Mixing Cell Model: A One-Dimensional Numerical Model for Assessment of Water Flow and Contaminant Transport in the Unsaturated Zone

Arthur S. Rood

April 2009

Idaho Cleanup Project

Mixing Cell Model: A One-Dimensional Numerical Model for Assessment of Water Flow and Contaminant Transport in the Unsaturated Zone

Arthur S. Rood

April 2009

Idaho Cleanup Project
Idaho Falls, Idaho 83415

ABSTRACT

This report describes the Mixing Cell Model code, a one-dimensional model for water flow and solute transport in the unsaturated zone under steady-state or transient flow conditions. The model is based on the principles and assumptions underlying mixing cell model formulations. The unsaturated zone is discretized into a series of independent mixing cells. Each cell may have unique hydrologic, lithologic, and sorptive properties. Ordinary differential equations describe the material (water and solute) balance within each cell. Water flow equations are derived from the continuity equation assuming that unit-gradient conditions exist at all times in each cell. Pressure gradients are considered implicitly through model discretization. Unsaturated hydraulic conductivity and moisture contents are determined by the material-specific moisture characteristic curves. Solute transport processes include explicit treatment of advective processes, first-order chain decay, and linear sorption reactions. Dispersion is addressed through implicit and explicit dispersion. Implicit dispersion is an inherent feature of all mixing cell models and originates from the formulation of the problem in terms of mass balance around fully mixed volume elements. Expressions are provided that relate implicit dispersion to the physical dispersion of the system.

Two FORTRAN codes were developed to solve the water flow and solute transport equations: (1) the Mixing-Cell Model for Flow (MCMF) solves transient water flow problems and (2) the Mixing Cell Model for Transport (MCMT) solves the solute transport problem. The transient water flow problem is typically solved first by estimating the water flux through each cell in the model domain as a function of time using the MCMF code. These data are stored in either ASCII or binary files that are later read by the solute transport code (MCMT). Code output includes solute pore water concentrations, water and solute inventories in each cell and at each specified output time, and water and solute fluxes through each cell and specified output time. Computer run times for coupled transient water flow and solute transport were typically several seconds on a 2 GHz Intel Pentium IV desktop computer. The model was benchmarked against analytical solutions and finite-element approximations to the partial differential equations (PDE) describing unsaturated flow and transport. Differences between the maximum solute flux estimated by the mixing-cell model and the PDE models were typically less than two percent.

CONTENTS

FIGURES

TABLES

ACRONYMS

DUST   Disposal Unit Source Term

MCM   Mixing-Cell Model

MCMF   Mixing-Cell Model for Flow

MCMT   Mixing-Cell Model for Transport

ODE   ordinary differential equation

PDE   partial differential equation

x

Mixing Cell Model: A One-Dimensional Numerical Model for Assessment of Water Flow and Contaminant Transport in the Unsaturated Zone

1. INTRODUCTION

Evaluation of contaminant transport in the unsaturated zone is both a complex and evolving science. Typically, one is presented with the problem of assessing the release and transport of contaminants to a potable aquifer from radionuclides and chemicals disposed in an engineered waste disposal facility or present in the form of residual contamination in surface soils. Many models ranging from the simple to complex have been developed to address this problem. Examples of relatively simple assessment models that include one-dimensional transport in the unsaturated zone are RESRAD (Yu et al. 2000), MEPAS (Whelan et al., 1996), SESOIL (Scott and Hetrick 1994), MMSOILS (EPA 1992), and GWSCREEN (Rood 1999). Other models, such as the Disposal Unit Source Term Model (DUST) (Sullivan 1996) include a more sophisticated treatment of source release mechanisms coupled with a one-dimensional finite-difference solution to the advection-dispersion equation for transport in the unsaturated zone. Models that numerically approximate the non-linear partial differential equations (PDE) governing fluid flow and solute transport in a variable saturated porous media are the most flexible in terms of conceptual model development, understanding the behavior of the system, and examination of transport process, but can be cumbersome to use in risk assessment. Several examples of such models include STOMP (PNNL 1996), HYDRUS (Simunek et al. 1999), and PORFLOW (ACRI 1996). Often times the subsurface environment is poorly characterized which limits the effectiveness of a complex model. Furthermore, many of assessments are prospective and entail model predictions out to tens of hundreds (and sometimes thousands) of years. The reliability of any model is limited under such conditions and by their very nature, such model predictions cannot be confirmed with field observations. The nature of the prospective analysis and the complexity of problem often times leads to simplifying but conservative assumptions about contaminant release and transport in the subsurface environment. The model described in this report is intended to provide an assessment tool (as opposed to a research tool) for evaluating one-dimensional contaminant transport in the unsaturated zone under steady-state and transient flow conditions.

Transient infiltration is defined here as a change in the net infiltration rate that affects the water and contaminant flux to the aquifer over the assessment time frame, typically tens of hundreds of years in arid climates that exist at the Idaho National Laboratory (INL). Net infiltration (sometimes referred to as drainage) is defined as the amount of water that drains from the near surface layers to underlying strata, typically below the root zone. Net infiltration is a function of precipitation, evapotranspiration, and runoff. Other models (UNSAT-H [Fayer 2000] and HELP [Schroeder et al. 1994]) explicitly address these processes and may be used to provide net infiltration rates to the model described here.

Transient infiltration as defined here can occur with the installation and subsequent failure of an infiltration-limiting cover over buried waste or contaminated soil, disturbance of the natural soil layer, discharge of liquid effluent to an infiltration basin, or long-term changes in natural precipitation. In situations such as these, water fluxes beneath the root zone are temporally and spatially variable over the assessment period. The aforementioned simple assessment models lack the capability to address spatially and temporally variable water fluxes in the unsaturated zone in a quantitative manner, and therefore, one is left with using the relatively complex fluid-flow and transport models to estimate the effects of transient infiltration on contaminant transport. The Mixing-Cell Model (MCM) offers a relatively simple assessment approach that includes transient infiltration.

Ordinary differential equations describe the water and contaminant mass balance in a series of "mixing cells" into which the model domain is discretized. Other authors refer to this type of model as a compartment model (Whicker and Shultz 1982), box model, and tanks-in-series model (Shanahan and Harleman 1984; Rao and Hathaway 1989). Mixing-cell models have been used extensively for lake water quality modeling, contaminant transfer in biota, and chemical engineering applications. The primary output from MCM is contaminant flux at the unsaturated-saturated interface, but output also includes pore water concentrations, moisture profiles, water fluxes, and contaminant inventories in mixing cells as a function of time. While MCM is designed primarily for unsaturated transport, it is also amenable to one-dimensional saturated flow as well. The model was designed to incorporate readily available data and the dominant processes that tend to impact the results of such assessments. Such processes include time-variable net water infiltration rates, subsurface heterogeneity, and differential transport of contaminant degradation products formed during transport. MCM output is compared and contrasted against other models employing solutions to the partial differential equations describing unsaturated water flow and solute transport.

2. CONCEPTUAL AND MATHEMATICAL MODEL

The basis for the MCM is described in Rood (2004). The conceptual model envisions the unsaturated subsurface environment to be composed of a series of individual mixing cells (Figure 1). Within each mixing cell, the moisture content (fraction of the mixing cell volume composed of water) and contaminant concentration are uniform and assumed to equilibrate instantaneously in response to a change in the amount of water or contaminant entering the cell. Each mixing cell may have its own unique properties that include vertical dimensions, bulk density, hydraulic characteristics (e.g., porosity, residual moisture content, and hydraulic conductivity), and sorptive properties. Water balance within each cell is maintained by the difference between inflow and outflow. The water flux or specific discharge entering the uppermost mixing cell (q) is assumed to be the net infiltration rate past the root zone. The net infiltration rate may change with time and, in turn, affect the specific discharge through all remaining cells below it. Water movement is assumed to be downward and under unit gradient conditions within a mixing cell. Specific discharge is assumed to be less than the saturated hydraulic conductivity of any of the materials comprising the unsaturated zone.

The conceptual model for contaminant transport considers two processes: advection and dispersion. Advective processes (*F* in Figure 1) move the contaminant downward while dispersive processes (*D* in Figure 1) can move the contaminant upward or downward depending on the concentration gradient between two adjacent cells. Dispersion results in greater spreading of the contaminant among the mixing cells. As shown later, dispersion effects can be simulated through the implicit dispersion inherent in a mixing-cell model, or may be simulated by including interchange between adjacent mixing cells.

Contaminant degradation is assumed to be a first-order process described by a half-life. The contaminant may degrade into one or more degradation products, each formed from the preceding product and thereby forming a chain of degradation products. A radionuclide decay chain is perhaps the best example of this process. However, the framework can also be adapted to chemical constituents that degrade in a similar manner.

Contaminants entering a cell mix, sorb, decay, and are eventually removed by the downward movement of water. Contaminants sorb on to the solid matrix as described by the equilibrium partitioning coefficient or *Kd*. Sorption retards the overall downward movement of contaminants. The rate of transport of the degradation products that form during vertical transport are governed by the sorptive properties of the degradation product, and not those of the originating contaminant.
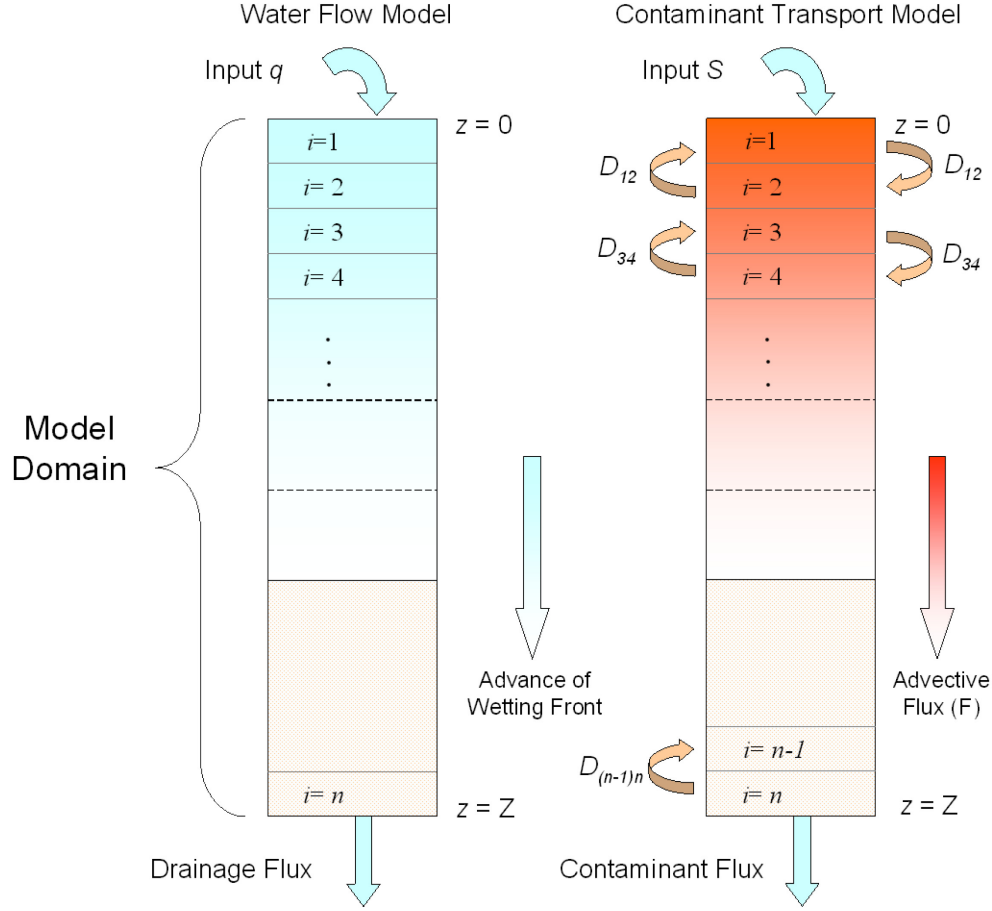
Figure 1. The MCM conceptual model for water flow (left) and contaminant transport (right). The model domain is discretized into *n* cells and extends to a depth of $z = Z$. Interchange between cells is indicated the variable $D_{i,j}$ where i is the index of the donor cell and j is the index of the receiving cell.

As formulated, contaminants may be present in each of the mixing cells at the start of the simulation, or alternatively, the contaminant may be placed over time through an external source (S in Figure 1). Concentrations of contaminants in pore water are not allowed to exceed their element or compound-specific solubility limit.

Conceptually, the model is very similar to the SESOIL model. However, significant differences exist, namely in the manner in which water flow in the unsaturated zone is treated, the selection of the number of mixing cells, and transport of degradation products. The SESOIL model calculates a net infiltration rate using precipitation records and site-specific evapotranspiration data. The MCM model assumes this value is known or estimated external to the model. More importantly, SESOIL assumes the unsaturated zone is a single homogenous cell whereas MCM allows for multiple cells and can represent a heterogeneous unsaturated zone with spatially and temporally variable water flux. In terms of solute transport, SESOIL computes concentrations and fluxes for a single contaminant with first-order decay whereas the MCM model has been written in terms of a contaminant with multiple degradation products.

2.1　Water Flow

A simple one-dimensional water-balance model coupled with material-specific moisture characteristic curves are used to calculate the net water flux through each mixing cell assuming unit gradient conditions exist throughout each cell. Additionally, water is assumed to be incompressible, its density remain constant, vapor-phase flow is inconsequential, and hydrostatic conditions are assumed to never exist (i.e., a net water flux of zero). The unit gradient model assumes water infiltration in the soil column is downward and driven by gravitational forces only. The specific discharge (sometimes referred to as the Darcy velocity or Darcy flux) in a one dimensional, vertically aligned, unsaturated soil column may be described by:

$$q = -K\left(\frac{\partial H}{\partial z} + \frac{\partial \psi}{\partial z}\right) \tag{1}$$

where

q　　= 　specific discharge ($L\ T^{-1}$)

θ　　= 　volumetric moisture content ($L^3\ L^{-3}$)

H　　= 　elevation head (L)

ψ　　= 　suction or pressure head from capillary forces (L)

K　　= 　unsaturated hydraulic conductivity of the column ($L\ T^{-1}$)

z　　= 　distance positive downward from the top of the column (L).

Under unit gradient conditions, $\partial\psi/\partial z = 0$, and $\partial H/\partial z = 1$. Therefore, $q = K$, provided q is less than the saturated hydraulic conductivity. That is, the amount of water discharged from a mixing cell is equal to the unsaturated hydraulic conductivity at a given volumetric moisture content. The volumetric moisture content is the fraction of the bulk media that is filled with water. When a porous media is saturated (i.e., all the pore spaces are filled with water), the volumetric moisture content is equal to the effective porosity of the media. In this model, we have assumed the effective porosity is equal to the total porosity. Unit gradient conditions are assumed to exist at all times within a mixing cell. That is, once water enters the mixing cell, it is instantaneously and uniformly distributed within the mixing cell. Capillary forces are explicitly excluded from the model by assuming unit gradient conditions exist at all times. However, as shown later, these forces are implicitly accounted for through discretization of the domain into a series of mixing cells. Each cell is treated as an independent unit that may receive water from a cell above it and discharge water to the cell beneath it.

The continuity equation for a constant water density states that the change in the water stored in a unit volume of soil must equal the difference between the flux into and out of the unit volume and is given by:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z}\ . \tag{2}$$

Combining Equations 1 and 2 with $\partial H/\partial z = 1$ gives the traditional formulation for one-dimensional unsaturated flow in a porous medium known as Richard's equation:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K \frac{\partial \psi}{\partial z} - K \right).$$

(3)

The unsaturated hydraulic conductivity is a function of the moisture content and described by the moisture characteristic curve. Combining Equations 1 and 2, with the assumption of unit gradient conditions (i.e., $\partial \psi / \partial z = 0$) gives:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial K(\theta)}{\partial z}$$

(4)

The term, $\partial K(\theta)/\partial z$ is approximated for the mixing cell model by:

$$\frac{\partial \theta_i}{\partial t} = \frac{K_{i-1}(\theta_{i-1}) - K_i(\theta_i)}{z_i - z_{i-1}}$$

(5)

where i is the cell index number and zi is the depth of cell i below a datum at index i = 0, z = 0. The water storage in the ith mixing cell (ϕ_i) is given by:

$$\phi_i = \theta_i T_i$$

(6)

where T_i is the thickness of the ith mixing cell which is equivalent to $z_i - z_{i-1}$. Equation 5 is now rewritten in terms of the change in water storage with respect to time and given by:

$$\frac{d\phi_i}{dt}\frac{1}{T_i} = \frac{K_{i-1}(\theta_{i-1}) - K_i(\theta_i)}{T_i}$$

$$\frac{d\phi_i}{dt} = K_{i-1}(\theta_{i-1}) - K_i(\theta_i).$$

(7)

For the uppermost mixing cell (i = 1), $K_{i-1}(\theta_{i-1}) = K_0(\theta_0) = q(t)$ where $q(t)$ is the net infiltration rate as a function of time into the uppermost mixing cell. Note that volumetric flow rates are achieved by multiplying Equation 7 by the horizontal surface area of the cells.

The functional relationship between the unsaturated hydraulic conductivity and moisture content is made using established empirical relationships that relate suction head to volumetric moisture content and unsaturated hydraulic conductivity. The relationship between these three parameters is referred to hereafter as the moisture characteristic curve. For this model, the unsaturated hydraulic conductivity as a function of moisture content as described by van Genuchten (1980) was used and is given by:

$$K(\theta) = K_{sat}\left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^{1/2}\left\{1 - \left[1 - \left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^{\frac{1}{m}}\right]^m\right\}^2$$

(8)

and

$$\left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right) = \left(\frac{1}{1 + (\alpha\psi)^{ng}}\right)^m \quad (\theta_r \leq \theta \leq \theta_s)$$

(9)

where

θ = volumetric moisture content ($L^3 L^{-3}$)

θ_r = residual moisture content ($L^3 L^{-3}$)

θ_s = saturated moisture content ($L^3 L^{-3}$)

K_{sat} = saturated hydraulic conductivity ($L\ T^{-1}$)

ψ = soil water matric suction pressure (L)

α = empirical fitting parameter (L^{-1})

ng = empirical fitting parameter

m = $1 - 1/ng$.

Equations 8 and 9 are valid when $q < K_{sat}$. Hydraulic properties that consider hysteresis were not included in this formulation. Other functional relationships of unsaturated soil hydraulics were derived by Brooks and Corey (1964), Gardener (1960), and Campbell (1974). Ideally, site-specific parameter values of the moisture characteristic curve would be available. However, more often than not, generic values are used in the early stages of an assessment when field data are lacking. Some representative van Genuchten fitting parameter values for various lithologies are given in Table 1.

Table 1. Mean representative values of the saturated hydraulic conductivity (K_{sat}), residual moisture content (θ_r), saturated moisture content (θ_s), and the van Genuchten fitting parameters α and n for various soil types (from Carsel and Parrish 1988).

Soil Type	Percent sand	Percent clay	n	α (cm^{-1})	θ_r	θ_s	K_{sat} (cm yr^{-1})
Clay	14.9	55.2	1.09	0.008	0.068	0.38	1,752
Clay loam	29.8	32.6	1.31	0.019	0.095	0.41	2,278
Loam	40	19.7	1.56	0.036	0.078	0.43	9,110
Loamy sand	80.9	6.4	2.28	0.124	0.057	0.41	127,808
Silt	5.8	9.5	1.37	0.016	0.034	0.46	2,190
Silt loam	16.6	18.5	1.41	0.020	0.067	0.45	3,942
Silty clay	6.1	46.3	1.09	0.005	0.070	0.36	175
Silty clay loam	7.6	33.2	1.23	0.010	0.089	0.43	613
Sand	92.7	2.9	2.68	0.145	0.045	0.43	260,172
Sandy clay	47.5	41.0	1.23	0.027	0.100	0.38	1,051
Sandy clay loam	54.3	27.4	1.48	0.059	0.100	0.39	11,476
Sandy loam	63.4	11.1	1.89	0.075	0.065	0.41	38,719

The moisture content in the ith mixing cell is used in combination with the moisture characteristic curve to determine $K_i(\theta_i)$, the specific discharge through the ith mixing cell. The value of $K_i(\theta_i)$ as a function of time is then passed to the transport model.

2.2   Contaminant Transport

The model for solute transport explicitly treats advective processes and implicitly or explicitly treats dispersive processes. The model is based on the one-dimensional PDE for mass transport in a variably saturated porous medium. The general transport equation for a single contaminant with first-order decay is given by (Codell et al. 1983):

$$Rd\, A\theta \frac{\partial C}{\partial t} = A\frac{\partial}{\partial z}\left(\theta\, D\frac{\partial C}{\partial z}\right) - A\frac{\partial qC}{\partial z} - \left(Rd\,\theta\,\lambda + Rd\frac{\partial\theta}{\partial t}\right)AC \tag{8}$$

where

C = solute concentration (M L^{-3})

D = dispersion and diffusion coefficient (L^2 T^{-1})

A = cross sectional area perpendicular to flow (L^2)

Rd = retardation coefficient (unitless)

q = specific discharge or Darcy velocity (L T^{-1})

λ = first-order decay constant (T^{-1}).

The mixing cell approximation is written in terms of the mass balance around fully mixed volume elements. Assuming unidirectional flow in the positive z direction, the mixing-cell model formulation for interior cells (i.e., $i\neq 1$ and $i\neq n$ where n is the number of cells) of equal thickness, T is given by:

$$T_i Rd_i\, A\theta_i \frac{dC_i}{dt} = A\sum_k \frac{D_{ik}}{T_{ik}}\left(\theta_k\, C_k - \theta_i C_i\right) + A\left(q_{i-1}C_{i-1}\right) - A\left(q_i C_i\right) - T_i A Rd_i\,\theta_i\,\lambda C_i + S_i \tag{9}$$

where i is the cell index, k is the index for cells adjacent cell i (i.e., $i-1$ and $i+1$), D_{ik} is the dispersion coefficient between cell i and k (L^2 T^{-1}) T_{ik} is the distance separating the center of cell i and k (L), and S_i is an external source to cell i (M T^{-1}). The first term in Equation 9 represents dispersion, the second and third terms represent advection, and the last term represents decay. The variables, θ and q, can be time-variable or constant depending on whether transient infiltration or steady-state flow is considered.

The term, $Rd\,\partial\theta/\partial t$ in Equation 8, enforces continuity between the moisture content and solute concentration. This term is zero under steady-state flow conditions. Continuity between the two quantities (θ and C) under transient flow conditions is achieved by determining the time-dependent moisture content at each time step. Moisture content as a function of time is calculated in the water flow portion of the code. The concentration in each cell at a given time-step is adjusted for the moisture content by:

$$C_i^m = \frac{Q_i^m}{\theta_i^m\, AT\left(1 + \dfrac{Kd_i\rho_i}{\theta_i^m}\right)} \tag{10}$$

where

C_i^m = contaminant pore water concentration in cell i at time-step m (M L^{-3})

Q_i^m = mass of contaminant in cell i at time step m (M)

Kd_i = equilibrium partition coefficient for mixing cell i (L^3 M^{-1})

ρ_i = bulk density of mixing cell i (M L^{-3})

θ_i^m = the moisture content in mixing cell i at time step m (M L^{-3}).

