, and satisfactory results may be obtained using estimated values taken from the reported ranges presented here.

For easy reference, the parameters are grouped according to the data group in which they appear in the input data sets (see Section 4). Concepts, such as initial and boundary conditions, isotherms, distributed and point sources and sinks, and subregional data, were introduced in Section 3 and guidance is not provided in this section for related parameters.

5.1 3DFEMWATER

5.1.1 Data Set 1: Title of the Simulation Run

5.1.1.1 Geometry, Boundary, and Pointer Array Control, IGEOM [--]

The integer IGEOM has two functions. It is used to specify if geometry, boundary, and pointer arrays should be printed so that the user can examine them. It also controls whether the boundary and pointer arrays are written to or read from binary files. Boundary arrays store data related to the boundary conditions. Pointer arrays store the global matrix in compressed form and are used to construct the subregional block matrices. For large problems, it takes too much time to generate these arrays for each computer execution of a particular scenario. Usually, they should be generated only once and stored in binary files using logical units LUBAR and LUPAR (see Table B-1).

In order to compute and store the boundary and pointer arrays, the user should choose a value for IGEOM less than or equal to one. In subsequent runs, the boundary and pointer arrays can be read from the binary files by changing the value of IGEOM to a number greater than three. Whenever changes are made to the model which involve the geometry of the problem, the boundary conditions, and the configuration of the subregions, the arrays must be generated and stored again. Note that the option presented in the input to read boundary

arrays and compute and write pointer arrays is not used in 3DFEMWATER under normal conditions.

For the options explained above, if the number chosen by the user is even, the arrays will be printed as output. If the number is odd, the arrays will not be printed.

5.1.2 Data Set 2: Basic Integer Parameters

5.1.2.1 Number of Material Types, NMAT [--]

This parameter is the total number of different porous media being modeled. For example, if the region of interest is predominantly sand with clay lenses, then the value of NMAT should be set equal to two. When material properties are assigned to each material type, using data set 5 (see Section 4.1.5), the first material type should be the predominant porous medium (e.g., for the example here, the sand).

5.1.2.2 Number of Elements with Material Property Correction, NCM [--]

In the code, all the grid elements automatically are initialized as having a material type of one. If the region being modelled is homogeneous, the parameter NCM is set equal to zero. To model a heterogeneous porous medium, NCM and the parameters in data set 10 of the input (see Section 4.1.10) are used to specify which elements have different material types associated with them. The parameter NCM is the total number of elements which have a material type different than the first material type.

5.1.2.3 Number of Time-Steps, NTI [--]

For a constant time-step size, this number is obtained by dividing the simulation time by the time-step size, DELT. If the time-step size is variable, this number is computed using the formula given in the note at the end of data set 2 in Section 4.1.2. If a steady-state solution is desired, NTI should be set equal to zero.

5.1.2.4 Steady-State Control, KSS [--]

As noted in Section 4.1.2, a steady-state option may be used to provide either the final state of a system under study or the initial condition for a transient-state calculation. In the former case, both KSS and the number of time steps, NTI, should be set to zero. In the latter case (i.e., when KSS = 0 and NTI > 0), the code performs a steady-state calculation before beginning the transient computations. If KSS = 1, no steady-state calculation is performed. Rather, the code begins transient calculations using initial conditions supplied in data set 11 of the input.

5.1.2.5 Gravity Term Control, KGRAV [--]

This parameter indicates if the gravity term should be included. For most cases, KGRAV should be equal to 1. For cases when flow due to the pressure gradient is much greater than that due to gravity, KGRAV is set to 0.

5.1.2.6 Mass Lumping Flag, ILUMP [--]

This parameter indicates if the mass matrix is to be lumped or not. Normally, one should set this parameter to 0. Without lumping, the solution is more accurate. However, for occasions when negative concentrations or oscillating solutions occur, this parameter should be set to 1. It has been suggested that for saturated-unsaturated flow computations, the parameter ILUMP should always be set equal to 1.

5.1.2.7 Mid-differencing Flag, IMID [--]

This parameter indicates if the more accurate mid-difference method should be used in flow computations. For practical purposes, IMID = 0 should be sufficient. IMID = 1 is used only for research purposes.

5.1.2.8 Number of Iterations for the Nonlinear Equation, NITER [--]

This parameter is the number of iterations allowed for solving the nonlinear equation. Normally, NITER = 50 should be sufficient. If this number is exceeded and the solution does not converge, the program will issue a warning message. When this occurs, the user should first recheck the input values. If the input is correct, the program can be re-executed using a larger value for NITER.

5.1.2.9 Number of Cycles, NCYL [--]

This parameter indicates how many cycles are used for iterating the boundary conditions. A value of 20 should be adequate for most problems.

5.1.2.10 Number of Times to Reset the Time Step, NDTCHG [--]

This parameter indicates how many times the time-step size should be reset to the initially small time-step size. When we start a simulation, we normally use a small time-step size. However, for every consecutive time step, we may gradually increase the time-step size by some amount specified by the variable CHNG in Data Set 3 in Section 4.1.3. When a steep change in boundary conditions or source/sink conditions occurs, however, the time-step size should be reset to the initially small value. (See the example problem in Section 6.1.1.) NDTCHG tells us how many times we want to reset the time-step size during a simulation.

The value of NDTCHG must be at least one. If the user does not want to reset the time step, a value of one should be entered here and a very large number, larger than the total simulation

time, should be entered for TDTCH(1) in data set 4 (see Section 4.1.4).

5.1.2.11 Number of Iterations for Pointwise Solution, NPITER [--]

This parameter is used to input the number of iterations allowed for solving the matrix equations with the block iteration method. A value of 300 should be sufficient for most problems. If this number is exceeded and the solution does not converge, the program will issue a warning message. When this occurs, the users should re-execute the program using a larger value for NPITER.

5.1.3 Data Set 3: Basic Real Parameters

5.1.3.1 Initial Time-Step Size, DELT [T]

This is the time-step size used for the first time-step computation if the variable CHNG is not equal to 0.0. It is the time-step size used for every time step if the variable CHNG is set equal to 0.0. It is advisable to choose the value of DELT such that:

$$(F*DELX*DELX)/(DELT*K) \leq 1$$

where

DELX = the element size (L)
K = hydraulic conductivity (L/T)
F = specific storage (1/L)

For example, if F = 0.001 1/m, K = 0.00001 m/sec, and an element size of 10 m is used, then DELT should be less than 10,000 seconds.

5.1.3.2 Fractional Change in Time-Step Size, CHNG [--]

This parameter specifies how much of an increase one would like to make to the time-step size for each subsequent time step. Normally, a value from 0.0 to 0.5 can be used.

5.1.3.3 Maximum Allowable Time Step, DELMAX [T]

The maximum time-step size allowed depends on how fast the system responds to change. Use of a value one to ten times the size of the initial time step is advised.

5.1.3.4 Maximum Simulation Time, TMAX [T]

This is the actual length of time to be simulated. If this time is exceeded before you have made NTI step computations, the simulation will be terminated.

5.1.3.5 Steady-State Convergence Criterion, TOLA [L]

This is the absolute error allowed for assessing if a steady-state solution for hydraulic head has converged. The value used for TOLA depends on how much the system is disturbed. Normally, setting TOLA equal to one-ten-thousandth (0.0001) of the maximum disturbance should be sufficient. For example, if one is conducting a simulation of drawdown due to pumping and one expects the maximum drawdown at steady-state will be 1 m, then a value of TOLA equal to 0.0001 m should be sufficient.

5.1.3.6 Transient Convergence Criterion, TOLB [L]

This is the absolute error allowed for assessing if the solution for hydraulic heads has converged for each transient time step. A value equal to one-hundred-thousandth (0.00001) of the maximum disturbance should be sufficient for most problems.

5.1.3.7 Density of Water, RHO [M/L^3]

The density of water, D_w, is the ratio of its mass to its volume and has SI units of kg/m^3. Density varies with temperature (Table 5-1) and can be computed using regression equations presented in CRC (1981). Density also varies with the concentration of dissolved chemical

TABLE 5-1. WATER DENSITY AS A FUNCTION OF TEMPERATURE

Temperature (^oC)	Density (kg/m^3)
0	999.87
10	999.73
20	998.23
30	995.67
40	992.24
50	988.07
60	983.24
70	977.81
80	971.83
90	965.34
100	958.38

Source: Mercer et al., 1982; Original Reference: CRC, 1965

species. Water density appears in the definition of specific storage and in the relationship

between hydraulic conductivity and intrinsic permeability (Section 5.1.4.2).