The term, $1 + Kd_i\,\rho_i/\theta_i$ is the retardation coefficient (Rd) and is unity for a Kd of zero. Darcy fluxes in each cell and at each time-step are calculated using the time-dependent value of θ and the material-specific moisture characteristic curve. If C_i as given by Equation 10 exceeds the solubility limit, then $C_i = C_{Sl}$ where C_{Sl} is the solubility limit of the contaminant. The solubility adjustment does not affect the total mass of contaminant in the cell. The left-hand side of Equation 9 and the decay terms can now be rewritten in terms of the state variable (contaminant mass) by substituting the right hand side of Equation 10 for C.

$$\frac{dQ_i}{dt} = A\sum_k \frac{D_{ik}}{T_{ik}}\left(\theta_k C_k - \theta_i C_i\right) + A\left(q_{i-1}C_{i-1}\right) - A\left(q_i C_i\right) - \lambda Q_i + S_i \tag{11}$$

where Q_i is the contaminant mass in the cell i. Equation 11 is valid for all non-boundary cells. Imposing the following boundary conditions

$$D\frac{dC}{dz} = 0 \quad \text{at} \quad z = 0 \quad \text{and} \quad z = Z \tag{12}$$

then gives the mass balance equations for the first ($i = 1$) and last ($i = n$) cell in the system.

$$\frac{dQ_1}{dt} = A\frac{D_{12}}{T_{12}}\left(\theta_2 C_2 - \theta_1 C_1\right) - A\left(q_1 C_1\right) - \lambda Q_1 + S_1 \qquad \text{for } i = 1$$

$$\frac{dQ_n}{dt} = A\frac{D_{n-1n}}{T_{n-1n}}\left(\theta_{n-1}C_{n-1} - \theta_n C_n\right) - A\left(q_n C_n\right) + A\left(q_{n-1}C_{n-1}\right) - \lambda Q_n + S_n \qquad \text{for } i = n \tag{13}$$

Implementation of Equation 11 in the MCM code is performed differently than what is presented in Rood (2004). A simple procedure is used where each cell is treated as an independent unit and advective and dispersive rate constants are defined. Sources are only considered for the first cell. The advective (κ) and dispersion (δ) rate constants are defined as follows.

$$\kappa_i = \frac{q}{T_i \theta_i Rd_i} \quad \text{and} \quad \delta_i = \frac{D_i}{T_i^2} \tag{14}$$

The advective rate constant is equivalent to the leach rate constant as described in Baes and Sharp (1983). An optional rate constant (designated kx) is also introduced into the governing equations that describes the transfer from cell i to cell $i+1$. This rate constant is provided by the user and

is calculated external to the code. Assigning rate constants to the advection, dispersive, and optional transfer processes, and expanding the summation term results in the following equation for interior cells

$$\frac{dQ_i}{dt} = A\left[\delta_{i-1}C_{i-1}\theta_{i-1}T_{i-1} + \delta_{i+1}C_{i+1}\theta_{i+1}T_{i+1} - 2\delta_i C_i\theta_i T_i\right] + (kx_{i-1} + \kappa_{i-1})Q_{i-1} - (kx_i + \kappa_i)Q_i - \lambda Q_i \tag{15}$$

and

$$\frac{dQ_1}{dt} = A\left[\delta_2 C_2\theta_2 T_2 - \delta_1 C_1\theta_1 T_1\right] - (kx_1 + \kappa_1)Q_1 - \lambda Q_1 + S_1 \quad \text{for } i = 1$$

$$\frac{dQ_n}{dt} = A\left[\delta_{n-1}C_{n-1}\theta_{n-1}T_{n-1} - \delta_n C_n\theta_n T_n\right] + (kx_{n-1} + \kappa_{n-1})Q_{n-1} - (kx_n + \kappa_n)Q_n - \lambda Q_n \quad \text{for } i = n \tag{16}$$

for the boundary cells. Equation 15 can now be expanded to include the transport of multiple decay products.

$$\frac{dQ_{i,j}}{dt} = A\left[\delta_{i-1,j}C_{i-1,j}\theta_{i-1}T_{i-1} + \delta_{i+1,j}C_{i+1,j}\theta_{i+1}T_{i+1} - 2\delta_{i,j}C_{i,j}\theta_i T_i\right]$$

$$+ (kx_{i-1,j} + \kappa_{i-1,j})Q_{i-1,j} - (kx_{i,j} + \kappa_{i,j})Q_{i,j} - \lambda_j Q_{i,j} + BR_j\lambda_{j-1}Q_{i,j-1} \tag{17}$$

where, j is the index for the decay chain member, BR_j is the fraction of decay product j–1 that decays to product j, and $kx_{i,j}$ is the optional rate constant describing transfer from cell i to cell i+1 for contaminant j. For the originating contaminant in a series of degradation products, the term, $BR_j.\lambda_{j-1}Q_{i,j-1}$ is omitted from Equation 17. The decay rate constant is given by:

$$\lambda_j = \frac{\ln(2)}{th_j} \tag{18}$$

where th_j is the half-life of contaminant j. Equation 17 describes the mixing-cell model with interchange. Equation 17 also gives the mixing-cell model without interchange except the dispersive terms are omitted (i.e., $\delta = 0$). The mixing-cell model without interchange is useful because relatively simple analytical solutions exist for the equations describing the system. These solutions are useful for simple conceptual models and model verification exercises.

The overall objective of the model is to provide a solute flux to the aquifer. The solute flux to the aquifer for degradation product j at $z = Z$ ($i = n$) for the stated boundary conditions is given by:

$$F_j = A(q_n C_{n,j}) = \frac{q_n Q_{n,j}}{\theta_n T_n Rd_{n,j}} \tag{19}$$

where F_j is the solute flux to the aquifer from cell n for decay product j.

3.   MODEL DISCRETIZATION AND SOLUTE DISPERSION

The dispersive behavior of the mixing-cell model is similar to that of the advection dispersion equation and is related to the physical dispersion of the system (Zvirin and Shinnar 1976; Van Ommen 1985; Appelo and Willemsen 1987; Shanahan and Harleman 1984). Shanahan and Harleman (1984) use the term *implicit dispersion* to describe the dispersion that is inherent in the formulation of mass transport around fully mixed volume elements (cells) and described in terms of ordinary differential equations (ODEs). The dimensionless Peclet number characterizes dispersion and is given by:

$$Pe = \frac{Z}{D}\frac{q}{\theta} \tag{20}$$

where Pe is the Peclet number, Z is the length of the unsaturated zone (L), and D is the dispersion coefficient ($L^2 T^{-1}$). The dispersion coefficient is given by:

$$D = \alpha_L\, q/\theta + D_m \tag{21}$$

where D_m is the effective molecular diffusion coefficient in pore water($L^2 T^{-1}$), and α_L is the longitudinal dispersivity (m). Molecular diffusion may be important for systems with extremely low specific discharge. Equation 20 is referred to here as the scale-length Peclet number because it is the ratio of advection to dispersion for the entire system. If molecular diffusion is neglected, Equation 20 reduces to Z/α_L.

Levenspiel and Bischoff (1963) established a relationship between the number of equal-thickness mixing cells and the scale-length Peclet number for the mixing cell-model without interchange. They concluded that the number of mixing cells is approximately related to the Peclet number as given by:

$$\frac{1}{n} = \frac{2}{Pe^2}\left(Pe - 1 + e^{-Pe}\right) \tag{22}$$

which can be approximated by (Shanahan and Harleman 1984)

$$n = \frac{Pe + 1}{2} \tag{23}$$

or as n becomes large

$$n \cong \frac{Pe}{2} \;. \tag{24}$$

Zvirin and Shinnar (1976) as reported in Shanahan and Harleman (1984) defined the relationship between an equivalent Peclet number (Pe) and n for the mixing-cell model with interchange as:

$$Pe = \frac{2n}{1 + 2\beta} \tag{25}$$

where β is the ratio of the exchange flow to through-flow and all cells are of equal size. The influence of cell interchange is to decrease the Peclet number (increase dispersion) by the factor $1 + 2\beta$. Shanahan

10

and Harleman (1984) define exchange flow as $D\,A/T$ and through-flow as $A\,q/\theta$, where T is the distance separating adjacent mixing cells. If molecular diffusion is neglected, β can be written in terms of the local dispersivity:

$$\beta = \frac{D\,A}{A\,q/\theta\,T} = \frac{\alpha_{L*}\,q\,\theta}{T\,q\,\theta} = \frac{\alpha_{L*}}{T}\,.$$

(26)

The term β is essentially the inverse of the local (or grid) Peclet number. The term α_{L*} represents the equivalent local dispersivity accounting for implicit dispersion. If the dispersivity of the overall system is α_L, then the equivalent local dispersivity can be derived from Equations 20, 25, and 26:

$$\alpha_{L*} = \left[\frac{2n\alpha_L}{Z} - 1\right]\frac{T}{2}\,.$$

(27)

It can be shown that as $n \to \infty$, $\alpha_{L*} \to \alpha_L$. If α_{L*} is negative, then implicit dispersion is greater than the dispersion defined by α_L and additional cells must be added. For the case where molecular diffusion is not negligible, an equivalent local dispersion coefficient (D^*) is calculated for each cell and given by Equation 28:

$$D^* = \left[\frac{2D_i}{q_i/\theta_i} - 1\right]\frac{T\,q_i/\theta_i}{2}\,.$$

(28)

3.1   Comparison of Mixing Cell Model with an Analytical Solution for Solute Flux

Assuming a unidirectional constant flow field in a homogeneous isotropic porous media, the flux from an instantaneous unit release at $z = 0$ with the initial conditions $C = 0$ at $t = 0$ for all z, and boundary conditions $C = 0$ at $z = \pm\infty$ is (Codell et al. 1983)

$$F(z,t) = \frac{\left(z + \dfrac{qt}{\theta\,Rd}\right)}{4\sqrt{D\pi t^3/Rd}}\exp\left(\frac{-\left(z - \dfrac{qt}{\theta\,Rd}\right)^2}{4Dt/Rd} - \lambda t\right).$$

(29)

A comparison of the analytical flux to the flux estimated by the mixing-cell model with interchange is illustrated in Figure 2. The model was discretized into sixty equal-thickness cells of 1-meter thickness. Each cell was assigned a specific discharge of 0.05 m yr^{-1} and moisture content of 0.3. A unit mass was placed in cell ten. The percent difference between the maximum flux for the two models was ~0.2% for $Pe = 100$. The percent difference increases with decreasing Pelect number to a maximum of ~4% for a Pe of 10.
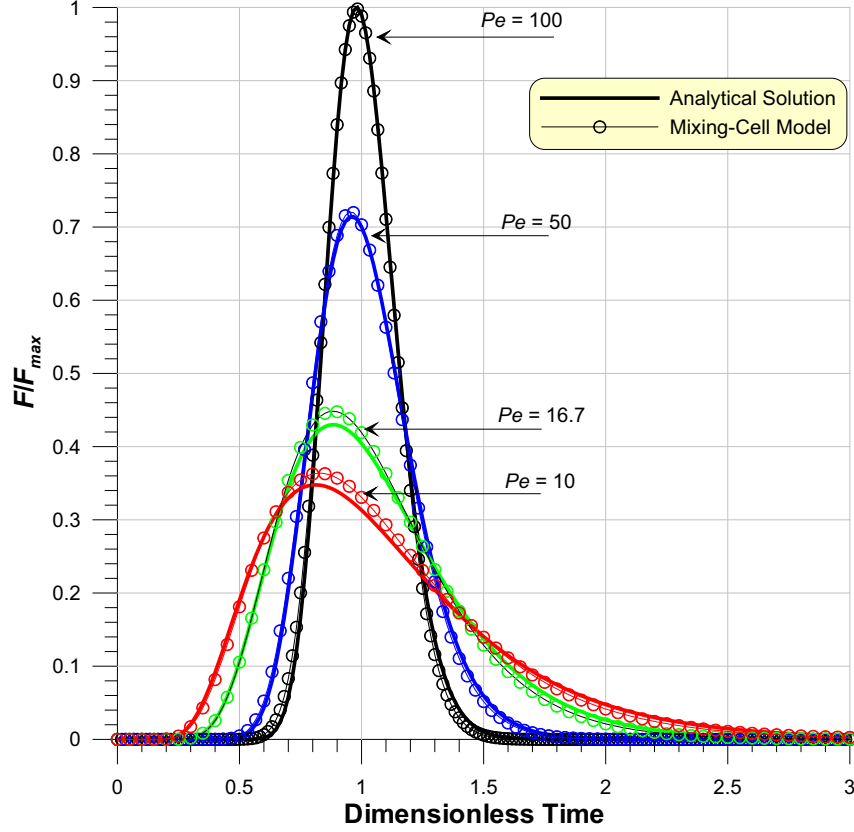
Figure 2. Normalized solute flux versus dimensionless time for various Peclet numbers for the mixing-cell model with interchange and an analytical solution to the advection-dispersion equation for flux. Solute fluxes are normalized to the peak advection dispersion equation flux for a *Pe* of 100. Dimensionless time is given by *t/tt* where *tt= Zθ/q*.

4.   MODEL DISCRETIZATION AND TRANSIENT WATER FLUX

Under steady-state infiltration conditions, Equation 7 is unnecessary, and solute transport calculations only require an infiltration rate and a corresponding moisture content, which may be obtained from an appropriate moisture characteristic curve. Under transient infiltration conditions, water flux is spatially and temporally variable, and Equation 7 must be solved for as a function of time for each mixing cell defining the unsaturated zone. Rood (2004) describes a method to estimate the number of mixing cells necessary to simulate a wetting front. His method is summarized in this section.

Figure 3 illustrates the conceptual model Rood (2004) used to examine transient water fluxes with the mixing-cell model. The model domain is discretized into *n*, equal-thickness mixing cells and initialized to a constant water flux, q_o. The water flux entering the top of the column is then increased to a new value, q_n, at the start of the simulation and continues for a time, t_p, after which, the water flux returns to its initial value, q_o. The water flux out the bottom of the domain (at $z = Z$ and $i = n$ in Figure 3) is the primary endpoint that was examined.

12
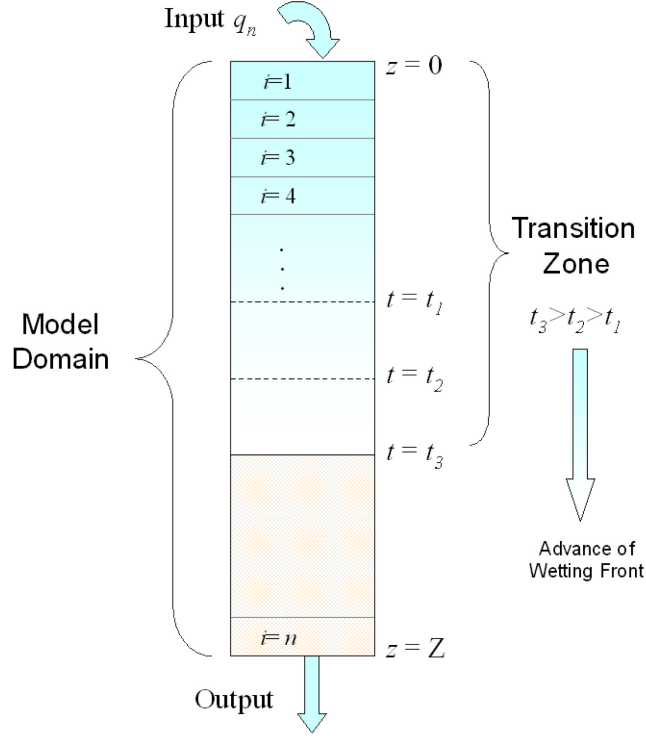
Figure 3. Conceptual model for examination of transient water flux. The mixing-cell model is composed of n equal-dimension cells and initial moisture contents correspond to an initial infiltration rate of q_o. A new water flux (q_n, where $q_n > q_o$) is applied to the top of the domain at $t > 0$ for a time, tp. The downward advance of a wetting front created by the new water flux is shown at three times (t_1, t_2, t_3).

Gravitationally-driven flow within a cell is the primary assumption underlying the mixing-cell water flow model, although capillary gradients are considered implicitly. A moisture profile is a function of both gravitationally-driven flow and capillary gradients. Capillary gradients tend to dampen the effects of pure gravitational flow (i.e., pure translation of the wetting front) and result in a more disperse wetting front.

Consider the conceptual model illustrated in Figure 3, where q is described by a step-function, $q(0) = q_o$, $q(t>0) = q_n$, $q(\infty) = q_n$, and $q_n < K_{sat}$. The asymptotic water flux at any point in the model domain behind the wetting front (designated the transition zone in Figure 3) is q_n which is equivalent to $K(\theta_n)$, where θ_n is the new moisture content corresponding to the new water flux, q_n. The asymptotic water flux at the wetting-front boundary is $K(\theta_n) - K(\theta_o)$ and the speed of the advancing wetting front is therefore (Philip 1957 as given in Smith et al., 2002; Hillel 1998):

$$u_{wf} = \frac{K(\theta_n) - K(\theta_o)}{\theta_n - \theta_o} \tag{30}$$

where u_{wf} is the velocity of the wetting front (L T^{-1}), θ_o and $K(\theta_o)$ are the initial moisture content and hydraulic conductivity respectively of the soil column that corresponds to a water flux of q_o, and θ_n and $K(\theta_n)$ are the new moisture content and hydraulic conductivity respectively of the soil column that corresponds to the new water flux, q_n. The wetting front time-of-arrival at $z = Z$ is given by:

13

$$t_{wf} = \frac{Z}{u_{wf}} \tag{31}$$

where t_{wf} is the wetting-front arrival time (T). In a heterogeneous unsaturated zone composed of m layers of different materials, the wetting-front travel time can be approximated as:

$$t_{wf} \approx \sum_{k=1}^{m} \frac{Z_k}{u_{wf_k}} \tag{32}$$

where m is the number of different layers, Z_k is the layer thickness (L), and k is the index for the layer. Equation 31 and 32 provide the arrival time of a wetting front provided $t_p > t_{wf}$. Under these conditions ($t_p > t_{wf}$), the water flux at Z approaches an equilibrium value equivalent to q_n. When $t_p < t_{wf}$, the water flux at Z is less than q_n and the arrival time of the wetting front is less than t_{wf} because the characteristic wave velocity overtakes the shock velocity of the wetting front (Smith et al., 2002).

Capillary forces may be characterized in terms of the hydraulic diffusivity, which is used to convert the two-variable (pressure and moisture) based Richard's equation into a single-variable (moisture) version. The hydraulic diffusivity is given by (Hillel 1998):

$$D_h(\theta) = K(\theta) \frac{d\psi}{d\theta} \tag{33}$$

where

$D_h(\theta) = $ the hydraulic diffusivity of the medium for a given moisture content ($L^2\ T^{-1}$)

$K(\theta) = $ the hydraulic conductivity of the medium at the moisture content, θ.

The shape of an advancing wetting front is influenced by the initial hydraulic diffusivity (i.e., the hydraulic diffusivity at $q = q_o$) of the medium. Materials with relatively high D_h values like clays will exhibit more diffuse wetting fronts while materials like sand, with relatively low D_h values exhibit sharp wetting fronts. After passage of the wetting front, capillary forces are not as important because the capillary gradient ($\partial\psi/\partial z$) relaxes and is zero under steady-state conditions. The effects of capillary forces on the shape of the water flux profile are implicitly accounted for in the mixing-cell model by discretization of the model domain. That is, the number of cells used in a mixing-cell model simulation affects the shape of the wetting front as it exits the model domain.

Figure 4 illustrates the sensitivity of the number of equal-thickness mixing cells on the shape of the wetting front at $z = Z$ for a homogeneous and heterogeneous unsaturated zone. In all cases, the maximum water flux achieved during the simulation was q_n. For comparison, the same conditions were simulated with the numerical flow and transport code, HYDRUS (Simunek et al., 1999). HYDRUS is a finite-element approximation to the nonlinear partial differential equation (Richard's equation) for unsaturated flow and coupled solute transport. The HYDRUS simulation shows a near step-function of water flux with respect to time as the advancing wetting-front exits the model domain at $z = Z$. The mixing-cell model produces a curve that approaches the step function with increasing number of cells. In general, discretization of the model domain into more cells results in a sharper wetting front.

14
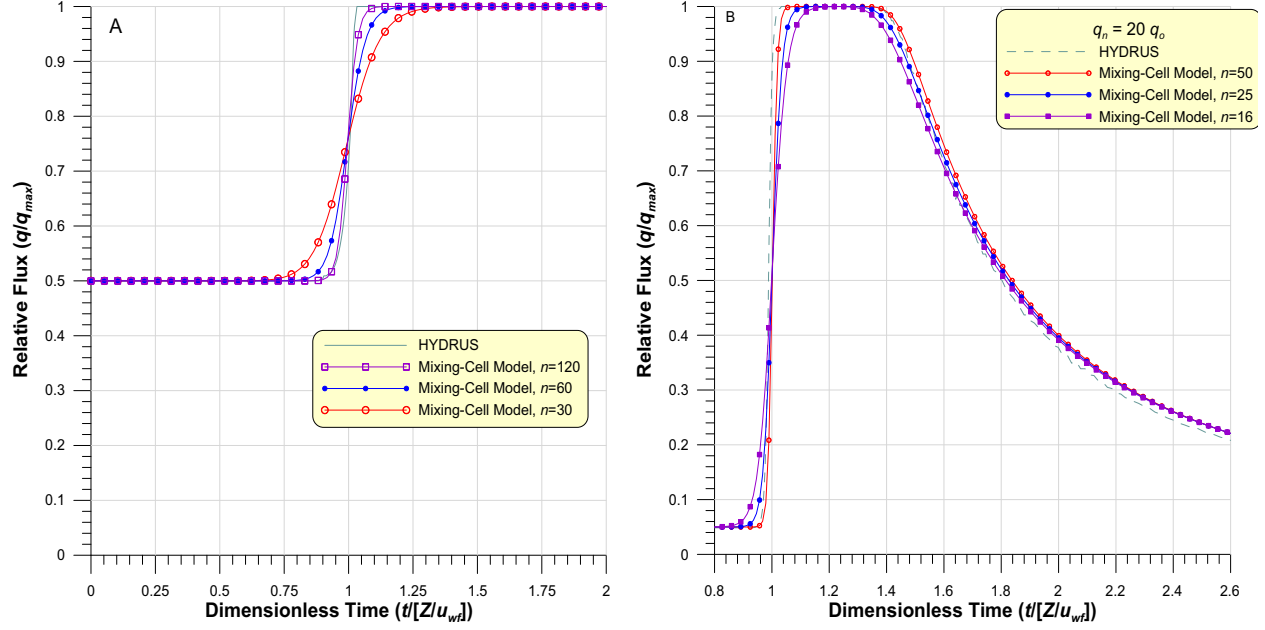
Figure 4. Relative water flux at z = Z as a function of dimensionless time for various numbers of mixing cells. In the left graph (A), tp = ∞ whereas in right graph (B), tp = 1.16 twf. For comparison, the same conditions were simulated with HYDRUS. Time has been normalized to the wetting front arrival time. The variable n is the number of equal-dimension mixing cells in the simulation. The left graph (A) is for a heterogeneous (i.e., layered) unsaturated zone whereas the right graph (B) is for a homogeneous unsaturated zone.