5.1.3.8 Dynamic Viscosity of Water, VISC [M/L/T]

The viscosity of a fluid is a measure of the forces that work against flow when a shearing stress is applied (Lyman et al., 1982). The more viscous a fluid is, the greater the shear stress needed to maintain a given velocity gradient. Dynamic viscosity is often expressed in terms of poise (gram per centimeter per second) or centipoise (0.01 poise). Water has a viscosity of approximately 1 centipoise at 20°C.

Viscosity varies with temperature, as indicated in Table 5-2, and with concentration of dissolved chemicals. The effect of pressure on fluid viscosity is generally unimportant (Mercer et al., 1982). Note that dynamic viscosity is a term in the relationship between hydraulic conductivity and intrinsic permeability (Section 5.1.4.2).

5.1.3.9 Time Integration Weighting Factor, W [--]

A value of W equal to 1.0 should be used for most practical problems (see Equation 3-16). Setting W equal to 0.5 is normally done for research purposes to assess the accuracy of the Crank-Nicolson scheme.

5.1.3.10 Relaxation Parameter for Solving the Nonlinear Equation, OME [--]

Normally this parameter should be set to 1.0 (see Equation 3-17). If the convergence history shows sign of oscillation, then a value of 0.5 should be used. If the convergence history

TABLE 5-2. DYNAMIC VISCOSITY OF WATER AS A FUNCTION OF TEMPERATURE

Temperature (°C)	Dynamic Viscosity (centipoise)
0	1.7921
10	1.3077
20	1.0050
30	0.8007
40	0.6560
50	0.5494
100	0.2838

Source: CRC, 1965

shows monotonic decreases but at a very slow rate, then OME should be set to somewhere

between 1.7 to 1.9.

5.1.3.11 Iteration Parameter to Solve the Linearized Matrix Equation, OMI [--]

Normally this parameter should be set to 1.0 (see Equation 3-18). If the convergence history shows signs of oscillation, then set OMI to 0.5. If the solution converges monotonically but at a very slow rate, then set OMI to between 1.7 and 1.9.

5.1.4 Data Set 5: Material Properties

In the material properties data set, the user must input values for either hydraulic conductivity or permeability for each aquifer/soil material type. The flag which tells the code which of these two properties is being input is the permeability input control, KCP, located in Data Group 6.

5.1.4.1 The Saturated Hydraulic Conductivity Tensor [L/T]

Hydraulic conductivity is the coefficient of proportionality which appears in Darcy's Law. It expresses the ease with which a fluid can be transported through a porous medium and is a function of properties of both the porous medium and the fluid (Mills et al., 1985b). It is defined as the volume of water that will move in unit time under a unit hydraulic gradient through a unit area measured at right angles to the direction of flow. For three-dimensional flow in an anisotropic medium, hydraulic conductivity varies with direction at any point in space and is expressed as a symmetric second-rank tensor:

$$K_{ij} = \begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix} \qquad (5\text{-}1)$$

where K_{ij} is the hydraulic conductivity tensor and x, y, and z are the coordinate axes of the model grid. Because of symmetry, only 6 of the 9 terms are needed (K_{xx}, K_{yy}, K_{zz}, and $K_{xy} = K_{yx}$, $K_{xz} = K_{zx}$, and $K_{yz} = K_{zy}$).

If the coordinate axes coincide with the principal directions of anisotropy, then the nine components of the tensor reduce to K_{xx}, K_{yy}, and K_{zz}, with the other components equal to zero. For isotropic media, hydraulic conductivity is independent of the direction of measurement (i.e., $K_{xx} = K_{yy} = K_{zz}$).

Hydraulic conductivity estimates should be based on site-specific data collection (e.g., pumping tests or piezometer tests). Some typical horizontal hydraulic conductivity values for various materials are shown in Table 5-3. Note that hydraulic conductivity varies over a very wide range. As a result, values are rarely known with more than an order-of-magnitude

accuracy. Hydraulic conductivity values for fractured rock can be found in Mercer et al. (1982).