The relationship between the number of mixing cells and the water-flux versus time profile at $z = Z$ was established empirically by fitting the mixing-cell model temporal water-flux profile to same quantity determined by simulations with HYDRUS (Figure 5). An empirical relationship was established between a dimensionless variable, similar in form to the Peclet number, and the number of mixing cells required to adequately simulate the water-flux versus time profile generated by HYDRUS. The dimensionless variable (designated φ) relates the wetting-front velocity and distance traveled to the initial hydraulic diffusivity and is given by:

$$\varphi = \frac{Z \, u_{wf}}{\left| D_{ho} \right|} \tag{34}$$

where

D_{ho} = the hydraulic diffusivity at the initial moisture content of the unsaturated zone ($L^2 \, T^{-1}$).
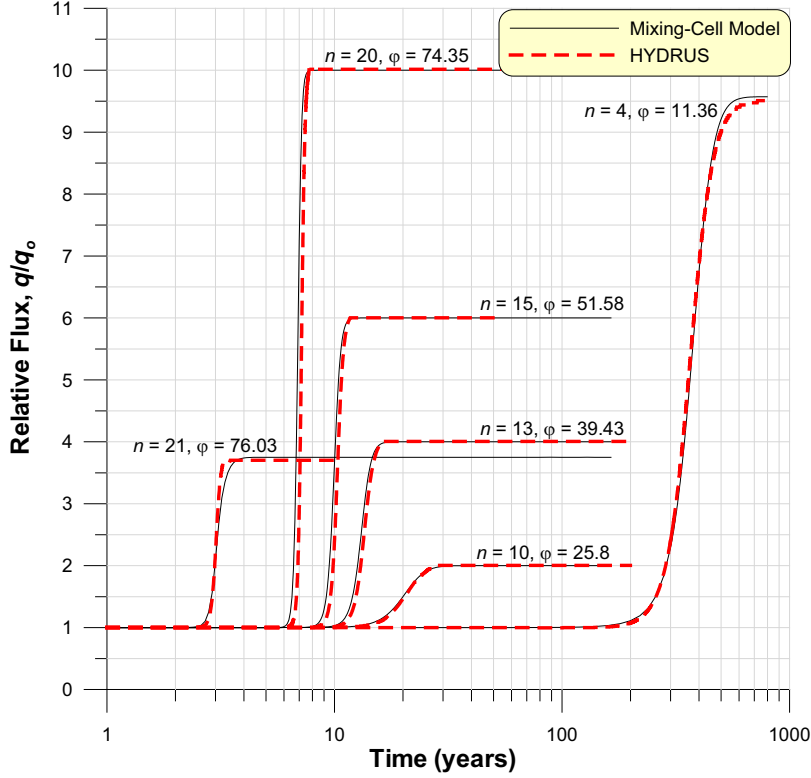
Figure 5. Relative water flux versus time for HYDRUS and mixing-cell model simulations involving a 30-m clay unsaturated zone. These data were used to develop the regression given in Equation 35.

The relationship between n and φ is based on the assumptions described earlier in Figure 3. The hydraulic diffusivity was calculated from the van Genuchten θ-ψ curves at the specified initial water flux ($q_o = K(\theta_o)$). The number of mixing cells required to match the HYDRUS results were then fit to φ for various lithologies, initial conditions, and water fluxes (Table 2 and Figure 6). An adequate match was achieved when the slope of the water flux versus time curve at $z = Z$ and $t \approx t_{wf}$ for the two models were visually matched. A linear and polynomial fit between n and φ yielded the following equations ($r^2 = 0.997$):

$$n = 0.229\varphi + 3.6 \qquad 30 < \varphi < 550$$
$$n = 1.89 + 0.1037\varphi + 0.00814\varphi^2 \qquad 3 < \varphi \leq 30$$

(35)

where n is the number of cells rounded to the nearest whole number. In general, φ values greater than about 100 for a 30-m model domain resulted in a near square-wave shape of the water-flux profile as it passes the lower boundary of the model domain at $z = Z$. For a heterogeneous (layered) environment, the number of cells for each layer may be determined independently for each layer and used directly, or alternatively, summed and divided into the total unsaturated thickness to yield single mixing-cell thickness that can be applied to all layers. For φ values greater than 550, Equation 35 may estimate an unreasonable number of cells for a model simulation, and the wetting front can be approximated with fewer cells.

16

Table 2. Model data used to develop regression between n and φ. All mixing cells were of equal thickness.

| Lithology	q_o (m yr^{-1})	q_n (m yr^{-1})	θ_o	θ_n	D_{ho} (m^2 yr^{-1})	T (m)	t_{wf} (years)	φ	n
clay	0.010	0.020	0.3474	0.3539	1.7723	3.0	19.680	25.804	10
clay	0.010	0.040	0.3474	0.3602	1.7723	2.3077	12.880	39.427	13
clay	0.010	0.060	0.3474	0.3638	1.7723	2.0	9.846	51.576	15
clay	0.010	0.100	0.3474	0.3679	1.7723	1.5	6.830	74.352	20
clay	0.040	0.150	0.3602	0.3708	4.1256	1.429	2.869	76.034	21
clay	2.089×10^{-4}	0.002	0.3090	0.3311	0.2134	7.5	371.338	11.356	4
clay	0.010	0.050	0.3474	0.3623	1.7723	2.40	22.20	91.46	25
clay	2.089×10^{-4}	4.96×10^{-4}	0.3089	0.3173	0.2134	10	873.6	4.827	3
clay	2.089×10^{-4}	2.287×10^{-4}	0.3089	0.3098	0.2134	15	1318	3.199	2
sandy clay loam	0.010	0.011	0.1997	0.2014	0.3323	1.6667	41.129	61.488	18
sandy clay loam	0.010	0.015	0.1997	0.2058	0.3323	1.4286	36.600	69.097	21
sandy clay loam	0.010	0.020	0.1997	0.2104	0.3323	1.2500	32.100	78.783	24
sandy clay loam	0.010	0.040	0.1997	0.2223	0.3323	1.0000	22.600	111.900	30
sandy clay loam	0.010	0.060	0.1997	0.2297	0.3323	0.8330	18.000	140.496	36
sandy clay loam	0.010	0.100	0.1997	0.2397	0.3323	0.6383	13.333	189.670	47
sandy clay loam	0.010	0.200	0.1997	0.2544	0.3323	0.4286	8.637	292.808	70
sand	0.010	0.020	0.0619	0.0654	0.1570	0.2400	10.452	548.454	125
sand	0.00209	0.004	0.0561	0.0582	0.0643	0.2857	33.136	422.187	105
sand	0.010	0.012	0.0619	0.06278	0.1570	0.2777	6.645	215.67	54
sand	0.00209	0.002386	0.0561	0.0565	0.06433	0.333	20.45	171	45
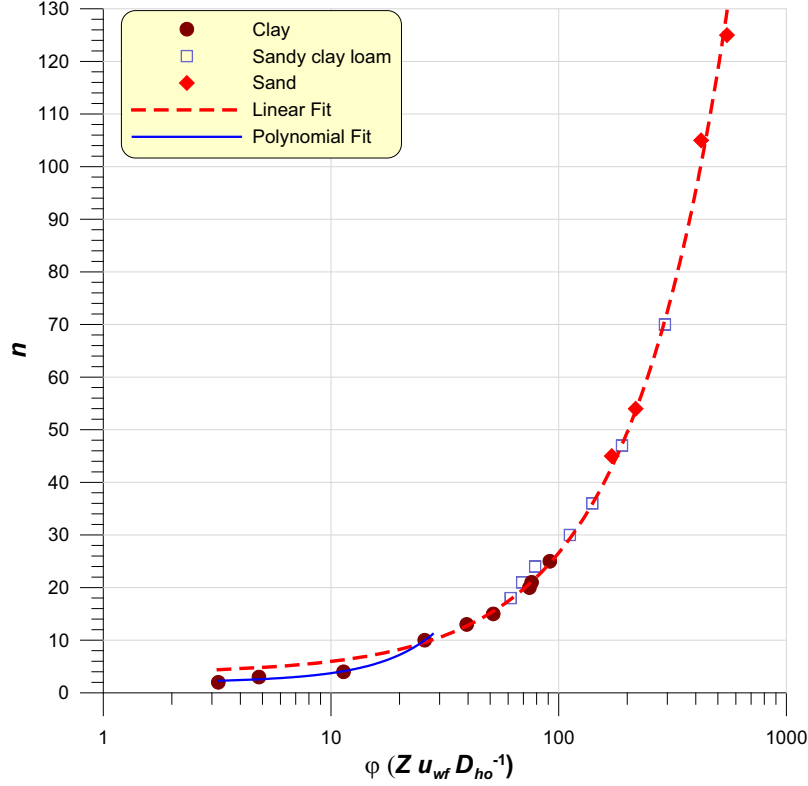
Figure 6. The number of mixing cells (n) versus the dimensionless variable φ required to approximate the behavior of the water-flux profile at $z = Z$. The abscissa was plotted in log-scale so as to better visualize the points for $\varphi < 100$.

Equation 35 provides guidance on the number of mixing cells to use in a model simulation under the extreme situation of a step increase in the input water flux. Ultimately, model discretization should consider the assessment question and overall uncertainty accompanying a contaminant fate and transport estimate in the unsaturated zone. That is, how sensitive is the assessment question to model discretization? As shown in Figure 4A and 4B, adequate solutions to the water flow problem are obtained with relatively few mixing cells for an assessment question involving the mean wetting-front travel time and the maximum water flux.

4.1 Coupling Water Flow and Solute Transport

The transport model requires the water flux as a function of time for each mixing cell. However, the number of mixing cells required to simulate transient flow behavior may not match the number of cells required to simulate dispersion effects. In most cases, the number of cells required to simulate transient flow behavior exceeds the number of cells required to simulate dispersive effects. In these cases, the mixing-cell model with interchange is used because dispersive effects can be simulated through cell interchange. In some cases, the number of mixing cells required to simulate transient flow behavior is less than the number of cells required to simulate dispersive processes. For example, clays exhibit a relatively high hydraulic diffusivity resulting in diffuse infiltration fronts and therefore require relatively few mixing cells to simulate transient flow. In these cases, the mixing-cell model without interchange can be used. The water flux assigned to each transport cell is based on the water flux in the cell that occupies the same space as the transport cell.

5.   NUMERICAL SOLUTION

The numerical solution uses a fifth-order Runge-Kutta algorithm coupled with adaptive stepsize-control described in Press et al. (1992). The adaptive stepsize algorithm adjusts the time step according to a user-provided tolerance of the local truncation error. The time step shortens when integrating the stiffer portions of the derivative function and lengthens when integrating the smoother portions. The fifth-order algorithm described in Press et al. (1992) has an embedded forth-order method that is used for error estimation. Beginning with an initial value of the state variable, y_n at time t_n, the general form of the fifth-order Runge-Kutta method is (Press et al. 1992):

$$k_1 = h f(t_n, y_n)$$
$$k_2 = h f(t_n + a_2 h, y_n + b_{21} k_1)$$
$$\ldots \tag{36}$$
$$k_6 = h f(t_n + a_6 h, y_n + b_{61} k_1 + \ldots + b_{65} k_5)$$
$$y_{n+1} = y_n + c_1 k_1 + c_2 k_2 + c_3 k_3 + c_4 k_4 + c_5 k_5 + c_6 k_6 + O(h^6)$$

where

y_n	=	value of the state (dependent) variable at the nth time step
t_n	=	value of time (independent variable) at the nth time step (Note: $t_{n+1} \equiv t_n + h$)
$f(t_n, y_n)$	=	right-hand side of the derivative
h	=	value of time in the time step
n	=	time step number
$O(h^6)$	=	the error correction term
a, b, c	=	Cash-Karp parameters for the embedded Runge-Kutta method.

The embedded forth-order method is:

$$y_{n+1}^* = y_n + c_1^* k_1 + c_2^* k_2 + c_3^* k_3 + c_4^* k_4 + c_5^* k_5 + c_6^* k_6 + O(h^5) \tag{37}$$

and the error (Δ) estimate is:

$$\Delta \equiv y_{n+1} - y_{n+1}^* = \sum_{i=1}^{n} (c_i - c_i^*) k_i \,. \tag{38}$$

The Cash-Karp parameters are provided in Press et al. (1992). The overall error is scaled to a user-provided tolerance level which is also used to estimate the starting time step of the next step. The desired accuracy of the solution for the *ith* equation (Δ_o) is estimated by:

$$\Delta_o = eps \times \left(|y_i| + \left| h \times \frac{dy_i}{dt} \right| \right) \tag{39}$$

where *eps* is the user-provided tolerance level. The optimal time step (h_o) to achieve the desired accuracy is then computed based on the error estimate from the actual time step taken (h_1):

$$h_o = \begin{cases} S\,h_1 \left| \dfrac{\Delta_o}{\Delta_1} \right|^{0.20} & \Delta_o \geq \Delta_1 \\[2em] S\,h_1 \left| \dfrac{\Delta_o}{\Delta_1} \right|^{0.25} & \Delta_o < \Delta_1 \end{cases} \tag{40}$$

where

Δ_1 = the error estimate for the time step, h_1

S = a "safety factor" that is a few percent smaller than unity.

The exponents 0.20, and 0.25 essentially grow and shrink the time step depending on the ratio of Δ_o/Δ_1.

The code uses a linear interpolation routine to interpolate tabulated values of water flux and contaminant flux as a function of time. If radionuclides are modeled, radionuclide inventories and fluxes are entered in the activity units of Curies or Becquerels. Activities are converted to mass units (i.e., grams) for all computations, and are then converted back to activity units before output. Activity is converted to mass using

$$Q_{mass} = \frac{Q_{activity}\,(APD)\,MW}{\lambda\,N_A} \tag{41}$$

where

MW = molecular weight (g mol^{-1})

N_A = Avogadro's number (6.023×10^{23} atoms mol^{-1})

APD = disintegrations per second (dps) per activity unit (3.7×10^{10} dps/Ci, or 1 dps/Bq)

Q_{mass} = number of atoms of a radionuclide (atoms)

$Q_{activity}$ = activity of a radionuclide (Ci or Bq)

λ = decay rate constant (s^{-1}).

6.   CODE IMPLEMENTATION

The MCM model was coded into two FORTRAN programs; one to solve for water fluxes in each cell (MCMF), and the other to solve for solute transport (MCMT). The water flow code is only required if transient infiltration is considered. For transient infiltration problems, the MCMF (water flow code) is run first followed by the solute transport code (MCMT). The output from MCMF is stored either in an ASCII or binary file that is later read by MCMT. Input to both codes is provided through ASCII files whose construction is described later in this section. Both programs perform the same general tasks that include: (1) read user input from ASCII input files, (2) compute unit conversions and internal parameter values, (3) solve the ODEs, and (4) writes output to ASCII or binary files. Input to both MCMF and MCMT is through several ASCII files. The primary input file is termed the parameter definition file and defines model options, cell properties, contaminant properties (MCMT only), and initial inventories of water or contaminant in each cell. The parameter definition file also identifies auxiliary files that may be required. These files include the MCMF water flux file, name of the output file, and release rate history file. Both codes use the same general input file structure, which consists of a series of records that are read in sequential order.

Each code writes a list file (MCMF.LST and MCMT.LST) that: (1) identifies the version of the code, (2) echoes back all input data, (3) presents computed intermediate parameter values, and (4) summarizes time steps taken, execution time, and mass balance. The primary MCMF output file contains the water fluxes, moisture content, and water inventory as a function of time for each cell. The primary MCMT output files contains contaminant inventories, pore water concentrations, and contaminant fluxes as a function of time for each cell. MCMF generates an additional file that contains water fluxes as a function of time for each cell. This file is formatted to be read by MCMT. The primary MCMF output file and water flux file can be written in either binary or ASCII format. A binary file is recommended if the number of cells in the simulation exceed about 60. A utility program has also been written to extract time histories and profiles from the MCMF and MCMT primary output files. MCMT also produces a file for each contaminant (or decay chain member) of contaminant flux leaving the base of the model domain. This is file is useful for quick examination of contaminant fluxes and may be used as input for an aquifer transport model.

Although the model formulation does not specify the units of calculation, both MCMF and MCMT have adhered to convenient units for computations. Parameter units are identified in the input file structure in the next section.

6.1   Input File Structures for MCMF

File structure for the MCMF parameter definition file is described in Table 3. All input files are free-form ASCII and may be created and edited in any standard text editor. Each record in the file represents one or more lines of input. Records must be placed in ascending order and the order of each of variable comprising the record must be in the same order as prescribed in Table 3. Blank lines between records are permitted. The code ignores lines where a dollar sign ($) is placed in the first column, thereby facilitating comments in the file. Comments may also be placed after the last value present on a line. Suggested default values (when applicable) are put in the description column of Table 3 in parentheses. Further explanation of some of the code variables follows.

Table 3. Format for the MCMF parameter definition file.

Record	Code Variable	Type/Format	Units	Description
1	Title	CHAR/A80		Title of run
2	fileout	CHAR/A80		Name of the water flux file that will be read by MCMT
3	fileppt	CHAR/A80		File containing the net water flux into the first cell as a function of time
4	eps	REAL/*		Desired accuracy of solution (1×10^{-6})
4	h1	REAL/*	yr	Beginning time step (0.0001 yr)
4	hmin	REAL/*	yr	Minimum time step (1×10^{-60} yr)
5	mlayer	INT/*		Number of cells in the simulation ($250 \geq mlayer \geq 1$)
5	nmat	INT/*		Number of material types (must be $\leq mlayer$)
5	nkt	INT/*		Number of points to store that describe hydraulic conductivity curve as a function of moisture content (100)
5	qmax	REAL/*	m yr^{-1}	Maximum infiltration rate for simulation
5	qmin	REAL/*	m yr^{-1}	Minimum infiltration for simulation
5	iflag	INT/*		Flag variable for initial moisture option: (0) Initial moisture content based on first record in fileppt; (1) user will provide initial moisture contents.
5	abin	CHAR/*		Flag variable for ASCII or binary output: (A) for ASCII output or, (B) for binary output. All output is written in the specified format (ASCII or binary) except for the .LST file, which is always in ASCII format.

NOTE: Record 6 is read only if iflag = 1

Record	Code Variable	Type/Format	Units	Description
6	theta(i)	REAL/*	m^3 m^{-3}	Initial moisture content in each cell. Twenty values are read per line until all cells are defined.

NOTE: Record 7, 8, and 9 define the cell property range and the cell properties. These records are repeated nmat number of times. Cells must be defined in ascending order

Record	Code Variable	Type/Format	Units	Description
7	h	INT/*		Beginning cell number to define cell properties (inclusive).
7	j	INT/*		Ending cell number to define cell properties (inclusive).

NOTE: Cell properties in records 8 and 9 for each material type apply to cells h through j (inclusive)

Record	Code Variable	Type/Format	Units	Description
8	thick	REAL/*	m	Thickness of all cells in the range from h to j.
9	sk(i)	REAL/*	m yr^{-1}	Saturated hydraulic conductivity of all cells in the range from h to j.
9	ths(i)	REAL/*	m^{-3} m^{-3}	Saturated porosity of all cells in the range from h to j.
9	thr(i)	REAL/*	m^{-3} m^{-3}	Residual moisture content of all cells in the range from h to j.

Table 3. (continued).

Record	Code Variable	Type/Format	Units	Description
9	alpha(i)	REAL/*	m^{-1}	van Genuchten fitting parameter, α for all cells in the range from h to j.
9	rn(i)	REAL/*		van Genuchten fitting parameter n for all cells in the range from h to j.
10	ntimes	INT/*		Number of output time periods (1)
NOTE: Record 11 is repeated for each output time period. Total number of output time periods = ntimes				
11	t1(k)	REAL/*	yrs	Begin time of output time k
11	t2(k)	REAL/*	yrs	End time of output time k
11	tp(k)	REAL/*	yrs	Print step of output time k
12	tmax	REAL/*	yrs	Maximum time of simulation
13	ncout	INT/*		Number of cells to produce time histories of water flux (0, maximum value of 10)
NOTE: Record 14 read only if ncout>0				
14	ncoutput(k)	INT/*		Cell numbers for each time history (**ncout** number of values read)

6.1.1 Record 2 (fileout)

The fileout variable stores the name of the water flux file (and complete or relative path to the file) that will later be read by MCMT. This file contains the water flux in each cell as a function of time and can either be binary or ASCII depending on the value of the variable **abin**.

6.1.2 Record 3 (fileppt)

The **fileppt** variable stores the name of the file (and complete or relative path to the file) containing the net infiltration rate as a function of time that is fed into the first (uppermost) cell of the model. The structure for the file is described in Table 4.

Table 4. Format of the water flux file for MCMF.

Line Number	Code Variable	Description
1	junk	Column headers and comments (discarded)
2 to n+1[a]	precip(k,1)	Time in years from the start of the simulation for the kth record
2 to n+1[a]	precip(k,2)	Water flux (m y^{-1}) entering the first compartment of the model domain for the kth time record

a. n is the number of time and water flux records. A minimum of two records are required.

6.1.3 Record 4 (eps, h1, hmin)

The code variables, **eps**, **h1**, and **hmin** all control time stepping and iteration of the Runge-Kutta solver. The code variable **eps** is defined in terms of Equation 39 and has a default value of 10^{-6}. The variable **h1** defines the initial time step to be taken. A relatively large value (say 1 year) can result in faster simulation times, but a user runs the risk of an inaccurate solution. A default value of 0.0001 yr is

recommended. The code variable, **hmin** defines the minimum time step to be taken. The code will abort if the estimated time step is less than **hmin**. If this occurs, the user should set **hmin** to a smaller value step.

6.1.4 Record 5 (mlayer, nmat, nkt, qmax, qmin, iflag, and abin)

The variable **mlayer** defines the total number of cells to discretize the model domain into. The variable **nmat** defines the number of material-type definitions that will be used to assign material properties to each cell. Materials are defined in increasing order, starting with the cell nearest the ground surface and ending with the cell at the aquifer-unsaturated zone interface (see Figure 1 and 3). For example, if a 50 m thick unsaturated zone is composed (from top to bottom) of 20 m of sandstone, 10 m of clay, and 20 m of sandstone, then **nmat** is set to **3**, because there are three material definitions required to define the unsaturated zone. Material properties are defined in records 7, 8, and 9.

In MCMF, the moisture characteristic curve, (which is the relationship between θ and K and given by Equation 8 and 9), is computed first and stored in an array. Evaluation of the θ-K function is then performed by linear interpolation. The number of points that comprise the tabulated function is specified by the code variable, **nkt**. Naturally, one would only want to compute the function over the range of hydraulic conductivities expected to be encountered. The range of hydraulic conductivities to compute the θ-K function over is specified by the code variables **qmin** (the minimum value of K) and **qmax** (maximum value of K). Inaccurate interpolation can occur if too few points are specified for the range of **qmin** and **qmax**, however, this also depends largely on the shape of the θ-K curve in the region bounded by **qmin** and **qmax**. The MCMF list file prints the θ-K values that are used for interpolation. The user should be aware of the shape of the θ-K curve in the region bounded by **qmin** and **qmax** and adjust **nkt** accordingly.

The **iflag** variable selects whether the user provides the initial moisture profile or the initial moisture profile is defined by the first record in the net infiltration file (fileppt). An initial moisture profile is required if **iflag**=1. Otherwise, if **iflag**=0, then the initial moisture content is calculated from the first record in the net infiltration file. If **iflag**=1, then the initial moisture content is read in Record 6.

The **abin** variable defines whether an ASCII (**abin**=A) or binary (**abin**=B) output file is written. A binary file is recommended if the number of cells exceeds about 60. The corresponding value of **abin** in the MCMT parameter definition file must also be the same. The **abin** variable should always be in upper case.

6.1.5 Record 6 (theta)

The code variable **theta** is an array that holds the current moisture content in each cell. The initial moisture content values are read from the parameter definition file in Record 6 if **iflag**=1. Twenty values are read per line until all cells are defined. Values are assigned in ascending order. That is, the first **theta** value read is assigned to cell 1 (uppermost cell), the next value read is assigned to cell 2, and so on until the last (lowermost) cell is assigned the last value provided. For example, if a problem had a total of 43 cells, and **theta** was 0.2 for the first 10 cells, 0.1 for the next 30 cells, and 0.3 for the last three cells, then the input file for the 6th record would look like

```
0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.2 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1  ! cells 1-20
0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1  ! cells 21-40
0.3 0.3 0.3                                                                      ! cells 41-43
```

If **iflag** is zero, then the 6th record is omitted from the parameter definition file.

24

6.1.6   Records 7, 8, and 9 (h, j thick, sk ths, thr, alpha, rn)

The code variables **h** and **j** define the beginning and ending cells (inclusive) to include in a material definition. Each material is defined in terms of its thickness and hydraulic properties (saturated hydraulic conductivity, porosity, etc.) as defined in the variables **thick**, **sk**, **ths**, **thr**, **alpha**, and **rn.** These properties are read in records 8 and 9 and are repeated for each material type. For example, suppose that a 45 m thick unsaturated zone is composed of (from top to bottom) 10 m of sandy clay loam, 15 m of sandy clay, and 20 m of sand. The code variable, **nmat** should be set to 3. Assuming 45 cells of 1 m thickness and the hydraulic properties in Table 1, records 7, 8, and 9 would then be:

```
$ Material definition for material type #1 - sandy clay loam
1  10                           [Record 7 h,j]
1.00                            [Record 8 thick]
114.76 0.39 0.10 5.9 1.48       [Record 9 sk ths thr alpha rn]
$ Material definition for material type #2 - sandy clay
11 25                           [Record 7 h,j]
1.00                            [Record 8 thick]
10.51 0.38 0.10 2.7 1.23        [Record 9 sk ths thr alpha rn]
$ Material definition for material type #3 - sand
26 45                           [Record 7 h,j]
1.00                            [Record 8 thick]
2601.72 0.43 0.045 14.5 2.68    [Record 9 sk ths thr alpha rn]
```

Note that records 7, 8, and 9 are repeated **nmat** number of times (**nmat**=3). Comments are placed on lines that begin with a dollar sign ($), and comments may be placed after the last value on each line.

6.1.7   Records 10, 11, and 12 (ntimes, t1, t2, tp, and tmax)

The code variable, **ntimes** defines how many time-history output periods are printed in **fileout**. Each output period is defined by a beginning time (**t1**), an ending time (**t2**), and a print intervals (**tp**). In this way, different time resolutions can be applied to various time periods of the simulation. Record 11 is repeated **ntimes**. It is important to apply proper time resolution for transient flows because these data are used by MCMT to estimate the time-variable Darcy velocity and moisture content in each cell. Suppose for example that one wants to capture the transient water fluxes during the first 100 years of a simulation, and extend the simulation out to 1000 years. A possible choice for records 10 and 11 would be:

```
3                              [Record 10 ntimes]
$ Time period 1, 0-100 years print every year
0.0  100.0  1.0                [Record 11 t1, t2, tp]
$ Time period 2, from 110 to 500 years print every 10th year
110.0   500.0  10.0.           [Record 11 t1 t2 tp]
$ Time period 3, from 525 to 1000 years print every 25th year
525.0   1000.0  25.0.          [Record 11 t1 t2 tp]
```

The code variable, **tmax** is the maximum time of the simulation. The water flow equations are not actually solved at **tmax**, rather the water inventory and flux at **t2**(**ntimes**) values are printed to the output file at the time, **tmax**. This variable should be greater than **t2**(**ntimes**) and is used to extend the simulation in time once steady-state conditions are achieved.

6.1.8   Records 13 and 14 (ncout, ncoutput)

The code variables **ncout** and **ncoutput** are used to define cells for which time histories are output in separate files. The variable **ncout** defines how many cells to output time histories for (maximum of 10), and the variable **ncoutput** defines an array of cell numbers for which to provide water flux time histories. Cell 1 is defined as the uppermost cell near at the top of the model domain. Cell numbers should

be separated by spaces or commas. For example, suppose a user wants to output water flux histories for cells 5, 10, 15, and 20. Records 13 and 14 would read:

```
4                                    [Record 13 ncout]
5 10 15 20                           [Record 14 ncoutput]
```

Water fluxes are written to predefined file names in the default working directory and named qXX.dat where XX is the sequential number of the cell read in the array **ncoutput**. Using the previous example, the code would write the flux histories to the files q01.dat, q02.dat, q03.dat, and q04.dat.

6.1.9   Water Flux File

Water fluxes entering the top of the model domain are provided to MCMF via an external ASCII file. The water flux file is specified in the parameter definition file (Record 3) and the name of the file is stored in the code variable, **fileppt**. The file can be any name the user chooses. The file format is described in Table 4.

6.2   Code Execution and MCMF Output Files and Utilities

Execution of the MCMF code is performed on the command line by typing:

[*path*]MCMF [*parameter definition file*]

where *path* is the full or relative path to the MCMF executable from the current operating directory, and *parameter definition file* is the name of the parameter definition file (Table 3). If the parameter definition file is left off, then MCMF will look for the default parameter definition file named MCMF.PAR in the current working directory. If the default parameter definition file is not found, or the user fails to provide a valid parameter definition file, the code will abort.

MCMF produces three output files: (1) the water flux output file read by MCMT and specified by record 2 in the parameter definition file, (2) the general output file (MCMF.OUT), and (3) the list file (MCMF.LST). The general output file and list file have hardwired file names and are written in the current operating directory each time MCMF is executed. The MCMF.OUT file contains the time histories of water inventory, moisture content, and water flux for each cell in the simulation. The MCMF.LST file contains the model input data, calculated intermediate values, the number of converged and unconverged time steps, code execution time, and mass balance information. The MCMF.LST file is always written in ASCII whereas the MCMF.OUT file is written in binary if the code variable **abin** is set to "B". A utility program (MCMFPRT) was written to allow access to the binary (or ASCII) data stored in the MCMF.OUT file. The MCMFPRT utility is executed by typing on the command line:

[*path*]MCMFPRT [*parameter definition file*]

where *path* is the full or relative path to the MCMFPRT executable from the current operating directory, followed by the name of the parameter definition file. If the parameter definition file is left off, then MCMFPRT will look for the default parameter definition file (MCMFPRT.PAR) in the current working directory. If the default parameter definition file is not found, or the user fails to provide a valid parameter definition file name, the code will abort. The format for the MCMFPRT parameter definition file is described in Table 5.

Table 5. Format for the MCMFPRT parameter definition file.

Record	Code Variable	Type/Format	Description
1	Title	CHAR/A80	Title of run
2	filedat	CHAR/A80	MCMF general output file (MCMF.OUT)
3	abin	CHAR/*	Flag variable for ASCII or binary output: (A) for ASCII output or, (B) for binary output.
3	aqnt	CHAR/*	Quantity to extract: M = moisture content, I = water inventory, Q = water flux
3	pfix	CHAR*4/*	A four character prefix to identify each output file name.
4	nout	INT/*	Number of cells to output time histories (maximum = 50)
4	tout	INT/*	Number of times to output spatial profiles (maximum = 50)
4	cf	REAL/*	User-provided conversion factor to multiply output by (1.0)
5	noutput(i)	INT/*	The cell numbers for each of the **nout** time histories. All values are read from one line and each value is separated by a space or comma. If **nout** is zero, this record should be blank.
6	toutput(i)	REAL/*	The time of each of the **tout** spatial profiles. All values are read from one line and each value is separated by a space or comma. If **tout** is zero, this record should be blank.

Output files for MCMFPRT are defined by the concatenation of a four character prefix (variable **pfix** in Record 3), a file sequence number, and a ".dat" file extension. The sequence number is a concatenation of the output quantity symbol (M for moisture content, I for water inventory, or Q for water flux), a time output (T) or profile output (P) symbol, and a sequence number. For example, if moisture time histories are requested for two different cells and the user defines the **pfix** variable as "test", then two files will be created. The file for the first cell requested will be called testMT001.dat and the file for the second cell requested will be testMT002.dat.

6.3 Input File Structures for MCMT

File structure for the MCMT parameter definition file is similar to the MCMF and is described in Tables 6. All MCMT input files are free-form ASCII, with the exception of binary water flux files generated by MCMF. Each record in the parameter definition file represents one or more lines of input. Records must be placed in ascending order and the order of each of variable comprising the record must be in the same order as prescribed in Table 6. Blank lines between records are permitted. The code ignores lines where a dollar sign ($) in placed in the first column, thereby facilitating comments in the file. Comments may also be placed after the last value on a line. Suggested default values (where applicable) are put in the description column of Table 6 in parentheses. Further explanation of some of the code variables follows.

Table 6. Format for the MCMT parameter definition file.

Record	Code Variable	Type/Format	Units	Description
1	title	CHAR/A80		Title of run
2	fileppt	CHAR/A80		Name of the MCMF water flux file. If fileppt=NONE (case sensitive) then a steady-state water flux is assumed. The steady-state water flux is read from the saturated $K(ksat)$ and moisture content is read from the saturated θ (thetas) that are defined in record 18.
3	filerel	CHAR/A80		Name of file containing the contaminant release rate into the first cell as a function of time. If filerel=NONE (case sensitive), then no external source of contaminant is assumed.
4	eps	REAL/*		Desired accuracy of solution (1×10^{-6})
4	h1	REAL/*	yr	Beginning time step (0.0001 yr)
4	hmin	REAL/*	yr	Minimum time step $(1 \times 10^{-60}$ yr)
5	mlayer	INT/*		Number of cells in the simulation $(250 \geq$ mlayer $\geq 1)$
5	nprog	INT/*		Number of contaminants or members in the decay-series $(10 \geq$ nprog $\geq 1)$
5	nmat	INT/*		Number of material types (must be $\leq$ mlayer)
5	iunits	INT/*		Flag variable that sets the units of the calculation: (1) Curies; (2) Becquerel; (3) mg
5	abin	CHAR/*		Flag variable for ASCII or binary output: (A) for ASCII output or, (B) for binary output. Only the general output file is written in binary when binary is specified. The format (ASCII or binary) of the water fluxes generated with MCMF must match the format specified in MCMT
6	cname(i)	CHAR*6/*		A six character name (no spaces in name) for each contaminant or decay chain member (**nprog** number of values expected).
7	mw(i)	REAL/*	g mol^{-1}	Molecular weight of each contaminant or decay chain member (**nprog** number of values expected).
8	sol(i)	REAL/*	mg m^{-3}	Solubility in water for each contaminant or decay chain member (**nprog** number of values expected).
9	thalf(i)	REAL/*	years	Half life of contaminant or decay chain member (**nprog** number of values expected).
10	bratio(i)	REAL/*	—	Branching ratio of the fraction of decay product j-1, that decays to decay product j (**nprog** number of values expected, last value is not used if it is the last contaminant in the list)
11	dwater(i)	REAL/*	m^2 yr^{-1}	Free-water molecular diffusion coefficient (**nprog** number of values expected).

Table 6. (continued).

Record	Code Variable	Type/Format	Units	Description
NOTE: Record 12, 13, and 14 are repeated for each contaminant or decay chain member				
12	y(*i,j*)	REAL/*	Ci, Bq, or mg	Initial contaminant inventories in cell *i* for contaminant *j*. Twenty values are read per line until all cells for a given contaminant are defined. The first contaminant is read first followed by the remaining contaminants.
13	kd(*i,j*)	REAL/*	mL g^{-1}	Linear sorption coefficient for cell *i* and contaminant *j*. Twenty values are read per line until all cells for a given contaminant are defined. The first contaminant is read first followed by the remaining contaminants.
14	kx(*i,j*)	REAL/*	yr^{-1}	Optional rate constant describing transfer of contaminant *j* from cell *i* to cell *i*+1. Twenty values are read per line until all cells for a given contaminant are defined. The first contaminant is read first followed by the remaining contaminants (Default is 0)
NOTE: Record 15, 16, and 17 define the cell property range and the cell properties. These records are repeated nmat number of times. Cells must be defined in ascending order.				
15	h	INT/*		Beginning cell number to define cell properties (inclusive).
15	j	INT/*		Ending cell number to define cell properties (inclusive).
NOTE: Cell properties assigned in records 16 and 17 for each material type apply to cells h through j (inclusive)				
16	thick	REAL/*	m	Thickness of all cells in the range from h to j
16	rho	REAL/*	g cm^{-3}	Bulk density of all cells in the range from h to j
17	sk	REAL/*	m yr^{-1}	Saturated hydraulic conductivity of all cells in the range from h to j
17	ths	REAL/*	m^{-3} m^{-3}	Saturated porosity of all cells in the range from h to j.
17	thr	REAL/*	m^{-3} m^{-3}	Residual moisture content of all cells in the range from h to j.
17	alpha	REAL/*	m^{-1}	van Genuchten fitting parameter, α for all cells in the range from h to j.
17	rn	REAL/*		van Genuchten fitting parameter *n* for all cells in the range from h to j.
18	ntimes	INT/*		Number of output time periods
NOTE: Record 19 is repeated for each output time period. Total number of output time periods = ntimes				
19	t1(*k*)	REAL/*	yrs	Begin time of output time *k*
19	t2(*k*)	REAL/*	yrs	End time of output time *k*
19	tp(*k*)	REAL/*	yrs	Print step of output time *k*

6.3.1 Record 2 (fileppt)

The **fileppt** variable stores the name of the MCMF-generated water flux file. The file format (ASCII or binary) must correspond to the setting of the variable, **abin**. Setting **fileppt** to NONE (case sensitive) allows MCMT to be run in steady-state mode without an MCMF file. The variables **sk** and **theta** define the water flux and moisture content of each material. The **theta** value must be set to negative(theta) for this option to take effect.

6.3.2 Record 3 (filerel)

The **filerel** variable stores the name (and complete or relative path to the file) of the contaminant release rate file. If the file name is NONE (case sensitive), then no external contaminant flux is considered. The structure for the file is described in Section 6.3.8.

6.3.3 Record 4 (eps, h1, hmin)

The code variables, **eps**, **h1**, and **hmin** all control time stepping and iteration of the Runge-Kutta solver. The code variable **eps** is defined in terms of Equation 39 and has a default value of 10^{-6}. The variable **h1** defines the initial time step to be taken. A relatively large value (say 1 year) can result in faster simulation times, but a user runs the risk of an inaccurate solution. A default value of 0.0001 yr is recommended. The code variable, **hmin** defines the minimum time step to be taken. The code will abort if the estimated time step is less than **hmin**. If this occurs, the user should set **hmin** to a smaller value. A value of 10^{-60} yr is recommended.

6.3.4 Record 5 (mlayer, nprog, nmat, iunits, and abin)

The variable **mlayer** defines the total number of cells to discretize the model domain into. The variable **nprog** defines how many contaminants to simulate. If a radioactive decay chain is considered, **nprog** should be set to the number of progeny plus the parent. The variable **nmat** defines the number of different material definitions that will be used to assign material properties to each cell. Materials are defined in increasing order, starting with the cell nearest the ground surface and ending with the cell at the aquifer-unsaturated zone interface (see Figures 1 and 3). For example, if a 50 m thick unsaturated zone is composed (from top to bottom) of 20 m of sandstone, 10 m of clay, and 20 m of sandstone, then **nmat** is set to **3**, because there are three material definitions required to define the unsaturated zone. Material properties are defined in records 15, 16, and 17.

The **iunits** variable define the units of the calculation. Both radiological (i.e., Ci or Bq) and mass units are included. The **abin** variable defines whether an ASCII (**abin**=A) or binary (**abin**=B) output file is written. A binary file is recommended if the number of cells exceeds about 60. The format of the MCMF file must corresponding to the format defined by **abin** in the MCMT parameter definition file.

6.3.5 Record 6, 7, 8, 9, 10, and 11 (cname, mw, sol, thalf, bratio, dwater)

The variables read in records 6 through 10 are the material-independent contaminant properties. Each record contains **nprog** values. Decay chains are modeled by setting **bratio** to a value greater than zero (typically 1.0). If **bratio(i)** is zero, then the fraction of contaminant (i) that decays to contaminant i+1 is zero. In this way, a single MCMT simulation can include a decay chain and several contaminants that are not connected to the chain. The procedure is illustrated in the example below. Six radionuclides are modeled; Th-230, Ra-226, Pb-210, H-3, Tc-99, and C-14. The first three radionuclides comprise a decay chain (Th-230 $\rightarrow$ Ra-226 $\rightarrow$ Pb-210) with a branching ratio of 1.0 between Th-230 and Ra-226 (bratio(1)=1.0) and Ra-226 and Pb-210 (bratio(2)=1.0). The remainder of the radionuclides are independent, and therefore, bratio is set to zero.

```
$ Radionuclide names
Th-230, Ra-226, Pb-210, H-3, Tc-99, C-14                    !Record 6  [cname(i)]
$ molecular weight
230.0,  226.0 , 210.0 , 3.0, 99.0,  14.0                    !Record 7  [mw(i)]
$ Solubility (assume infinite solubility for all radionuclides)
1.0E+09, 1.0E+09, 1.0E+09, 1.0E+09, 1.0E+09, 1.0E+09        !Record 8  [sol(i)]
$ half lives
7.54E+04, 1600.0, 22.3, 12.35, 2.13E+05, 5730.0            !Record 9  [thalf(i)]
$ branching ratio - the 6th value is not used but needs to be included in the file
1.0,   1.0,  0.0 0.0  0.0                                   !Record 10 [bratio]
$ assume no diffusion in water
0.0, 0.0, 0.0, 0.0, 0.0, 0.0                                !Record 11 [dwater(i)]
```

The variable, **dwater** is the free-water molecular diffusion coefficient in water. The code calculates the effective diffusion coefficient in pore water using the empirical expression given by Millington and Quirk (1961).

$$D_m = D_o \frac{\theta^{10/3}}{\theta_s^2} \tag{42}$$

Where D_o is the contaminant diffusion coefficient in free-water, D_m is the effective diffusion coefficient in pore water ($L^2 T^{-1}$), θ is the moisture content, and θ_s is the saturated porosity.

Mixing radionuclide activity with nonradionuclide mass in an input file is not allowed because of unit conversion problems. However, if radionuclide activities are expressed as isotope mass (in mg), then radionuclides and nonradionuclides can be simulated in a single MCMT run.

6.3.6 Records 15, 16, and 17 (h, j thick, rho, sk ths, thr, alpha, rn)

The code variables **h** and **j** define the beginning and ending cells (inclusive) to include in a material definition. Each material is defined in terms of its physical (thickness and bulk density) and hydraulic (saturated hydraulic conductivity, porosity, etc.) properties as defined in the variables **thick**, **rho**, **sk**, **ths**, **thr**, **alpha**, and **rn.** These properties are read in records 16 and 17 and are repeated for each material type. For example, suppose that a 45 m thick unsaturated zone is composed of (from top to bottom) 10 m of sandy clay loam, 15 m of sandy clay, and 20 m of sand. The code variable, **nmat** should be set to 3. Assuming a 45 cell problem, a cell thickness of 1 m, a bulk density of 1.5 g cm^{-3} for all materials, and hydraulic properties listed in Table 1, records 15, 16, and 17 would be:

```
$ Material definition for material type #1 - sandy clay loam
1  10                       [Record 15 h,j]
1.00 1.5                    [Record 16 thick rho]
114.76 0.39 0.10 5.9 1.48   [Record 17 sk ths thr alpha rn]
$ Material definition for material type #2 sandy clay
11 25                       [Record 15 h,j]
1.00 1.5                    [Record 16 thick rho]
10.51 0.38 0.10 2.7 1.23    [Record 17 sk ths thr alpha rn]
$ Material definition for material type #3 sand
26 45                       [Record 15 h,j]
1.00 1.5                    [Record 16 thick rho]
2601.72 0.43 0.045 14.5 2.68 [Record 17 sk ths thr alpha rn]
```

Note that records 15, 16, and 17 are repeated **nmat** number of times (**nmat**=3).

6.3.7 Records 18, and 19 (ntimes, t1, t2, and tp)

The code variable, **ntimes** defines how many time-history output periods are requested. Each output period is defined by an array of beginning times (**t1**), ending times (**t2**), and print intervals (**tp**). In

this way, different time resolutions can be applied to various time periods of the simulation. Record 19 is repeated **ntimes**. Suppose for example that one wants to capture the transient during the first 100 years of a simulation, and extend the simulation out to 1000 years. A possible choice for records 18 and 19 would be:

```
3                           [Record 18 ntimes]
$ Time period 1, 0-100 years print every year
0.0  100.0  1.0             [Record 19 t1, t2, tp]
$ Time period 2, from 110 to 500 years print every 10th year
110.0   500.0  10.0.        [Record 19 t1 t2 tp]
$ Time period 3, from 525 to 1000 years print every 25th year
525.0   1000.0  25.0.       [Record 19 t1 t2 tp]
```

6.3.8   Contaminant Release Rate File

The contaminant release rate entering the top of the model domain is provided to MCMT via an external ASCII file. The contaminant release rate file is specified in the parameter definition file (Record 3) and the name of the file is stored in the code variable, **filerel**. The file can be any name the user chooses. The file format is described in Table 7.

Table 7. Format of the contaminant release rate file.

Line Number	Code Variable	Description
1	junk	Column headers and comments (discarded)
2 to $n+1$[a]	rel(k,1)	Time in years from the start of the simulation for the kth record
2 to $n+1$[a]	rel(k, 2), rel(k, 3), rel(k,4) ... rel(k, **nprog**+1)	Contaminant release rate (Ci, Bq, or mg y^{-1}) for each of the **nprog** contaminants

a. n is the number of time and contaminant release rate records. A minimum of two records are needed.

6.4   Code Execution and MCMT Output Files and Utilities

Execution of the MCMT code is performed on the command line by typing:

[*path*]MCMT [*parameter definition file*]

where *path* is the full or relative path to the MCMT executable from the current operating directory, and *parameter definition file* is the name of the parameter definition file (Table 6). If the parameter definition file is left off, then MCMT will look for the default parameter definition file named MCMT.PAR in the current working directory. If the default parameter definition file is not found, or the user fails to provide a valid parameter definition file, the code will abort.