For many materials, the vertical hydraulic conductivity is substantially smaller than the horizontal hydraulic conductivity (assuming horizontal bedding and measurements made along the principal axes) (Mercer et al., 1982). Mills et al. (1985b) state that the ratio of horizontal to vertical conductivity, known as the anisotropy ratio, is from 2 to 10 for alluvium and glacial outwash and from 1.5 to 3 for sandstone. The variability in horizontal and vertical conductivities for a few aquifer materials is shown in Table 5-4.

5.1.4.2 The Permeability Tensor [L^2]

Intrinsic permeability is a property of the porous medium only. It is a measure of the resistance to fluid flow through the medium. The greater the permeability, the less the resistance. Like hydraulic conductivity, permeability is a symmetrical second-rank tensor. Permeability is equal to hydraulic conductivity multiplied by a scalar value, as is seen in the following equation:

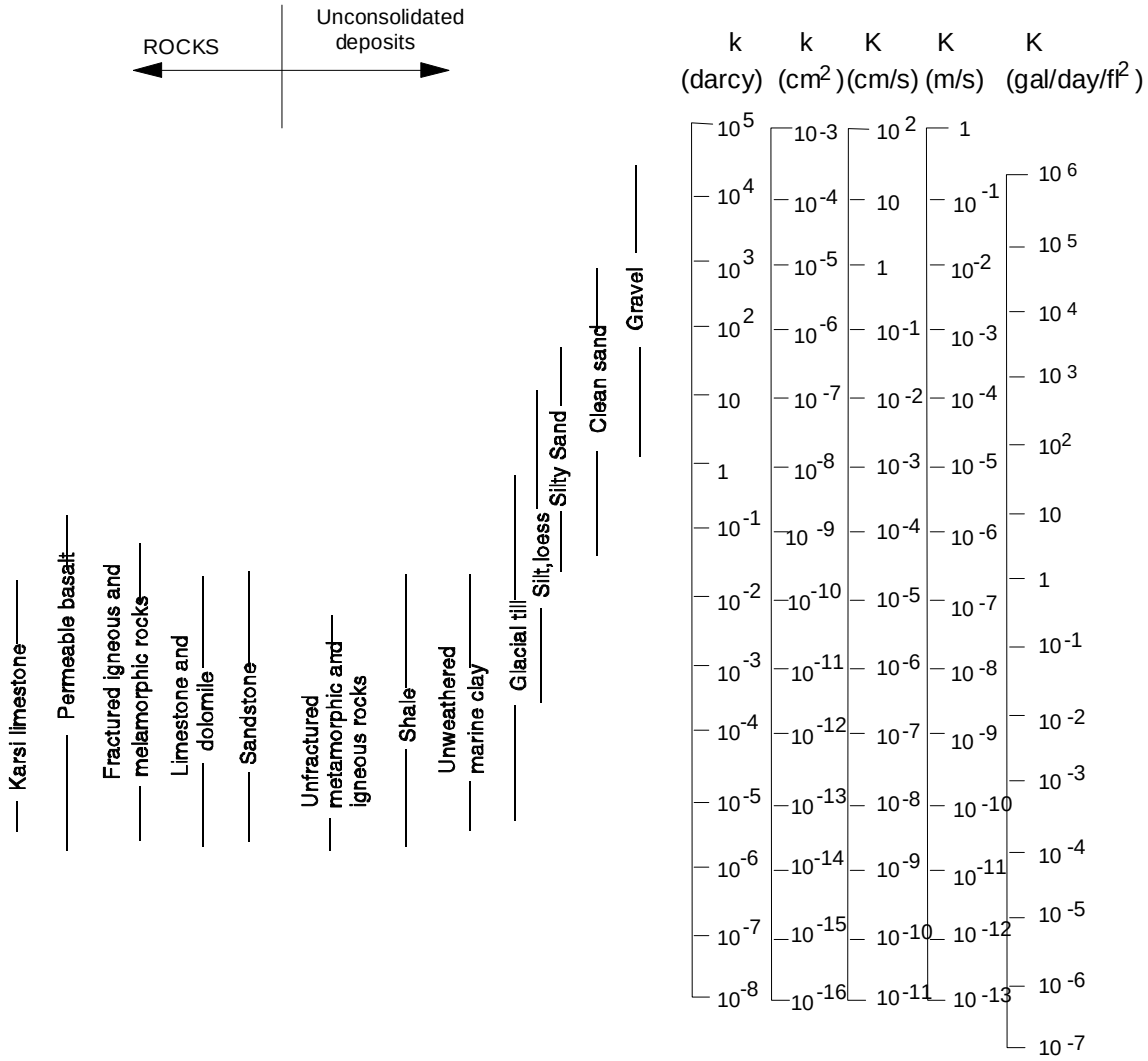
$$k_{ij} = K_{ij} F/(Dg) \qquad (5\text{-}2)$$