MCMT produces multiple output files: (1) a general output file (MCMT.OUT), (2) a list file (MCMT.LST), and (3) contaminant flux files for each contaminant simulated. The contaminant flux file names are automatically generated from a concatenation of the contaminant name with the ".rel" extension. The general output file and list file have hardwired file names and are written in the default directory each time MCMT is executed. The MCMT.OUT file contains the time histories of contaminant inventories, pore water concentrations, and fluxes for each cell in the simulation. The MCMT.LST file contains the model input data, calculated intermediate values, the number of converged and unconverged time steps, and the code execution time. The MCMT.LST file is always written in ASCII whereas the MCMT.OUT file is written in binary if the code variable **abin**=B. A utility program (MCMTPRT) was written to allow a user to access the binary (or ASCII) data stored in the MCMT.OUT file. The MCMTPRT utility is executed by typing on the command line:

[*path*]MCMTPRT [*parameter definition file*]

where *path* is the full or relative path to the MCMTPRT executable from the current operating directory, and *parameter definition file* is the name of the MCMTPRT parameter definition file. If the parameter definition file is left off, then MCMTPRT will look for the default parameter definition file (MCMTPRT.PAR) in the current working directory. If the default parameter definition file is not found, or the user fails to provide a valid parameter definition file, the code will abort. The format for the MCMTPRT parameter definition file is described in Table 8.

Table 8. Format for the MCMTPRT parameter definition file.

Record	Code Variable	Type/Format	Description
1	title	CHAR/A80	Title of run
2	filedat	CHAR/A80	MCMT general output file (MCMT.OUT)
3	abin	CHAR/*	Flag variable for ASCII or binary output: (A) for ASCII output or, (B) for binary output.
3	aqnt	CHAR/*	Quantity to extract: I = contaminant inventory, C = contaminant pore water concentration, F = contaminant flux
3	pfix	CHAR*4/*	A four character prefix to identify output file names.
4	nout	INT/*	Number of cells to output time histories (maximum = 50)
4	tout	INT/*	Number of times to output spatial profiles (maximum = 50)
4	cf	REAL/*	User-provided conversion factor (1.0)
5	noutput(*i*)	INT/*	The cell numbers for each of the **nout** time histories. All values are read from one line and each value is separated by a space or comma. If **nout** is zero, this record should be blank.
6	toutput(*i*)	REAL/*	The time of each of the **tout** spatial profiles. All values are read from one line and each value is separated by a space or comma. If **tout** is zero, this record should be blank.

7.   SOFTWARE MANAGEMENT

Software management requirements for the INL are stated in Management Control Procedure 550 (MCP-550). The MCM codes are classified as Quality Level C software as defined in MCP-550. The required elements of software management for Level C software are listed in Table 9. Fulfillment of these requirements is stated in column two of Table 9.

Table 9. MCP-550 software quality assurance requirements and where they are addressed in the MCM documentation.

MCP-550 Requirement	Section/Appendix/Form where MCP-550 requirement is fulfilled
Software Management Plan (SMP)	Form 562.26 ID No.
Software Quality Assurance Plan (SQAP)	Form 562.27 ID No.

8. SAMPLE APPLICATION

This section illustrates application of the MCM codes to a hypothetical problem regarding clean-up of a decommissioned infiltration pond that was used to dispose of low-level liquid radioactive waste. The problem is illustrated in Figure 7. A 100 m × 100 m infiltration basin operated for a period of 40 years during which liquid radioactive waste was disposed. During its operations, it was estimated that 100 Ci/yr year of Sr-90 and 1 Ci/yr of Ra-226 were disposed in the basin. Much of the contamination currently resides in the surface alluvium and in a 21.45 m thick sedimentary interbed located 66 m below the surface. The aquifer lies 144 m below the surface. Because of the depths of contamination, complete site remediation is impractical. The site may be put under administrative control and not accessible to the public for the next 100 years. Groundwater will be monitored in wells downgradient from the facility during this time.
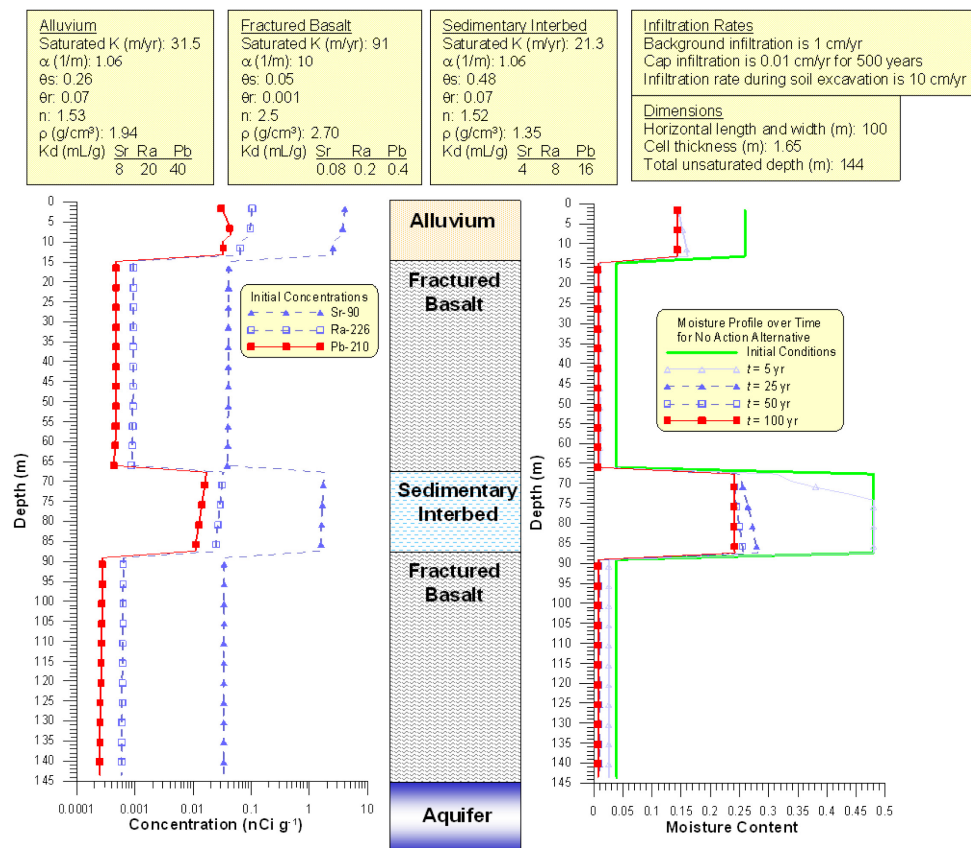
Figure 7. Problem description, model domain, and input parameters for the sample application of the MCM models. Initial concentrations of each radionuclide after the end facility operations is illustrated on

the left graph. The initial moisture content and moisture content profile in subsequent years for the no action alternative is shown in the graph on the right.

Three remediation options are considered: (1) no action, (2) remove contaminated soils down to fractured basalt and refill with clean soil, and (3) leave contaminated soil in place and cover site with an engineered barrier (capping). Remedial Option 2 will result in enhanced infiltration over the infiltration basin during the time excavation takes place and until native vegetation reestablishes itself over the disturbed soil. The infiltration during remediation and before native vegetation reestablishes itself is estimated to be about an order of magnitude greater than that for undisturbed soil. Enhanced infiltration is estimated to persist for 10 years.

The engineered barrier is designed for a 500-year lifetime and result in a two-orders of magnitude reduction in the infiltration rate relative to background infiltration through undisturbed soils. After 500 years, the infiltration is assumed to return to its background conditions.

Residual concentrations of Sr-90 and Ra-226 in surface soils present an unacceptable risk from surface exposure pathways (i.e., external exposure, soil resuspension/inhalation, and soil ingestion). Therefore some remediation of the surface soils will be necessary. Both source removal and capping will reduce the surface pathway risks to acceptable levels. The question is, which remediation strategy will also minimize groundwater impacts?

The MCMF and MCMT codes were first run to provide the moisture content and radionuclide concentration profiles at the end of operation of the infiltration basin. The radionuclide and moisture profiles at the end of operations were the initial conditions used in each remediation option simulation. Initial conditions could also have been provided by measured radionuclide concentrations and moisture contents in the subsurface. The model domain was discretized into 87 cells each having a thickness of 1.65 m. It was not particularly important to capture the shape of the wetting front in the MCMF code. Therefore, cell size was chosen based on the level of lithologic detail for the unsaturated zone. Water flow rates into infiltration basin were 180,000 m^3 yr^{-1} and spread out over an area of 10,000 m^2. It was assumed that all water entering the basin infiltrated into the subsurface. Radionuclide release rates into the infiltration basin were 100 Ci yr^{-1} of Sr-90, and 1 Ci yr^{-1} of Ra-226.

Radium-226 has numerous daughter products, but only Pb-210 has a long enough half life (22.3 years) such that it can exist in the environment without the presence of Ra-226. Therefore, Pb-210 was modeled as the only daughter of Ra-226. Infiltration basin effluent did not include Pb-210 and therefore, all Pb-210 was derived from the decay of Ra-226. The MCMF and MCMT input files for the no action alternative are presented in Figure 8.

The results of the simulation are summarized in Figure 9. The radionuclide fluxes are relatively insensitive to the different remediation options during the 0 to 50 year time frame following cessation of infiltration basin operations. Therefore, some administrative control will probably be necessary for at least 50 years. Option 2 results in slightly higher radionuclide fluxes at 100 years because infiltration is enhanced while soil is being excavated. However, radionuclide fluxes for Option 2 drop off faster after about 500 years compared to the fluxes for the Option 1 (no action alternative). Option 3 yields the lowest radionuclide aquifer flux after the 100 year administrative control period until about the year 700. The water and radionuclide flux for Option 3 drops over an order of magnitude between the years ~100 to ~700 as a result of the emplacement of the engineered barrier.

This sample application illustrates how MCM may be used for assessment of transient flow problems. Comparison of the graphs for the three remediation options with the one labeled "Steady-State" in Figure 9 illustrates the importance of transient flow on the outcome of the assessment. The graph labeled "Steady-State" in Figure 9 shows the radionuclide flux as a function of time assuming the initial

35

moisture profile and transient flow effects are ignored. The MCM simulation for the Steady-State problem assumed the same vertical distribution of radionuclides in the unsaturated zone, a steady-state water infiltration flux of 1 cm yr^{-1}, and an initial moisture content in all cells that corresponds to a 1 cm yr^{-1} steady-state water flux. The radionuclide flux for the steady-state simulation is substantially lower than the radionuclide flux for Options 1–3, which may lead to the conclusion that no action needs to be taken. Without considering drainage of the water present in the unsaturated zone after the end of operations, potentially incorrect conclusions could be drawn about the mobility of radionuclides present in the unsaturated zone. The MCM model represents a relatively simple model to address these processes. Based on the results presented in Figure 9, it appears that Option 3 would provide the best overall protection for groundwater for foreseeable future. However, other considerations, such as public perception and cost may weigh into the ultimate decision of what remediation option to select.

```
MCMF Input File for Sample Application Case 1                                              title [title of progect (a80)]
mcmf.flx                                                      fileout [name of MCMT water flux file (a80)]
mcmf.ptt                                                      fileppt [net infiltration rate file (a80)]
1.0e-6   0.0001  1.0e-60            [Record 4] eps,hl,hmin [accuracy, initial time step, minimum time step]

87 4  1000  0.1200 7.5e-003 1 B     [Record 5] mlayer,nmat,nkt,qmax,qmin,iflag,abin

$ initial moisture content [Record 6]
$1       2       3       4       5       6       7       8       9      10      11      12      13      14      15      16      17      18      19      20
2.59E-01 2.59E-01 2.59E-01 2.59E-01 2.59E-01 2.59E-01 2.59E-01 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02
3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02
4.80E-01 4.80E-01 4.80E-01 4.80E-01 4.80E-01 4.80E-01 4.80E-01 4.80E-01 4.80E-01 4.80E-01 4.80E-01 4.80E-01 4.80E-01 4.80E-01 4.80E-01 4.80E-01 3.91E-02 3.91E-02 3.91E-02 3.91E-02
3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02
3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02 3.91E-02
1  8                   [Record 7]  h,j   [begining cell, ending cell]
1.65                   [Record 8]  thick(h) [thickness (m)]
31.50 0.26 0.07 1.06 1.53   [Record 9] sk(h),ths(h),thr(h),alpha(h),rn(h) [Sat conductivity (m/yr) sat moist content, resid moist content, vanG alpha, vanG n]
9 40                   [Record 7]  h,j
1.65                   [Record 8]  thick(h)
91.00 0.05 1.0e-03 10.00 2.50   [Record 9] sk(h),ths(h),thr(h),alpha(h),rn(h) [Sat conductivity (m/yr) sat moist content, resid moist content, vanG alpha, vanG n]
41 53                  [Record 7]  h,j
1.65                   [Record 8]  thick(h)
21.30 0.48 0.07 1.06 1.52   [Record 9] sk(h),ths(h),thr(h),alpha(h),rn(h) [Sat conductivity (m/yr) sat moist content, resid moist content, vanG alpha, vanG n]
54 87                  [Record 7]  h,j
1.65                   [Record 8]  thick(h)
91.00 0.05 1.0e-03 10.00 2.50   [Record 9] sk(h),ths(h),thr(h),alpha(h),rn(h) [Sat conductivity (m/yr) sat moist content, resid moist content, vanG alpha, vanG n]
3                      [Record 10] ntimes
0.0  100  1.0          [Record 11] t1 t2 tp
110. 1000  10.         [Record 11] t1 t2 tp
1100 10000 100.        [Record 11] t1 t2 tp
15000                  [Record 12] tmax
2                      [Record 13] nout
37 45                  [Record 14] noutput(i)

MCMT Input File sample application: Case 1, no action alternative                          title [title of progect (a80)]
..\..\mcmf\case1\mcmf.flx                                     fileppt [name of MCMF water flux file (a80)]
NONE                                                          filerel [net infiltration rate file (a80)]
1.0e-6  0.0001  1.0e-60            [Record 4] eps,hl,hmin [accuracy, initial time step, minimum time step]
87 3 4 1 B             [Record 5] mlayer,nprog,nmat,iunits,abin [number of layers,number of contaminants, number of materials, units of measure, (A)scii or (B)inary]
Sr-90 Ra-226 Pb-210    [Record 6] contam names
90.0 226.0  210.0      [Record 7] mw [ molecular weight (g/mol)]
1.000e+009 1.000e+009 1.000e+009  [Record 8] sol [solubility limit (mg/m**3)]
2.9120e+001  1600.  22.3          [Record 9] thalf [half lives years)]
0.0 1.0  1.0           [Record 10] bratio [branching ratio]
0.0 0.0  0.0           [Record 11] dwater [water diffusivity]
$                      [Record 12] initial inventories mbr 1
$1       2       3       4       5       6       7       8       9      10      11      12      13      14      15      16      17      18      19      20
$ Sr-90 Inv (Ci)
1.29E+02 1.26E+02 1.22E+02 1.19E+02 1.17E+02 1.15E+02 1.13E+02 1.12E+02 1.81E+00 1.81E+00 1.81E+00 1.80E+00 1.80E+00 1.80E+00 1.80E+00 1.80E+00 1.80E+00 1.80E+00 1.80E+00 1.80E+00
1.80E+00 1.79E+00 1.79E+00 1.79E+00 1.79E+00 1.79E+00 1.79E+00 1.78E+00 1.78E+00 1.78E+00 1.77E+00 1.77E+00 1.76E+00 1.75E+00 1.74E+00 1.73E+00 1.72E+00
3.91E+01 3.86E+01 3.82E+01 3.77E+01 3.73E+01 3.69E+01 3.65E+01 3.61E+01 3.58E+01 3.55E+01 3.52E+01 3.50E+01 3.49E+01 1.51E+00 1.51E+00 1.51E+00 1.51E+00 1.51E+00 1.51E+00 1.51E+00
1.51E+00 1.51E+00 1.50E+00 1.50E+00 1.50E+00 1.50E+00 1.50E+00 1.50E+00 1.50E+00 1.50E+00 1.50E+00 1.49E+00 1.49E+00 1.49E+00 1.49E+00 1.49E+00
1.49E+00 1.49E+00 1.49E+00 1.49E+00 1.49E+00 1.49E+00
$ Ra-226 Inv (Ci)
3.30E+00 3.22E+00 3.14E+00 3.07E+00 2.99E+00 2.92E+00 2.87E+00 2.84E+00 4.20E-02 4.20E-02 4.20E-02 4.19E-02 4.19E-02 4.19E-02 4.18E-02 4.18E-02 4.18E-02 4.17E-02 4.17E-02 4.17E-02
4.16E-02 4.16E-02 4.16E-02 4.15E-02 4.15E-02 4.14E-02 4.14E-02 4.13E-02 4.12E-02 4.11E-02 4.09E-02 4.08E-02 4.06E-02 4.04E-02 4.01E-02 3.97E-02 3.92E-02 3.85E-02
7.34E-01 7.17E-01 6.99E-01 6.81E-01 6.63E-01 6.45E-01 6.27E-01 6.10E-01 5.93E-01 5.78E-01 5.65E-01 5.54E-01 5.48E-01 2.81E-02 2.80E-02 2.79E-02 2.79E-02 2.78E-02 2.78E-02 2.77E-02
2.76E-02 2.75E-02 2.74E-02 2.74E-02 2.73E-02 2.72E-02 2.71E-02 2.71E-02 2.70E-02 2.70E-02 2.69E-02 2.68E-02 2.68E-02 2.67E-02 2.66E-02 2.66E-02 2.65E-02 2.65E-02
2.64E-02 2.64E-02 2.63E-02 2.63E-02 2.62E-02 2.62E-02 2.62E-02
$ Pb-210 Inv (Ci)
9.64E-01 1.14E+00 1.27E+00 1.35E+00 1.40E+00 1.43E+00 1.45E+00 1.45E+00 2.09E-02 2.09E-02 2.09E-02 2.09E-02 2.09E-02 2.09E-02 2.09E-02 2.09E-02 2.09E-02 2.09E-02 2.09E-02 2.09E-02
2.09E-02 2.09E-02 2.09E-02 2.09E-02 2.09E-02 2.09E-02 2.09E-02 2.08E-02 2.09E-02 2.09E-02 2.07E-02 2.07E-02 2.06E-02 2.04E-02 2.03E-02 2.01E-02 1.98E-02 1.94E-02
3.73E-01 3.62E-01 3.51E-01 3.39E-01 3.26E-01 3.13E-01 3.00E-01 2.88E-01 2.76E-01 2.65E-01 2.55E-01 2.48E-01 2.43E-01 1.23E-02 1.22E-02 1.22E-02 1.22E-02 1.21E-02 1.21E-02 1.20E-02
1.20E-02 1.20E-02 1.19E-02 1.19E-02 1.18E-02 1.18E-02 1.17E-02 1.17E-02 1.17E-02 1.16E-02 1.16E-02 1.15E-02 1.15E-02 1.14E-02 1.14E-02 1.13E-02 1.12E-02 1.12E-02
1.12E-02 1.11E-02 1.11E-02 1.11E-02 1.10E-02 1.10E-02 1.10E-02
$ [Record 13]  Kd Values
$ kd values Sr-90
8.000e-000 8.000e-000 8.000e-000 8.000e-000 8.000e-000 8.000e-000 8.000e-000 8.000e+000 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002
8.000e-002
8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002
8.000e-002
4.000e-000 4.000e-000 4.000e-000 4.000e-000 4.000e-000 4.000e-000 4.000e-000 4.000e-000 4.000e-000 4.000e-000 4.000e-000 4.000e-000 4.000e-000 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002
8.000e-002
8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002
8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002 8.000e-002
$ kd values Ra-226
2.000e+001 2.000e+001 2.000e+001 2.000e+001 2.000e+001 2.000e+001 2.000e+001 2.000e+001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001
2.000e-001
2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001
2.000e-001
8.000e-000 8.000e-000 8.000e-000 8.000e-000 8.000e-000 8.000e-000 8.000e-000 8.000e-000 8.000e-000 8.000e-000 8.000e-000 8.000e-000 8.000e-000 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001
2.000e-001
2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001
2.000e-001
2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001 2.000e-001
$ kd values Pb-210
4.000e+001 4.000e+001 4.000e+001 4.000e+001 4.000e+001 4.000e+001 4.000e+001 4.000e+001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001
4.000e-001
4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001
4.000e-001
1.600e+001 1.600e+001 1.600e+001 1.600e+001 1.600e+001 1.600e+001 1.600e+001 1.600e+001 1.600e+001 1.600e+001 1.600e+001 1.600e+001 1.600e+001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001
4.000e-001
4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001
4.000e-001
4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001 4.000e-001
$ [Record 14]  Kx values
$ kx values Sr-90
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0
$ kx values Ra-226
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0
$ kx values Pb-210
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
0.0  0.0  0.0  0.0  0.0  0.0  0.0
1.000e+002  1.000e+002  6.000e+000    [Record 15] lth  width  alphaL [length, width, disp (m)]
1  8                   [Record 16]  h,j   [begining cell, ending cell]
1.65  1.94             [Record 17]
31.50 0.26 0.07 1.06 1.53   [Record 18] sk(h),ths(h),thr(h),alpha(h),rn(h) [Sat conductivity (m/yr) sat moist content, resid moist content, vanG alpha, vanG n]
9 40                   [Record 16]
1.65  2.70             [Record 17]
91.00 0.05 1.0e-03 10.00 2.50   [Record 18] sk(h),ths(h),thr(h),alpha(h),rn(h) [Sat conductivity (m/yr) sat moist content, resid moist content, vanG alpha, vanG n]
41 53                  [Record 16]
1.65  1.35             [Record 17]
21.30 0.48 0.07 1.06 1.52   [Record 18] sk(h),ths(h),thr(h),alpha(h),rn(h) [Sat conductivity (m/yr) sat moist content, resid moist content, vanG alpha, vanG n]
54 87                  [Record 16]
1.65  2.70             [Record 17]
91.00 0.05 1.0e-03 10.00 2.50   [Record 18] sk(h),ths(h),thr(h),alpha(h),rn(h) [Sat conductivity (m/yr) sat moist content, resid moist content, vanG alpha, vanG n]
3                      [Record 19] ntimes
0.0  100  1.0          [Record 20]
110. 1000  10.         [Record 20]
1100 15000 100.        [Record 20]
```

Figure 8. MCMF (top) and MCMT (bottom) input files for the no action alternative of the sample application.
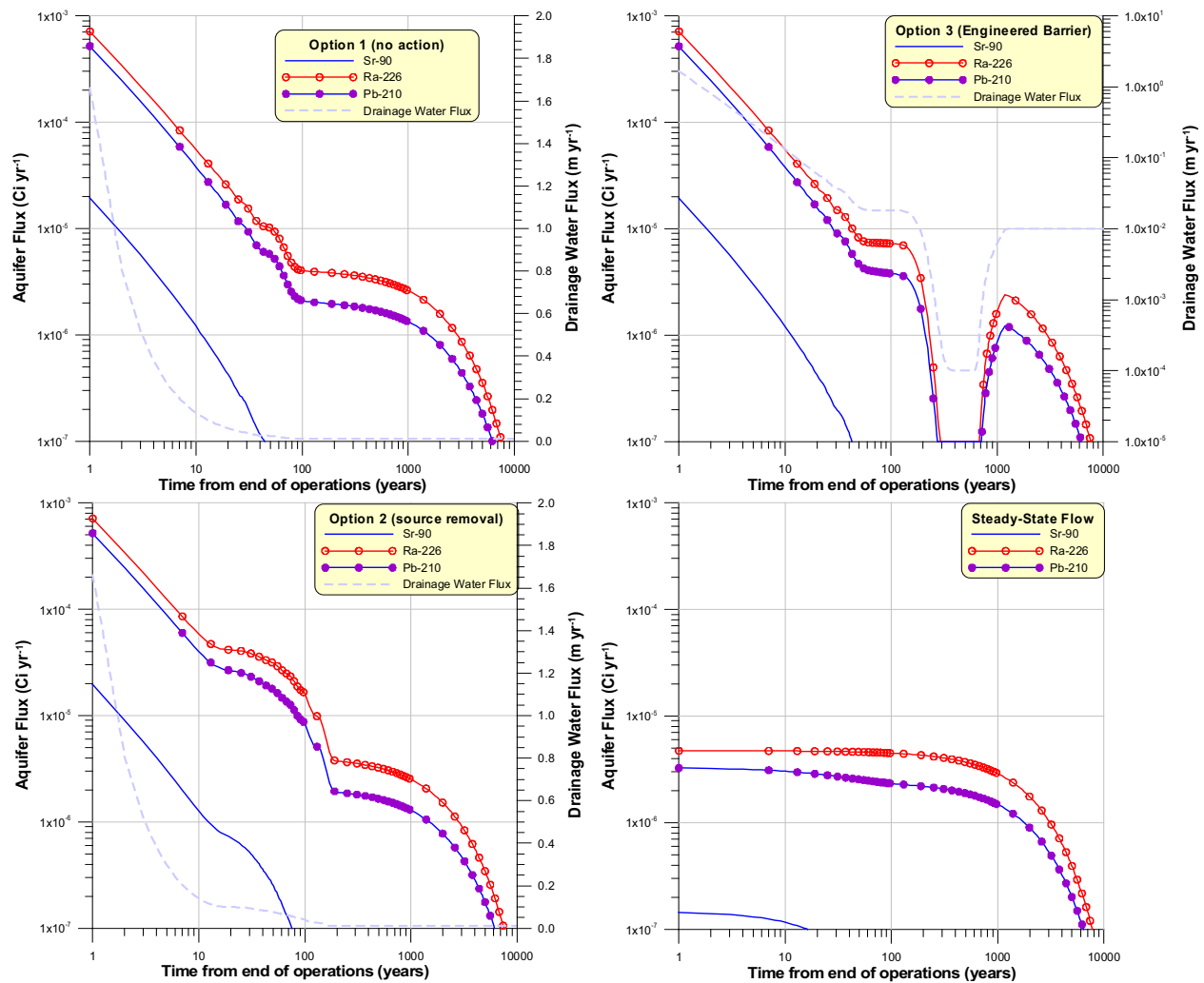
Figure 9. Radionuclide flux to the aquifer as a function of time for the three remediation options and the Steady-State case for the sample application of MCM.

9. REFERENCES

ACRI, 1996, "PORFLOW: A Software Tool for Multiphase Fluid Flow, Heat and Mass Transport in Fractured Porous Media," Analytical & Computational Research, Inc., Bel Air, CA, 1996.

Appelo, C. A. J. and A. Willemsen, 1987, "Geochemical Calculations and Observations on Salt Water Intrusions, I. A Combined Geochemical/Mixing Cell Model," *Journal of Hydrology*, *94*, pp. 313-330.

Baes, C. F., III and R. D. Sharp, 1983, "A proposal for estimation of soil leaching and leaching constants for use in assessment models," *Journal of Environmental Quality, 12*(1), pp. 17–28.

Brooks, R. H., and A. T. Corey, 1964, "Hydraulic Properties of Porous Media," *Hydrologic Paper 3*, Colorado State University, Fort Collins, CO.

Campbell, G. S., 1974, A "Simple Method for Determining Unsaturated Conductivity from Moisture Retention Data," *Soil Science 117*, 311–314.

Carsel, R. F. and R. S. Parrish, 1988, Developing joint probability distributions of soil water retention characteristics *Water Resources Research*, 25(5), 755–769.

Codell, R. B., K. T. Key, and G. Whelan, 1983, "Transport of Radionuclides in Groundwater," in *Radiological Assessment,* NUREG/CR-3332, J. E. Till and H. R. Meyer, eds., U.S. Nuclear Regulatory Commission, Washington, DC, 1983.

EPA, 1992, *MMSOILS: Multimedia Contaminant Fate, Transport, and Exposure Model. Documentation and User's Manual,*. U.S. Office of Research and Development, Washington, DC, 1992.

Fayer, M. J., 2000, UNSAT-H Version 3.0: Unsaturated Soil Waste and Heat Flow Model, Theory, User's Manual, and Examples. PNNL 13249, Pacific Northwest National Laboratories, Richland, Washington, 2000.

Gardner, W. R., 1960, "Soil Water Relations in Arid and Semi-arid Conditions," *UNESCO 15*, 37–61.

Hillel, D., 1998, *Environmental Soil Physics*. Academic Press, San Diego, CA.

Levenspiel, O. and K. B. Bischoff, 1963, "Patterns of Flow in Chemical Process Vessels" In T. B. Drew, J. W. Hoopes, Jr., and T. Vermeulen Eds., *Advances in Chemical Engineering,* Vol. 4, Academic Press, New York, 95–198.

MCP-550, 2004, "Software Management," Rev. 8, November 9, 2004.

Millington, R. J., and J. M. Quirk, 1961, "Permeability of Porous Solids" *Trans Faraday Soc*. 57:1200-1207.

Philip, J. R., 1957, "Theory of Infiltration 2. The Profile of Infinity." *Soil Science*, 83(6), 435–448.

PNNL, 1996, *Subsurface Transport Over Multiple Phase Description "STOMP" Theory Guide*, PNNL-11217, Pacific Northwest National Laboratories, Richland, WA, 1996.

Press, W. H., B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, 1992, *Numerical Recipes: The Art of Scientific Computing.* Cambridge: Cambridge University Press.

Rao, B. K. and D. L. Hathaway, 1989, "A Three Dimensional Mixing Cell Solute Transport Model and its Application," *Ground Water*, 27(4), 509–516.

Rood, A. S., 1999, *GWSCREEN: A Semi-Analytical Model for Assessment of the Groundwater Pathway from Surface or Buried Contamination, Theory and User's Manual*, Version 2.5. INEEL/EXT-98-00750, Idaho National Engineering and Environmental Laboratory, 1999.

Rood, A. S., 2004, "A Mixing-Cell Model for Assessment of Contaminant Transport in the Unsaturated Zone Under Steady-State and Transient Flow Conditions," *Environmental Engineering Science*, 21(6).

Schroeder, P. R., T. S. Dozier, P. A. Zappi, B. M. McEnroe, J. W. Sjostrom, and R. L. Peyton, 1994, *The Hydrologic Evaluation of Landfill Performance (HELP) Model*. EPA/600/R-94/168b. U.S. Environmental Protection Agency, Office of Research and Development, Cincinnati, Ohio, 1994.

Scott, S. J. and D. M. Hetrick, 1994, *The New SESOIL User's Guide*. PUBL-SW-200-94. Science & Technology Management Inc., Brookfield, WI 53005. Distributed by the Radiation Safety Information Computational Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 1994.

Shanahan, P. and D. R. F. Harleman, 1984, "Transport in Lake Water Quality Modeling," *Journal of Environmental Engineering*, *110*(1), pp. 42–57.

Simunek, J., M. Sejna, M. and M. Th. van Genuchten, 1999, *HYDRUS-2D/MESHGEN-2D Simulating Water Flow and Solute Transport in Two-Dimensional Variably Saturated Media*, IGWMC-TPS 53C, Version 2.0, International Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado, 1999.

Smith, R. E., K. R. J. Smetten, and D. A. Woolhiser, 2002, *Infiltration Theory for Hydrologic Applications*, American Geophysical Union, Washington DC.

Sullivan, T. M. 1996, *DUST Disposal Unit Source Term, Data Input Guide.* NUREG/CR-6041, BNL-NUREG-52375, Brookhaven National Laboratory, Upton, New York, 1996.

van Genuchten, M. Th., 1980, "A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils," *Soil Sci. Soc. Am J.*, 44, 892–898.

Van Ommen, H. C., 1985, "The Mixing Cell Concept Applied to Transport of Non-Reactive and Reactive Components in Soils and Groundwater," *Journal of Hydrology*, *78*, pp. 201–213.

Whelan, G., J. P. McDonald, and C. Sato, 1996, *Multimedia Environmental Pollutant Assessment System (MEPAS) Groundwater Pathway Formulations*, PNNL-10907, Pacific Northwest National Laboratory, Richland, Washington, 1996.

Whicker, F. W. and V. Schultz, 1982, *Radioecology: Nuclear Energy and the Environment*, CRC Press, Boca Raton, Florida.

Yu, C., A. J. Zielen, J. J. Cheng, Y. C. Yuan, L. G. Jones, D. L. Lepoire, Y. Y. Wang, C. O. Loureiro, E. Gnanapragasam, E. Failance, A. Wallo III, W. A. Williams, and H. Peterson, 2000, *Manual for Implementing Residual Radioactive Material Guidelines Using RESRAD Version 6.0*, ANL/EAD/LD-2 Argonne National Laboratory, Argonne, Illinois, 2000.

Zvirin, T., and R. Shinnar, 1976, "Interpretation of Internal Tracer Experiments and Local Sojourn Time Distributions," *International Journal of Multiphase Flow*, 2, pp. 495–520.

Appendix A

Software Design Description and Configuration Management Plan

Appendix A

Software Design Description and Configuration Management Plan

A-1. SOFTWARE DESIGN DESCRIPTION

The software design description depicts how the software is structured to satisfy the requirements of the software, and the components and subcomponents of the software. The MCM software is written in FORTRAN 77 with some use of language extensions as provided by the Lahey LF95 Compiler. Less than 15 modules comprise both MCMT and MCMF. Each module is described in Table A-1. The calling sequence and functional relationships are described in Table A-2.

Table A-1. Description of each subroutine and function in MCMF and MCMT.

Module	MCMT	MCMF	Description
main	x	x	Main program unit that: (1) reads the command line arguments, opens and reads the input files, calls the ODE solver, and writes output to files and screen
derivs	x	x	Subroutine that contains the ODEs to be solved
quantity	x		Subroutine for calculating retardation, pore water concentrations, and dispersive fluxes for each cell
odeint	x	x	Subroutine for control of Runge-Kutta ODE solver
lint	x	x	Subroutine for linear interpolation
vang	x	x	Subroutine for calculating the moisture characteristic curve
readline	x	x	Subroutine for reading a line of input from the parameter definition file
numvaline	x	x	Subroutine for determining the number of expected values on a line
checkfile	x	x	Subroutine to check for valid file names
filcase	x	x	Subroutine to convert the case of file names to lower or upper case
convert	x		Subroutine to calculate conversion factors from mass to activity
rkqs	x	x	Subroutine for QA checks for Runge-Kutta ODE solver
rkck	x	x	Subroutine of main Runge-Kutta ODE solver
timsscale	x		Subroutine for calculating advective and dispersive time scales

Table A-2. Functional relationship and subroutine calling sequence for MCMT and MCMF.

Level 0	Level 1	Level 2	Level 3	Level 4	Level 5	Level 6
			Program MCMT			
•	filcase					
•	checkfile					
•	readline					
•	numvaline					
•	convert					
•	odeint					
•	•	derivs				

Table A-2. (continued).

Level 0	Level 1	Level 2	Level 3	Level 4	Level 5	Level 6
•	•	•	lint			
•	•	•	quantity			
•	•	•	•	lint		
•	•	rkqs				
•	•	•	derivs			
•	•	•	•	lint		
•	•	•	•	quantity		
•	•	•	•	•	lint	
•	•	•	rkck			
•	•	•	•	derivs		
•	•	•	•	•	lint	
•	•	•	•	•	quantity	
•	•	•	•	•	•	lint
•	timsscale					
•	lint					
•	vang					
•	quantity					
•	•	lint				
Program MCMF						
•	filcase					
•	checkfile					
•	readline					
•	numvaline					
•	odeint					
•	•	derivs				
•	•	•	lint			
•	•	rkqs				
•	•	•	derivs			
•	•	•	•	lint		
•	•	•	rkck			
•	•	•	•	derivs		
•	•	•	•	•	lint	
•	lint					
•	vang					

A-2. SOFTWARE CONFIGURATION MANAGEMENT PLAN

Software configuration management provides the mechanism to identify, document, and control changes to the software. Software configuration management for MCM is addressed within the module headers and the version date. Each module in the MCM codes contain a header that documents: (1) The name and purpose of the module, (2) the code author, (3) the date it was written, (4) a change history to the module, (5) arguments and returned values, and (5) calls to and from the module. The module header forms the basis for most of the code documentation. An example module header is provided in Figure A-1.

```
 subroutine derivs(time,y,dydt)
c ================================================
c Modual Name: DERIVS
c Author: A. S. Rood
c Date Created: 09/29/2002
c Last Modified: 04/01/2004
c              11/16/02 - correcteed error in progeny calcuation when nprog>2
c                         changed array fluxi to a 2-D array that stores fluxes
c                         for all decay chain members and layers
c              06/28/03 - rearranged calculation and added dispersive fluxes
c              01/22/04 - added branching ratio
c              04/01/04 - added if-then logic to address single cell models

c Purpose: Routine that contains derivitives. Calculation is performed in atoms for radionuclides
c
c Arguments
c  time:  time derivative is evalauated at
c  y:     array of dependent varaibles
c  dydx:  derivative of dependent variable
c
c Common Blocks

c     common /rconstant/
c     kd(mlayer,nprog):   array of kd values for each cell and each contaminant (mL/g)
c     lambda(nprog):      decay constants for each contaminant (1/yr)
c     thick(mlayer):      thickness of each cell (m)
c     rho(nmax):          bulk density of each cell (g/cm**3)
c     lth:                length of domain (m)
c     width:              width of domain (m)
c     sola(nprog):        solubility limit of each contaminant (mass/m**3)
c     kx(mlayer,nprog):   alternative removal rate constant (1/yr)
c     pe(mlayer,nprog):   peclet number for each cell and contaminant
c     prT:                total effective peclet number
c     alphaL:             longitudinal dispersivity (m)
c     bratio(nprog):      branching ratio for each contaminant
c     dwater(nprog):      water diffusion coefficient (m**2/yr)
c     area:               horizontal area of domain (m**2)
c     mlayer:             number of cells in simulation
c     nprog:              number of contaminants in simulation

c     common /interpolate/
c     precip(npoints,mlayer+1):  array of net infiltration values as a function of time for each cell (m/yr)
c     rel(npoints,mlayer+1):     array of contaminant mass fluxes as a function of time (mass/yr)
c     moist(npoints,mlayer+1)    array of moisture contents as a function of time
c     npp:                       number of precipitation points
c     nrel:                      number of release points


c Called By: odeint, rkqs, rkck
c Calls To:  quantity
c ================================================
```

Figure A-1. Module header for subroutine derives in MCMT.

Version control is primarily handled in MCM through the version date instead of a version number. The version date can be thought of as essentially a version number and is stored in the variable **vdate** in the main program unit. The version date is a six digit number where the first two numbers represent the month, the second two the day, and the last two the year. The version date is in the header of the .LST file

generated by MCMT and MCMF and in all ancillary output files generated by both codes. The version date is identified as the "Level" in the ancillary output files. In this way, results from old version of the code can be identified.

Old versions of the code are identified by a concatenation of either "mf" for MCMF or "mt" for MCMT and the version date. For example, mf010404.for would represent the MCMF code with a version date of January 4, 2004. Old versions of the code archived on the code custodian's computer in the c:\mcm\mcmf\f77 directory for MCMF and c:\mcm\mcmt\f77 directory for MCMT. Only the most recent version is sent when distributing the code to other users.

The code custodian has the responsibility of maintaining and updating the code, identifying and archiving code versions, verifying new versions of the code operate correctly, and distributing the software to end users.

Appendix B

Code Verification and Benchmark Problems

Appendix B

Code Verification and Benchmark Problems

Code verification is defined here as confirmation that the model was written and implemented in the computer code correctly. To do this, quantities output from the MCM codes (such as pore water concentrations, contaminant fluxes, water fluxes, and moisture contents) were compared with like quantities calculated using other codes or analytical solutions to the governing equations. MCMF and MCMT input files for each of the verification exercises are attached to the end of this appendix.

B-1. MCMT VERIFICATION PROBLEMS

Four verification problems and one benchmark problem were constructed to verify the MCMT code. Verification problems compare code output to analytical solutions to the governing equations. Benchmark problems compare code output to that of other codes that solve essentially the same type of problem. Differences between MCMT output and verification/benchmark output were expressed as the percent difference (%d) as given by Equation B-1:

$$\%d = \frac{V_v - V_m}{V_v} \times 100 \tag{B-1}$$

where V_v = the value calculated by verification/benchmark code output, and V_m = the value calculated by MCMT. Analytical solutions to the governing equations are developed first followed by the results of the verification exercises. An additional verification problem is also presented in Section 3.1 in the main body of the report.

B-1.1 Analytical Solutions for Governing Equations

For the case where dispersion is ignored (i.e., no cell interchange) the transport equation takes the form a unidirectional catenary system of equations. A general solution has been developed by Skrable et al. (1974) for the limiting case of an initial amount in each cell and where all leach rate constants are different. For other cases, analytical solutions to the first and second cell in a system are developed. For the case of no cell interchange, the governing equation is:

$$\frac{dQ_{i,j}}{dt} = \kappa_{i-1,j}Q_{i-1,j} - \kappa_{i,j}Q_{i,j} - \lambda_j Q_{i,j} + S_{i,j} + BR_j\lambda_{j-1}Q_{i,j-1} \tag{B-2}$$

where

$Q_{i,j}$ =   the mass of contaminant j in cell i (M)

i =   the cell index

j =   the index for the decay chain member

BR_j =   the fraction of decay product j–1 that decays to product j

$\kappa_{i,j}$ =   the leach rate constant describing transfer from cell i to cell i+1 for decay product j (T^{-1})

$S_{i,j}$ =   is the source term (M T^{-1})

λ =   decay rate constant (T^{-1}).

For the originating contaminant containing a series of degradation products, the term, $BR_j . \lambda_{j-1} Q_{i,j-1}$ is omitted. Equation B-2 has three solutions for the first and second cell depending on the initial conditions and whether there is an external source involved. For the case where $Q_{1,1} = Qo_{1,1}$ at $t = 0$, $S(t) = 0$ for all time, and $C_{11} \leq C_{Sl}$, the solution is:

$$Q_{1,1}(t) = Qo_{1,1} \exp\left(-\left(\kappa_{1,1} + \lambda_1\right)t\right) . \tag{B-3}$$

For the case where $Q_{1,1} = 0$ at $t = 0$, and $S(t)$ is a constant, R, for all time, the solution is:

$$Q_{1,1}(t) = \frac{R}{\kappa_{1,1} + \lambda}\left(1 - \exp\left[-\left(\kappa_{1,1} + \lambda_1\right)t\right]\right) . \tag{B-4}$$

The solution to the second cell for the conditions in Equation B-4 and $Q_{2,1} = 0$ at $t = 0$ can be found using Laplace transforms. The governing differential equation is given by:

$$\frac{dQ_{2,1}}{dt} = \frac{\kappa_{1,1}R}{\gamma}\left[1 - \exp(-\gamma t)\right] - \delta Q_{2,1} \tag{B-5}$$

where

γ = $\kappa_{1,1} + \lambda_1$

δ = $\kappa_{2,1} + \lambda_{1.}$

The solution is

$$Q_{2,1}(t) = \kappa_{1,1}R\left(\frac{1}{\gamma\delta} + \frac{\gamma e^{-\delta t} - \delta e^{-\gamma t}}{\gamma\delta(\delta - \gamma)}\right) . \tag{B-6}$$

For a decay chain of more than one member, a generalized solution to the multi-cell catenary system has been developed by Skrable et al. 1974 and implemented in a computer algorithm by Birchall (1986) for the limiting conditions, $S(t) = 0$ for all times, $\kappa_i \neq \kappa_{i+1}$ for all i, and $Q_{i,j} = Qo_{i,j}$ at $t = 0$.

$$Q_n(t) = \sum_{i=1}^{n}\left[\left(\prod_{j=1}^{n-1}K_j\right)\sum_{j=i}^{n}\frac{Qo_i e^{-KT_j t}}{\prod_{\substack{p\neq j \\ p=i}}^{n}\left(KT_p - KT_j\right)}\right] \tag{B-7}$$

where

$Q_n(t)$ =   mass in the *nth* cell in the system (M)

Q_o =   the initial amount in the *nth* cell in the system (M)

K_j =   the rate constant from cell *j* to cell *j*+1 (T^{-1})

KT_j =   the total transfer rate constant out of cell *j* (T^{-1}).

When the pore water concentration exceeds the solubility limit of the contaminant, then a solubility-limited release is calculated. The solubility-limited release in the first cell where $S(t) = 0$ for all times is described by the differential equation:

$$\frac{dQ_{1,1}}{dt} = -\lambda_1 Q_{1,1} - R_s \tag{B-8}$$

where

R_s = $S_L \times q \times A$

S_L =   solubility limit ($M\ L^{-3}$)

q =   water flux ($L\ T^{-1}$)

A =   area of source (L^2).

The solution to Equation B-8 for the initial conditions, $Q_{1,1} = Qo_{1,1}$ at $t = 0$, is:

$$Q_{1,1}(t) = Qo_{1,1} \exp(-\lambda_1 t) - \frac{R_s}{\lambda_1}\left[1 - \exp(-\lambda_1 t)\right] . \tag{B-9}$$

When the pore water concentration is less than the solubility limit, then $Q(t)$ is described by:

$$Q_{1,1}(t) = Q_{1,1}(t_{sl}) \exp\left[-\left(\kappa_{1,1} + \lambda_1\right)\left(t - t_{sl}\right)\right] \tag{B-10}$$

where $t \geq t_{sl}$, and t_{sl} is the time when the pore water concentration drops below the solubility limit.

B-1.2   Verification Problem 1

Verification Problem 1 considers a two-cell model with an initial radioactivity inventory of zero in all cells and a constant release rate of 1 Ci y^{-1} into the first cell. A hypothetical radionuclide having a half-life of 100 years and a molecular weight of 138 g mol^{-1} is simulated. Water flux is assumed to be at steady state and different for each cell. Input data are presented in Table B-1. Radionuclide inventories were converted to pore water concentrations using Equation B-10. Radioactive inventories were calculated using Equation B-4 for the first cell and Equation B-6 for the second cell.

Table B-1. Parameter Values used in Verification Test Problems 1, 2, and 4.