where

k_{ij} = permeability (L^2)
K_{ij} = hydraulic conductivity (L/T)
F = dynamic viscosity (M/L/T)
D = density (M/L^3)
g = acceleration of gravity (L/T^2)

As was true for hydraulic conductivity, permeability estimates should be based on site-specific data collection. Ranges of values for permeability are shown in Table 5-3 and in Table 5-5. Permeability is sometimes expressed in units of darcies. Conversion from darcies to other units can be done by using the conversion factors provided at the bottom of Table 5-3.

TABLE 5-3. RANGE OF HYDRAULIC CONDUCTIVITY VALUES FOR VARIOUS GEOLOGIC MATERIALS (Freeze and Cherry, 1979)



Conversion Factors for Permeability and Hydraulic Conductivity Units

	Permeability, k^*			Hydraulic conductivity, K		
	cm^2	ft^2	darcy	m/s	ft/s	U.S. gal/day/ft^2
cm^2	1	1.08×10^{-3}	1.01×10^{8}	9.80×10^{2}	3.22×10^{3}	1.85×10^{9}
ft^2	9.29×10^{2}	1	9.42×10^{10}	9.11×10^{3}	2.99×10^{6}	1.71×10^{12}
darcy	9.87×10^{-9}	1.06×10^{-11}	1	9.66×10^{-6}	3.17×10^{-5}	1.82×10^{1}

m/s	1.02×10^{-3}	1.10×10^{-6}	1.04×10^{5}	1	3.28	2.12×10^{6}
ft/s	3.11×10^{-4}	3.35×10^{-7}	3.15×10^{4}	3.05×10^{-1}	1	6.46×10^{3}
U.S. gal/day/ft^2	5.42×10^{-10}	5.83×10^{-13}	5.49×10^{-2}	4.72×10^{-2}	1.55×10^{-6}	1

To obtain k in ft^2, multiply k in cm^2 by 1.08×10^{-3}.

TABLE 5-4. VARIABILITY IN HORIZONTAL AND VERTICAL HYDRAULIC CONDUCTIVITIES

Rock Types	K_H, m/s	K_V, m/s	K_V/K_H
Shale	2.0×10^{-8}	1.0 x 10-8	0.5
Siltstone-shale	2.1×10^{-6}	2.1×10^{-7}	0.1
Siltstone-shale	2.8×10^{-7}	3.0×10^{-8}	0.107
Sandstone	3.4×10^{-7}	3.4×10^{-7}	1.0

Source: Mercer et al., 1982; Original Reference: Golder Associates, 1977

TABLE 5-5. PERMEABILITY OF POROUS MATERIALS[a]

Material		k (m^2)
Argillaceous limestone	2% porosity	9.87×10^{-17}
Limestone	16% porosity	1.38×10^{-13}
Sandstone, silty	12% porosity	2.57×10^{-15}
Sandstone, coarse	12% porosity	1.09×10^{-12}
Sandstone	29% porosity	2.37×10^{-12}
Very fine sand	well sorted	9.77×10^{-12}
Medium sand	very well sorted	2.57×10^{-10}
Coarse sand	very well sorted	3.06×10^{-9}
Gravel	very well sorted	4.24×10^{-8}
Montmorillonite clay[b]		10^{-17}
Kaolinite clay[b]		10^{-15}

[a] These are provided as estimates; actual values will vary.
[b] For the clays, only the order of magnitude is indicated.
Source: Mercer et al., 1982; Adapted from: Davis and DeWiest, 1966
)

5.1.5 Data Set 6: Soil Property Parameters

As was explained in Section 3.1.1, relationships between relative permeability and water content and between pressure head and water content must be specified in order to solve the governing equation for unsaturated flow. The 3DFEMWATER code provides two options for specifying these relationships. The user can 1) input parameters for analytical expressions of these relationships, or 2) input the coordinates of characteristic curves in tabular format. The analytical parameters are discussed first, followed by the tabular data requirements.