Parameter	Cell 1	Cell 2
Thickness (m)	1.00E+00	1.00E+00
Length (m)	1.00E+01	1.00E+01
Width (m)	1.00E+01	1.00E+01
Bulk Density (g cm^{-3})	1.50E+00	1.50E+00
Saturated hydraulic conductivity (m y^{-1})	1.71E+03	1.71E+03
Total porosity (m^3 m^{-3})	2.72E-01	2.72E-01
Residual moisture content (m^3 m^{-3})	3.21E-02	3.21E-02
van Genuchten alpha (m^{-1})	7.51E+00	7.51E+00
van Genuchten n	2.30E+00	2.30E+00
Water flux (m y^{-1})	1.00E-01	5.00E-02
Half-life (y)	1.00E+02	1.00E+02
Molecular weight (g mol^{-1})	1.38E+02	1.38E+02
Solubility limit (mg L^{-1})	1.00E+00	1.00E+00
Partition coefficient (mL g^{-1})	1.00E-01	5.00E-01
Initial moisture content[a]	6.06E-02	5.61E-02
Leach rate constants[a] (y^{-1})	4.75E-01	6.20E-02
Solubility limit[a] (Ci m^{-3})	2.59E+01	2.59E+01

a. Calculated values

Results of Verification Problem 1 (Table B-2) for the first two cells indicate good agreement between MCMT and the analytical solution. The differences are ≤0.004%.

B-1.3   Verification Problem 2

Verification Problem 2 considers the same model as Verification Problem 1 but $R(t) = 0$ and $Q_{1,1}(0) = 1.0$ Ci. Radionuclide inventories and pore water concentrations for cell 1 were calculated using Equations B-2 and 10, respectively. The results (Table B-3) indicate very little difference between the analytical solution and MCMT. Differences between the analytical solution and MCMT increase as the inventory decreases. However, differences are still less than 0.05 percent, and the inventory at those times (42 and 54 years) is nine orders of magnitude smaller than the initial inventory.

B-1.4   Verification Problem 3

Verification Problem 3 uses the general solution developed Skrable et al. (1974) and implemented by Birchall (1986) to solve a four cell model with a two member decay chain consisting of Pu-241 ($T1/2 = 14.4$ years) and Am-241 ($T1/2 = 432$ years). Parameters values (Table B-4) include the initial inventories of Pu-241 and Am-241 in each of the cells, cell-specific partition coefficients, and a constant water flux.

Table B-2. Results of Verification Problem 1.

Time (y)	MCMT Inventory (Ci)	Analytical Solution (Ci)	% Difference	MCMT Conc. (Ci m^{-3})	Analytical Solution (Ci m^{-3})	% Difference	MCMT Inventory (Ci)	Analytical Solution (Ci)	% Difference
		Cell 1						Cell 2	
2	1.28E+00	1.28E+00	0.003%	6.10E-02	6.10E-02	0.002%	6.723E-01	6.723E-01	0.001%
6	1.96E+00	1.96E+00	0.002%	9.31E-02	9.31E-02	0.001%	3.397E+00	3.397E+00	0.001%
10	2.06E+00	2.06E+00	0.002%	9.78E-02	9.78E-02	0.002%	5.942E+00	5.942E+00	0.000%
14	2.07E+00	2.07E+00	0.000%	9.84E-02	9.84E-02	0.002%	7.943E+00	7.943E+00	0.001%
20	2.08E+00	2.08E+00	0.000%	9.86E-02	9.86E-02	0.001%	1.009E+01	1.009E+01	0.002%
28	2.08E+00	2.08E+00	0.002%	9.86E-02	9.86E-02	0.002%	1.187E+01	1.187E+01	0.000%
36	2.08E+00	2.08E+00	0.002%	9.86E-02	9.86E-02	0.002%	1.290E+01	1.290E+01	-0.002%
42	2.08E+00	2.08E+00	0.002%	9.86E-02	9.86E-02	0.002%	1.337E+01	1.337E+01	0.000%
54	2.08E+00	2.08E+00	0.002%	9.86E-02	9.86E-02	0.002%	1.389E+01	1.389E+01	0.004%

Table B-3. Results of Verification Problem 2 for Cell 1.

Time (y)	MCMT Inventory (Ci)	Analytical Solution (Ci)	% Difference	MCMT Conc. (Ci m^{-3})	Analytical Solution (Ci m^{-3})	% Difference
2	3.82E-01	3.82E-01	-0.002%	1.81E-02	1.81E-02	0.002%
6	5.55E-02	5.55E-02	-0.005%	2.64E-03	2.64E-03	0.005%
10	8.09E-03	8.09E-03	-0.008%	3.84E-04	3.84E-04	-0.08%
14	1.18E-03	1.18E-03	-0.010%	5.59E-05	5.59E-05	-0.010%
20	6.54E-05	6.54E-05	-0.016%	3.10E-06	3.10E-06	-0.016%
28	1.39E-06	1.39E-06	-0.019%	6.58E-08	6.58E-08	-0.019%
36	2.94E-08	2.94E-08	-0.029%	1.39E-09	1.39E-09	-0.029%
42	1.63E-09	1.63E-09	-0.031%	7.75E-11	7.74E-11	-0.031%
54	5.03E-12	5.03E-12	-0.044%	2.39E-13	2.39E-13	-0.044%

Table B-4. Parameters Values for Verification Problem 3.

Parameter	Cell 1	Cell 2	Cell 3	Cell 4
Length (m)	1.0	1.0	1.0	1.0
Width (m)	1.0	1.0	1.0	1.0
Thickness (m)	0.02	0.13	0.15	0.2
Bulk density (g cm^{-3})	1.2	1.5	1.5	1.8
Saturated hydraulic conductivity (m y^{-1})	1710	1710	1710	1710
Porosity	0.2724	0.2724	0.2724	0.2724
Residual moisture content	0.0321	0.0321	0.0321	0.0321
Alpha (m^{-1})	7.71	7.71	7.71	7.71
rn	2.28	2.28	2.28	2.28
Calculated moisture content	0.0659	0.0659	0.0659	0.0659
Water flux, $t = 0$ to $t = \infty$ (m y^{-1})	0.2	0.2	0.2	0.2
Pu-241 partition coefficient (mL g^{-1})	10	15	22	22
Am-241 partition coefficient (mL g^{-1})	50	60	70	70
Pu-241 solubility (mg L^{-1})	infinite	infinite	infinite	infinite
Am-241 solubility (mg L^{-1})	infinite	infinite	infinite	infinite
Pu-241 initial inventory (Ci)	2.40E-05	5.46E-04	6.75E-05	2.72E-11
Am-241 initial inventory (Ci)	4.80E-07	2.93E-06	2.25E-07	2.86E-14

As shown in Figure B-1 (for Pu-241) and Figure B-2 (for Am-241), there is excellent agreement between the analytical solution and MCMT. Differences between the analytical expression and MCMT for the maximum inventory beyond 1-year ranged from 0.0000% for Pu-241 in cell 3, to 0.1277% for Am-241 in cell 4.
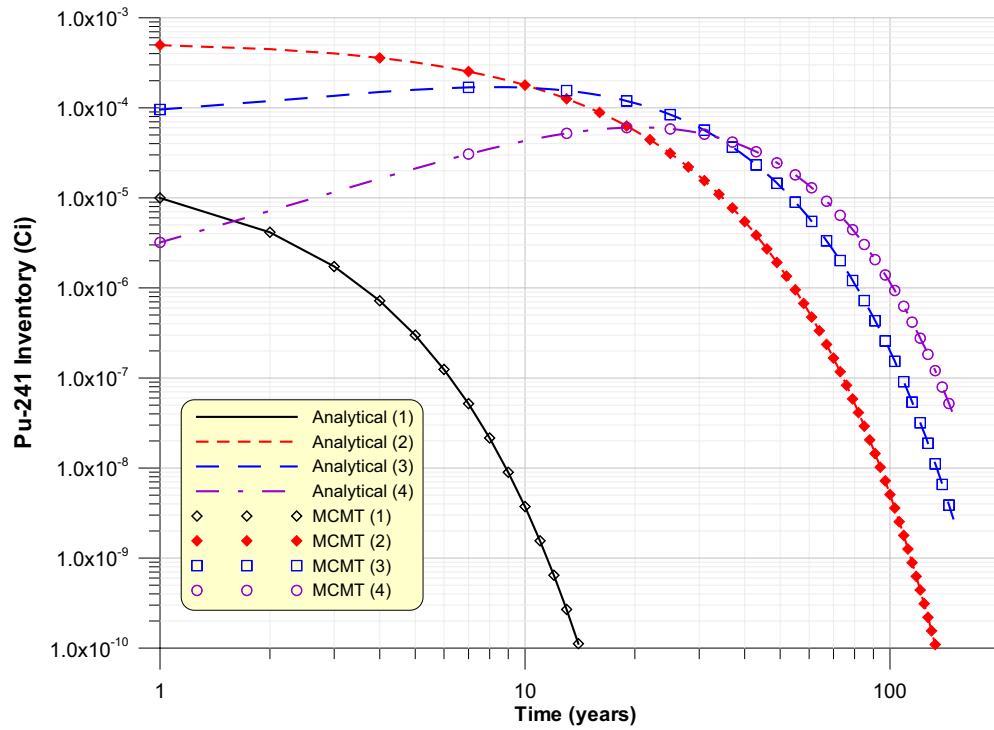
Figure B-1. Plutonium-241 inventory as a function of time calculated with the analytical solution developed by Birchall (1986) and MCMT. The numbers in parentheses in the legend refer to the cell number.
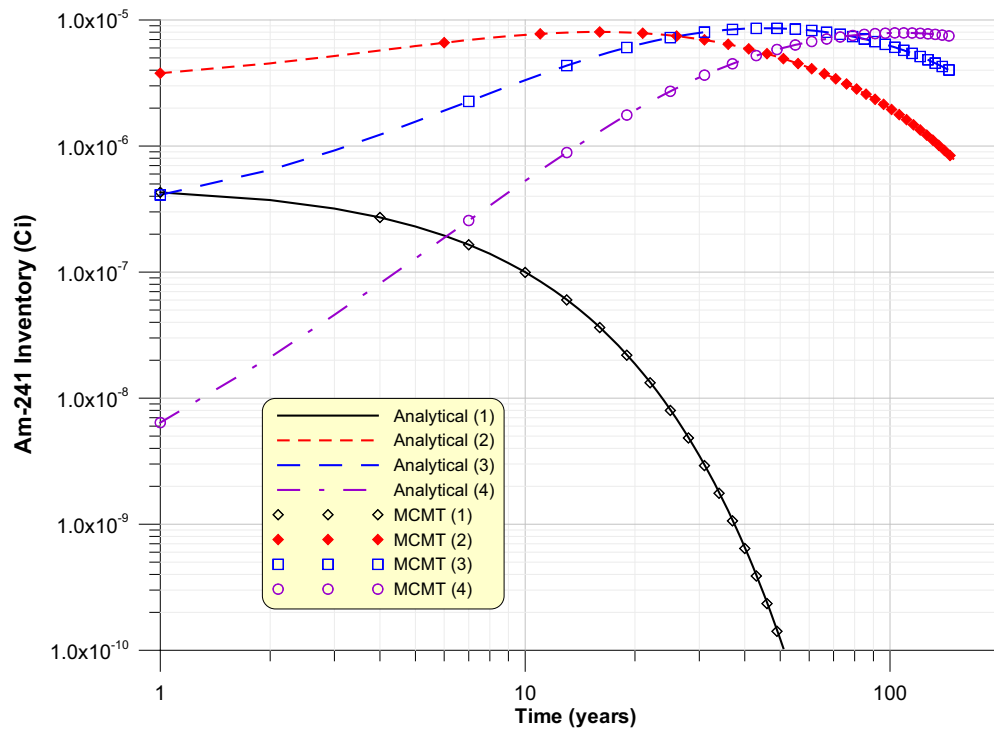
Figure B-2. Americium-241 inventory as a function of time calculated with the analytical solution developed by Birchall (1986) and MCMT. The numbers in parentheses in the legend refer to the cell number.

B-1.5 Verification Problem 4

Verification Problem 4 checks the solubility limited release function in MCMT with the analytical solution expressed by Equations B-9 and B-10. The problem uses the same parameters used in Verification Problem 2, except the initial inventory is set to 1×10^4 Ci. The flux from cell 1 was also output and compared with output from the GWSCREEN model (Rood 1999), which includes the solubility release model described in Equations B-9 and B-10. Results (Table B-5) show good agreement between MCMT, the analytical solution, and GWSCREEN. Differences are no greater than 0.163 percent.

Table B-5. Inventory and Flux from Cell 1 for Verification Problem 4.

Time (y)	MCMT Inventory (Ci)	Analytical Solution (Ci)	% Difference	MCMT Flux (Ci y^{-1})	GWSCREEN Flux (Ci y^{-1})	% Difference
2	9.35E+03	9.35E+03	-0.001%	2.59E+02	2.59E+02	0.012%
6	8.07E+03	8.07E+03	-0.002%	2.59E+02	2.59E+02	0.012%
10	6.83E+03	6.83E+03	-0.005%	2.59E+02	2.59E+02	0.012%
14	5.62E+03	5.62E+03	-0.008%	2.59E+02	2.59E+02	0.012%
20	3.86E+03	3.86E+03	-0.015%	2.59E+02	2.59E+02	0.012%
28	1.64E+03	1.64E+03	-0.048%	2.59E+02	2.59E+02	0.012%
36	8.30E+01	8.29E+01	-0.162%	3.94E+01	3.95E+01	0.119%
42	4.61E+00	4.60E+00	-0.162%	2.19E+00	2.19E+00	0.146%
54	1.42E-02	1.42E-02	-0.163%	6.76E-03	6.76E-03	0.115%

B-2. MCMT BENCHMARK PROBLEM

The primary output of MCMT is the radionuclide flux from the unsaturated zone to the aquifer. In this section, the radionuclide flux to the aquifer calculated with MCMT is compared to the radionuclide flux calculated using the Disposal Unit Source Term (DUST) (Sullivan 1996) model. The DUST model solves the one-dimensional transport equation for parent and progeny using an implicit finite difference scheme. Temporal changes in water fluxes and spatial distribution of moisture content are specified by the user in DUST and not calculated within the code; hence transient water flux is not modeled in DUST but rather is specified.

The benchmark exercise with DUST considered a 11.5 m of contaminated soil containing 6.42 Ci of U-238. The soil contamination covers an area of ~0.2 km^2 (382 m × 512 m). An 81 m thick unsaturated zone underlies the contaminated soil. Model parameters are described in Table B-6. Moisture contents in DUST are not allowed to change over time. Therefore, a fixed value of 0.05 was used throughout the model domain. Uranium-238 has several important radioactive daughters that will grow in over time and are therefore, also modeled. These daughters are (in descending order) U-234 (T1/2 = 245,000 yr), Th-230 (T1/2 = 75,400 yr), and Ra-226 (T1/2 =- 1600 yr). Uranium-238 has a long half life (4.47E+09 yr) and little will decay during transport in the unsaturated zone. Therefore, if the simulation is run for sufficient time, the integrated U-238 flux at the bottom of the model domain should equal the total initial activity at the beginning of the simulation.

Table B-6. Parameter values used in the DUST benchmark exercise.

Parameter	Value
Thickness of source cell (m)	11.5
Finite difference node spacing in DUST (m)	0.5
Length of source (m)	382
Width of source and unsaturated cells (m)	518
Initial U-238 activity (Ci)[a]	6.42
Bulk density of contaminated soil (g cm^{-3})	1.26
Moisture content throughout model domain (m^3 m^{-3})	0.05
Uranium partition coefficient, 0 m to 23.14 m (mL g^{-1})	0.2
Thorium partition coefficient, 0 m to 23.14 m (mL g^{-1})	5.0
Radium partition coefficient, 0 m to 23.14 m (mL g^{-1})	0.4
Uranium partition coefficient, 23.14 m to 92.5 m (mL g^{-1})	3
Thorium partition coefficient, 23.14 m to 92.5 m (mL g^{-1})	1000
Radium partition coefficient, 23.14 m to 92.5 m (mL g^{-1})	20
Water flux (m y^{-1})	0.02
Dispersivity	4.1
Number of MCMT cells	24
Thickness of each cell (m)	3.854
Total thickness of domain (m)	92.5

a. In DUST, this was simulated by setting the initial U-238 pore water concentration at 10 pCicm^{-3} in the first 22 nodes of the model domain.

Results of the simulation are presented in Table B-7 and Figure B-3. In general, differences in the three essential quantities (maximum flux, time of maximum flux, and integrated flux) differ by less than about 5% between the two models, although MCMT consistently calculates higher fluxes and longer travel times relative to DUST. The total integrated flux out the bottom of the model domain for MCMT agrees well with the total initial amount (6.42 Ci) of U-238 present at the start of the simulation. However, DUST only calculated 6.36 Ci released, which equates to about a 1% mass balance error.

Table B-7. Results of MCMT benchmark with DUST.

Model	Quantity	U-238	U-234	Th-230	Ra-226
MCMT	Maximum Flux (Ci yr^{-1})	5.03E-04	2.17E-05	7.22E-09	3.51E-07
MCMT	Time of maximum	1.47E+04	1.63E+04	3.18E+04	3.43E+04
MCMT	Cumulative Flux (Ci)	6.42E+00	3.04E-01	7.36E-04	3.59E-02
DUST	Maximum Flux (Ci yr^{-1})	4.90E-04	2.06E-05	7.03E-09	3.43E-07
DUST	Time of maximum	1.42E+04	1.58E+04	3.17E+04	3.41E+04
DUST	Cumulative Flux (Ci)	6.36E+00	2.99E-01	7.27E-04	3.55E-02
	% Difference maximum flux	-2.68%	-5.30%	-2.64%	-2.41%
	% Difference time of maximum	-3.59%	-3.23%	-0.35%	-0.62%
	% difference cumulative flux	-0.94%	-1.58%	-1.29%	-1.04%
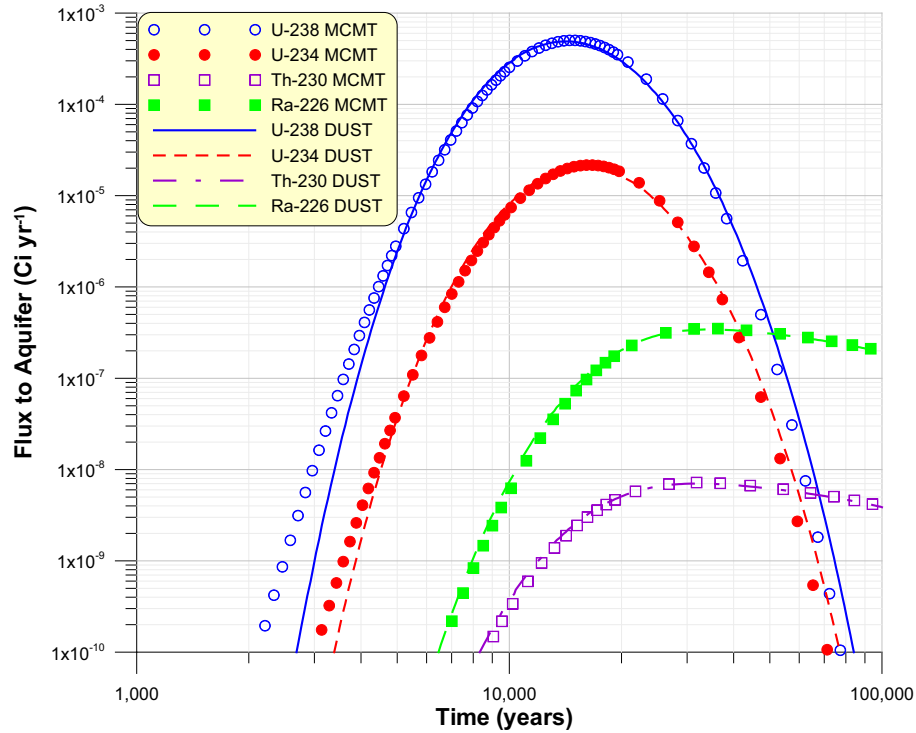
Figure B-3. Comparison of the aquifer flux calculated by MCMT and DUST.

The benchmark illustrates that the MCMT model produces results that are comparable to those derived from finite difference solutions of the advection-dispersion equation, and that the mixing-cell model is a good approximation to advection-dispersion behavior.

B-3. MCMF VERIFICATION PROBLEMS

The primary verification problem for MCMF is in Section 4 in the main body of the report. Figure 4 in the main body of the report illustrates the sensitivity of the number of cells to the water flux profile. Figure 5 illustrates the passage of a wetting front as a function of time as estimated by MCMF and the HYDRUS-2D finite element code. Excellent agreement between the two codes is found by fitting a proper number of cells to the problem. The number of cells needed to fit the water flux profile is defined by Equation 35.

In this section, MCMF is benchmarked against HYDRUS-2D for an arbitrary problem. Equation 35 is used to estimate the number of cells needed for the simulation. The water flux output is then used with MCMT to estimate solute fluxes at the base of the model domain. Solute fluxes calculated with MCMT are then compared to solute fluxes calculated with HYDRUS-2D.

B-3.1 Problem Description

The benchmark problem considered a 30-m thick homogeneous unsaturated zone consisting of sandy clay loam with an initial water flux (q_o) of 0.01 m yr^{-1} and an initial solute mass of ~0.25 g that occupied the first 1.5 m ($z = 0$ m to $z = 1.5$ m) of the model domain. The van Genuchten fitting parameters for sandy clay loam are found in Table 1 in the main body of the report. The system is subject to a new water flux (q_n) of 10-year duration after which it returns to its baseline value of q_o. Three cases were considered: $q_n = 0$, $q_n = 6 \times q_o$, and $q_n = 10 \times q_o$. The solute was assumed to have an infinite half-life

and a sorption coefficient of zero mL g^{-1}. A dispersivity of 1.1 m was used in all three cases resulting in a scale-length Peclet number of 30 m ÷ 1.1 m = 27.27. Because Case 1 involved steady-state flow conditions, the number of cells were chosen such that $n > Pe/2$. Cases 2 and 3 are transient flow simulations; therefore, Equations 34 and 35 were used to determine the number of mixing cells needed to simulate transient flow behavior.

The number of cells needed to simulate transient flow behavior used Equation 34 to calculate the value φ and the Equation 35 to calculate n. Calculation of the number of cells is organized in Table B-8. The hydraulic diffusivity is determined using the utility program, DHYD.FOR.

Table B-8. Data and calculations to determine the number of mixing cells.