5.1.5.1 Analytical Parameters

Analytical equations developed by van Genuchten (1980) are used in the code to describe the relationship between pressure head and moisture content and the relationship between relative hydraulic conductivity and moisture content (see Equations 3-3a through 3-3d). In order to solve these equations, five parameters must be specified in the input sequence for each material type: residual moisture content, saturated moisture content, air entry pressure head, and two soil-specific empirical parameters, alpha and beta.

5.1.5.1.1 Residual and Saturated Moisture (Water) Content [--]

The volumetric moisture content, θ, is defined as:

$$\theta = V_W/V_T \qquad (5\text{-}3)$$

where

V_T = the total unit volume of a rock or soil (L^3)
V_W = the volume of a rock or soil occupied by water (L^3)

The saturated moisture content is equal to the porosity of the medium since all of the void space is filled with fluid. Under unsaturated conditions, however, some of the void space is filled with air and thus, the moisture content is less than the medium's porosity. The residual moisture content is that amount which can not be removed from a soil by gravity drainage, even under large suction pressure, because it adheres to the grains of the soil.

Table 5-6 lists descriptive statistics for both saturated and residual moisture content for a variety of soil types. In addition, saturated and residual moisture content values for a large number of soils can be obtained using the interactive computer program DBAPE (Imhoff et al., 1990). DBAPE, which is a soils data base analyzer and parameter estimator, is available from the U.S. EPA Center for Exposure Assessment Modeling (CEAM) at the Environmental Research Laboratory in Athens, Georgia.

5.1.5.1.2 Air Entry Pressure Head [L]

The air entry pressure head is the threshold at which air starts to penetrate saturated soil. It is typically a very small negative value for fine-grained materials and zero for coarser materials. Its value can be estimated from the water retention curves of specific soils (Freeze and Cherry, 1979; Sharp-Hansen et al., 1990). In practice, it is regularly assumed to be zero.

TABLE 5-6. DESCRIPTIVE STATISTICS FOR SATURATION WATER CONTENT (θ_s) AND RESIDUAL WATER CONTENT (θ_r)

	Saturation Water Content (θ_s) Statistic*				Residual Water Content (θ_r)			
Soil Type	&	s	CV	n	x	s	CV	n
Clay**	0.38	0.09	24.1	400	0.068	0.034	49.9	353
Clay Loam	0.41	0.09	22.4	364	0.095	0.010	10.1	363
Loam	0.43	0.10	22.1	735	0.078	0.013	16.5	735
Loamy Sand	0.41	0.09	21.6	315	0.057	0.015	25.7	315
Silt	0.46	0.11	17.4	82	0.034	0.010	29.8	82
Silt Loam	0.45	0.08	18.7	1093	0.067	0.015	21.6	1093
Silty Clay	0.36	0.07	19.6	374	0.070	0.023	33.5	371
Silty Clay Loam	0.43	0.07	17.2	641	0.089	0.009	10.6	641
Sand	0.43	0.06	15.1	246	0.045	0.010	22.3	246
Sandy Clay	0.38	0.05	13.7	46	0.100	0.013	12.9	46
Sandy Clay Loam	0.39	0.07	17.5	214	0.100	0.006	6.0	214
Sandy Loam	0.41	0.09	21.0	1183	0.065	0.017	26.6	1183

* n = Sample size, & = Mean, s = standard deviation, CV = coefficient of variation (percent)

** Agricultural soil, less than 60 percent clay.

Source: Sharp-Hansen et al. (1990)
Original source Carsel and Parrish (1988)

5.1.5.1.3 Van Genuchten Parameters, " [1/L]; $ [--]

These are empirical parameters needed to solve the van Genuchten analytical equations which are used to model unsaturated flow (see Equations 3-3a through 3-3d). Descriptive statistics for these parameters have been reported by Carsel and Parrish (1988) for a variety of soils and are shown in Table 5-7.