Quantity	Steady State	$q_n = 6 \times q_o$	$q_n = 10 \times q_0$
Initial solute mass, Q_0 (g)	0.254	0.252	0.252
q_o (m yr^{-1})	1.00E-02	1.00E-02	1.00E-02
q_n (m yr^{-1})	1.00E-02	6.00E-02	1.00E-01
Duration of new flux (yr)	N/A	10	10
Initial moisture content, θ_o	1.9966E-01	1.9966E-01	1.9966E-01
New moisture content, θ_n	N/A	2.2973E-01	2.3974E-01
Wetting front speed, u_{wf} (m yr^{-1})	N/A	1.663E+00	2.246E+00
Time of arrival, t_{wf} (yr)	N/A	1.804E+01	1.336E+01
Initial hydraulic diffusivity, D_{ho} (m^2 yr^{-1})	3.3246E-01	3.3246E-01	3.3246E-01
φ	N/A	1.432E+02	1.934E+02
n	30	36	48
Cell thickness (m)	1.0	0.83333	0.63830

The HYDRUS domain was discretized into sixty, 0.5-m thick elements and a maximum time step of 100 days was specified for Cases 1 and 2, and 50 days for Case 3. The results of the simulation show that there is little difference between the water fluxes calculated by the two models (Figure B-4). The solute fluxes are illustrated in Figure B-5. While there are differences between the solute flux estimated by HYDRUS and that of the mixing-cell model, those differences are not meaningful when the overall uncertainty in an unsaturated flow and transport model are considered. The percent difference between the maximum solute flux estimated with HYDRUS and that of the mixing-cell model was 1.03% for Case 1, 1.26% for Case 2, and 1.78% for Case 3. However, what is more important is that the mixing-cell model mimics the behavior of HYDRUS for the three cases. That is, a pulse of water entering the top of the unsaturated zone results in shorter solute travel times and greater solute dilution. Consequently, solute fluxes are slightly lower for higher values of q_n.
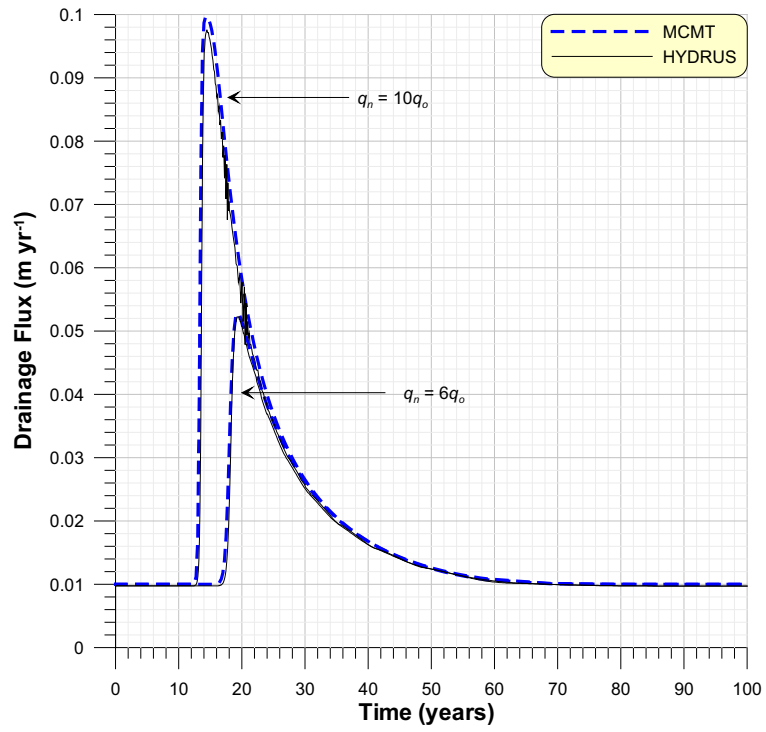
Figure B-4. Water fluxes as a function of time at $z = Z$ for Cases 2 and 3.
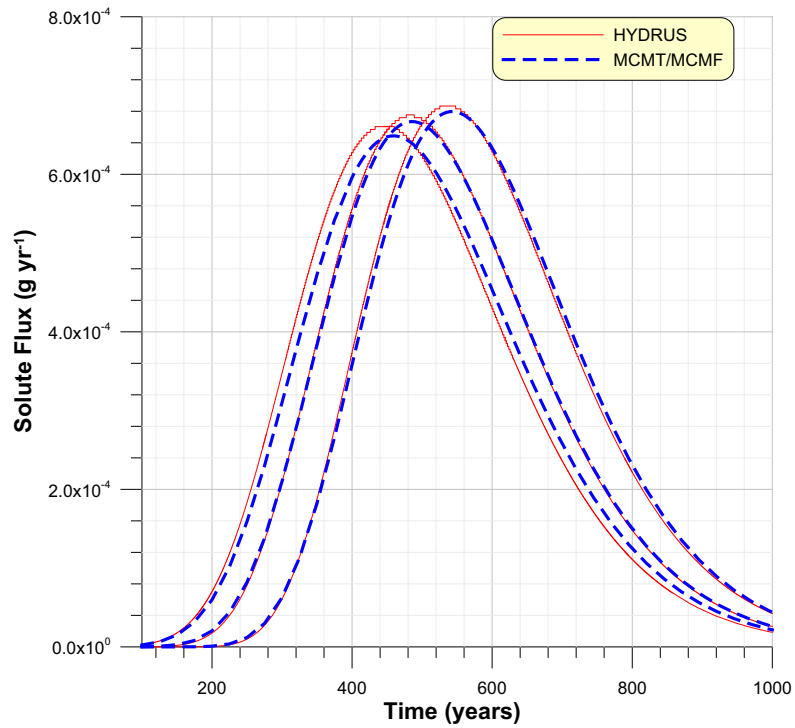
Figure B-5. Solute fluxes as a function of time for Cases 1, 2, and 3.

B-14

B-4. MCMT INPUT FILES

```
Verification Problem 1 for MCMF                                      title  [title of project]
water.flx                                                           fileppt   [water flux file from MCMF]
verify1.inv                                                         filerel   [contaminant source term file]
1.0e-6  1.0e-3 1.0e-60                                              eps,h1,hmin [accuracy, initial time step, minimum time step]
3  1  1  1  A                                                       mlayer,nprog,nmat,iunits,abin  [number of layers,number of contaminants, number of materials, units of measure, (A)scii or (B)inary
$[abin: (A)scii or (B)inary]
$[iunits: (1) Ci (2) Bq  (3) mg]
verify1                                                             cname [contaminant names (6 characters)]
138                                                                 mw [ molecular weight (g/mol)]
1000                                                                sol [solubility limit (mg/m**3)]
100                                                                 thalf [half lives years]
1.0                                                                 bratio [branching ratio]
0.0                                                                 dwater [water diffusivity]
$ [intial inventories in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
$     1      2      3      4      5      6      7      8      9     10     11     12     13     14     15     16     17     18     19     20
     0.     0.     0.     y(i)
$ [kd values in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
     0.1    0.5    1.0  kd(i)
$ [kx values in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
     0.0    0.0    0.0  kx(i)
10. 10.  0.0                                                        lth,width,alphaL [length (m), width (m), longitudinal dispersivity (m)
$ [Material properities are input by defining the range of cells where they apply]
1 3                                                                 h,j [begining cell, ending cell]
1.0 1.5                                                             thick(h),rho(h) [thickness (m) bulk density (g/cc)]
1710,0.2724,0.0321,7.51,2.298                                       sk(h),ths(h),thr(h),alpha(h),rn(h) [Sat conductivity (m/yr) sat moist content, resid moist content, vanG alpha, vanG n]
$ [Time output parameters]
1                                                                   ntimes [number of output time periods]
$ [Repeat for each ntime]
0. 466. 2.0                                                         t1(i),t2(i),tp(i) [begining time of output ending time of output, print step]
$ [End of Parameter Definition File]


Verification Problem 2 for MCMF                                      title  [title of project]
water.flx                                                           fileppt   [water flux file from MCMF]
verify2.inv                                                         filerel   [contaminant source term file]
1.0e-6  .1    1.0e-60                                               eps,h1,hmin [accuracy, initial time step, minimum time step]
3  1  1  1  A                                                       mlayer,nprog,nmat,iunits,abin  [number of layers,number of contaminants, number of materials, units of measure, (A)scii or (B)inary
$[abin: (A)scii or (B)inary]
$[iunits: (1) Ci (2) Bq  (3) mg]
verify2                                                             cname [contaminant names (6 characters)]
138                                                                 mw [ molecular weight (g/mol)]
1000                                                                sol [solubility limit (mg/m**3)]
100                                                                 thalf [half lives years]
1.0                                                                 bratio [branching ratio]
0.0                                                                 dwater [water diffusivity]
$ [intial inventories in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
$     1      2      3      4      5      6      7      8      9     10     11     12     13     14     15     16     17     18     19     20
     1.     0.     0.     y(i)
$ [kd values in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
     0.1    0.5    1.0  kd(i)
$ [kx values in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
     0.0    0.0    0.0  kx(i)
10. 10.  0.0                                                        lth,width,alphaL [length (m), width (m), longitudinal dispersivity (m)
$ [Material properities are input by defining the range of cells where they apply]
1 3                                                                 h,j [begining cell, ending cell]
1.0 1.5                                                             thick(h),rho(h) [thickness (m) bulk density (g/cc)]
1710,0.2724,0.0321,7.51,2.298                                       sk(h),ths(h),thr(h),alpha(h),rn(h) [Sat conductivity (m/yr) sat moist content, resid moist content, vanG alpha, vanG n]
$ [Time output parameters]
1                                                                   ntimes [number of output time periods]
$ [Repeat for each ntime]
0. 466. 2.0                                                         t1(i),t2(i),tp(i) [begining time of output ending time of output, print step]
$ [End of Parameter Definition File]


Verification Problem 3 for MCMF                                      title  [title of project]
water.flx                                                           fileppt   [water flux file from MCMF]
verify3.inv                                                         filerel   [contaminant source term file]
```

```
1.0e-6  .1   1.0e-60                                         eps,h1,hmin [accuracy, initial time step, minimum time step]
4   2   4   1   A                                           mlayer,nprog,nmat,iunits,abin  [number of layers,number of contaminants, number of materials, units of measure, (A)scii or (B)inary]
$[abin: (A)scii or (B)inary]
$[iunits: (1) Ci (2) Bq  (3) mg]
Pu-241,Am-241                                               cname [contaminant names (6 characters)]
241 241                                                     mw [ molecular weight (g/mol)]
10000 10000                                                 sol [solubility limit (mg/m**3)]
14.4   432                                                  thalf [half lives years]
1.0    1.0                                                  bratio [branching ratio]
0.0    0.0                                                       dwater [water diffusivity]
$ [intial inventories in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
$     1      2       3       4       5       6       7       8       9      10      11      12      13      14      15      16      17      18      19      20
   2.40E-05 5.46E-04  6.75e-5 2.72e-11     y(i)
   4.80E-07 2.93E-06  2.25e-7 2.86e-14          initial am241 layer 1-4
$ [kd values in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
      10      15      22      22                  kd(i)
      50      60      70      70                  kd am241 layer 1-4
$ [kx values in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
      0.0      0.0      0.0      0.0   kx(i)
      0.0      0.0      0.0      0.0   kx(i)
1.  1.  0.0                                                 lth,width,alphaL [length (m), width (m), longitudinal dispersivity (m)]
$ [Material properities are input by defining the range of cells where they apply]
$ layer 1
1 1                                                        h,j [begining cell, ending cell]
0.02  1.2                                                  thick(1),rho(1)
1710,0.2724,0.0321,7.51,2.298                             sk(1),ths(1),thr(1),alpha(1),rn(1)
$  layer 2
2   2                                                      h,j [begining cell, ending cell]
0.13  1.5                                                  thick(2),rho(2)
1710,0.2724,0.0321,7.51,2.298                             sk(2),ths(2),thr(2),alpha(2),rn(2)
$  layer 3
3   3                                                      h,j [begining cell, ending cell]
0.15  1.5                                                  thick(3),rho(3)
1710,0.2724,0.0321,7.51,2.298                             sk(3),ths(3),thr(3),alpha(3),rn(3)
$  layer 4
4   4                                                      h,j [begining cell, ending cell]
0.2  1.8                                                   thick(3),rho(3)
1710,0.2724,0.0321,7.51,2.298                             sk(3),ths(3),thr(3),alpha(3),rn(3)
$ [Time output parameters]
1                                                         ntimes [number of output time periods]
$ [Repeat for each ntime]
0. 150. 1.0                                               t1(i),t2(i),tp(i) [begining time of output ending time of output, print step]
$ [End of Parameter Definition File]


Verification Problem 4 for MCMF                            title  [title of project]
water.flx                                                  fileppt   [water flux file from MCMF]
verify2.inv                                                filerel   [contaminant source term file]
1.0e-6  .000001   1.0e-90                                  eps,h1,hmin [accuracy, initial time step, minimum time step]
3  1  1  1  A                                              mlayer,nprog,nmat,iunits,abin  [number of layers,number of contaminants, number of materials, units of measure, (A)scii or (B)inary]
$[abin: (A)scii or (B)inary]
$[iunits: (1) Ci (2) Bq  (3) mg]
verify2                                                    cname [contaminant names (6 characters)]
138                                                        mw [ molecular weight (g/mol)]
1000                                                       sol [solubility limit (mg/m**3)]
100                                                        thalf [half lives years]
1.0                                                        bratio [branching ratio]
0.0                                                        dwater [water diffusivity]
$ [intial inventories in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
$     1      2       3       4       5       6       7       8       9      10      11      12      13      14      15      16      17      18      19      20
   10000.      0.       0.        y(i)
$ [kd values in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
      0.1      0.5      1.0  kd(i)
$ [kx values in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
      0.0      0.0      0.0   kx(i)
10.  10.  0.0                                              lth,width,alphaL [length (m), width (m), longitudinal dispersivity (m)]
$ [Material properities are input by defining the range of cells where they apply]
1 3                                                        h,j [begining cell, ending cell]
1.0 1.5                                                    thick(h),rho(h) [thickness (m) bulk density (g/cc)]
1710,0.2724,0.0321,7.51,2.298                             sk(h),ths(h),thr(h),alpha(h),rn(h) [Sat conductivity (m/yr) sat moist content, resid moist content, vanG alpha, vanG n]
$ [Time output parameters]
1                                                         ntimes [number of output time periods]
$ [Repeat for each ntime]
0. 466. 2.0                                               t1(i),t2(i),tp(i) [begining time of output ending time of output, print step]
$ [End of Parameter Definition File]
```

```
U-238 Benchmark with DUST                                           title  [title of project (a80)]
NONE                                                                fileppt   [water flux file from MCMF(a80)]
NONE                                                                filerel   [contaminant source term file (a80)]
1.0e-6  0.0001  1.0e-60                                             eps,h1,hmin [accuracy, initial time step, minimum time step]
24  4  2  1  A                                                      mlayer,nprog,nmat,iunits,abin  [number of layers,number of contaminants, number of materials, units of measure, (A)scii or (B)inary]
$[abin: (A)scii or (B)inary]
$[iunits: (1) Ci (2) Bq  (3) mg]
'U-238' 'U-234' 'Th-230' 'Ra-226'                                   cname [contaminant names (6 characters)]
238  234  230  226                                                  mw [ molecular weight (g/mol)]
2.5e6  2.5e6  1e7  1e7                                              sol [solubility limit (mg/m**3)]
4.468E+09  2.450E+05  7.538E+04  1.600E+03                          thalf [half lives years]
1.0  1.0  1.0  1.0          bratio [branching ratio]
0.0  0.0  0.0  0.0          dwater [water diffusivity]
$ [intial inventories in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
$       1       2       3       4       5       6       7       8       9      10      11      12      13      14      15      16      17      18      19      20

$ U-238
   2.14E+00  2.14E+00  2.14E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00
   0.0E+00  0.0E+00  0.0E+00  0.0E+00
$ U-234
   0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00
   0.0E+00  0.0E+00  0.0E+00  0.0E+00
$ Th-230
   0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00
   0.0E+00  0.0E+00  0.0E+00  0.0E+00
$ Ra-226
   0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00
   0.0E+00  0.0E+00  0.0E+00  0.0E+00


$ [kd values in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
   2.0E-01  2.0E-01  2.0E-01  2.0E-01  2.0E-01  2.0E-01  3.0E-00  3.0E-00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00   U-238
kd(i)
   3.0E+00  3.0E+00  3.0E+00  3.0E+00

   2.0E-01  2.0E-01  2.0E-01  2.0E-01  2.0E-01  2.0E-01  3.0E-00  3.0E-00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00  3.0E+00   U-238
kd(i)
   3.0E+00  3.0E+00  3.0E+00  3.0E+00

   5.0E+00  5.0E+00  5.0E+00  5.0E+00  5.0E+00  5.0E+00  1.0E+03  1.0E+03  1.0E+03  1.0E+03  1.0E+03  1.0E+03  1.0E+03  1.0E+03  1.0E+03  1.0E+03  1.0E+03  1.0E+03  1.0E+03  1.0E+03   Th-230
kd(i)
   1.0E+03  1.0E+03  1.0E+03  1.0E+03

   4.0E-01  4.0E-01  4.0E-01  4.0E-01  4.0E-01  4.0E-01  2.0E+01  2.0E+01  2.0E+01  2.0E+01  2.0E+01  2.0E+01  2.0E+01  2.0E+01  2.0E+01  2.0E+01  2.0E+01  2.0E+01  2.0E+01  2.0E+01   Ra-226
kd(i)
   2.0E+01  2.0E+01  2.0E+01  2.0E+01
$ [kx values in each cell, 20 values per line are read begining with the uppermost cell]
$ [all values for the 1st member are read first, then the second and so on]
   0.00E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00   U-238
kx(i)
   0.0E+00  0.0E+00  0.0E+00  0.0E+00
   0.00E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00   U-234
kx(i)
   0.0E+00  0.0E+00  0.0E+00  0.0E+00
   0.00E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00   Th-230
kx(i)
   0.0E+00  0.0E+00  0.0E+00  0.0E+00
   0.00E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00  0.0E+00   Ra-226
kx(i)
   0.0E+00  0.0E+00  0.0E+00  0.0E+00
382 518  4.1               lth,width,alphaL [length (m), width (m), longitudinal dispersivity (m)]
$ [Material properities are input by defining the range of cells where they apply]
1 3                        h,j  [begining cell, ending cell]
3.854 1.26  382 518        thick(h),rho(h) [thickness (m) bulk density (g/cc)]
0.02,-0.05,0.0321,7.51,2.298    sk(h),ths(h),thr(h),alpha(h),rn(h) [Sat conductivity (m/yr) sat moist content, resid moist content, vanG alpha, vanG n]
4  24                      h,j  [begining cell, ending cell]
3.854   1.6                thick(h),rho(h) [thickness (m) bulk density (g/cc)]
0.02,-0.05,0.0321,7.51,2.298    sk(h),ths(h),thr(h),alpha(h),rn(h) [Sat conductivity (m/yr) sat moist content, resid moist content, vanG alpha, vanG n]
$ [Time output parameters]
$ output times
9                                  ntimes
0.     200.   2.                   t1,t2,tp
205.   500.   5.                   t1,t2,tp
510.   1000.  10.                  t1,t2,tp
1025.  5000.  25.                  t1,t2,tp
5050.  10000. 50.                  t1,t2,tp
10100. 20000. 100.                 t1,t2,tp
20500. 40000. 500.                 t1,t2,tp
41000. 1.0e5 1000.                 t1,t2,tp
```

```
1.05e5 2.0e5  5000.                      t1,t2,tp
$ [End of Parameter Definition File]


Benchmark 3a with HYDRUS
'..\mcmfa\mcmf.flx'
NONE                                                               No release file
1.0e-6 0.1   1.E-70            eps  h1 hmin
30  1  1   1   A              mlayer nprog nmat
'tracer'
14                            mw
1e9                           sol
1.e8                          thalf
1.0                           bratio
0.0                           dwater
$ initial inventory progeny 1
2.54e-01 0.00e+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00  y(i)
0.00e+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00  y(i)
$ kd values progeny 1  layer 1-15
0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00   0.0E+00 0.0E+00 0.0E+00 0.0E+00     kd(i)
0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00   0.0E+00 0.0E+00 0.0E+00 0.0E+00     kd(i)
$ kx values progeny 1-15
0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00   0.0E+00 0.0E+00 0.0E+00 0.0E+00 kx(i)
0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00   0.0E+00 0.0E+00 0.0E+00 0.0E+00 kx(i)
$ dimensions and dispersivity
1.0   1.0   1.1              len width alphaL
$ Materail properties
1 30                          layer 1 to 1  Sand
1.00  1.5                     thick(1),rho(1)
114.76,0.39,0.10,5.9,1.48      sk(1),ths(1),thr(1),alpha(1),rn(1)
$ output times
3                            ntimes
0.    400   25.                 t1,t2,tp
405   700   5.
725   1500  25.
0


Benchmark 3a with HYDRUS  6x
'..\mcmfd\mcmf.flx'
NONE
1.0e-6 0.001  1.E-60          eps  h1 hmin
36  1  1   1   A              mlayer nprog nmat
'tracer'
14                            mw
1e9                           sol
1.e8                          thalf
1.0                           bratio
0.0                           dwater
$ initial inventory progeny 1
$ 1       2       3       4       5       6       7       8       9       10      11      12      13      14      15      16      17      18      19      20
0.126e-00 0.126e-00 0.00E-00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00   y(i)
0.00e+00 0.0E+00  0.0E+00  0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00  y(i)
$ kd values progeny 1  layer 1-30
0.00e+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00     kd(i)
0.00e+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00  0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00  kd(i)
$ kx values progeny 1-30
0.00e+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00   kx(i)
0.00e+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00  0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00  kd(i)
$ dimensions and dispersivity
1.0   1.0   1.10             len width alphaL
$ Materail properties
1 36                          layer 1 to 1  Sand
0.83333   1.5                 thick(1),rho(1)
114.76,0.39,0.10,5.9,1.48      sk(1),ths(1),thr(1),alpha(1),rn(1)
$ output times
3                            ntimes
0.    400   25.                 t1,t2,tp
405   700   5.
725   1500  25.
0


Benchmark 3a with HYDRUS  10x
'..\mcmfe\mcmf.flx'
NONE
1.0e-6 0.1   1.E-70            eps  h1 hmin
48  1  1   1   A              mlayer nprog nmat
'tracer'
14                            mw
1e9                           sol
1.e8                          thalf
```

```
1.0                          bratio
0.0                          dwater
$ initial inventory progeny 1
$ 1      2      3      4      5      6      7      8      9      10     11     12     13     14     15     16     17     18     19     20
1.26e-01 1.26E-01 0.00E-00 0.0E-00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00  y(i)
0.00e+00 0.0E+00  0.0E+00  0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00  y(i)
0.0E+00  0.0E+00  0.0E+00  0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00
$ kd values progeny 1  layer 1-50
0.00e+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00  kd(i)
0.00e+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00  kd(i)
kd(i)
0.0E+00  0.0E+00  0.0E+00  0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00
$ kx values progeny 1-50
0.00e+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00  kx(i)
0.00e+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00  kx(i)
kx(i)
0.0E+00  0.0E+00  0.0E+00  0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00 0.0E+00
$ dimensions and dispersivity
1.0   1.0   1.1              len width alphaL
$ Materail properties
1 48                         layer 1 to 1  Sand
0.6383  1.5                  thick(1),rho(1)
114.76,0.39,0.10,5.9,1.48    sk(1),ths(1),thr(1),alpha(1),rn(1)
$ output times
3                            ntimes
0.     400    25.                 t1,t2,tp
405    700    5.
725    1500   25.
0
```

B-5. MCMF INPUT FILES

```
Benchmark 3 with HYDRUS - steady state flux
'mcmf.flx'
'mcmf.pcp'
1.0e-6 .0001   1.0e-30           eps h1 hmin
30 1 100   0.011 0.009 0  A        mlayer nmat nkt qmax qmin iflag abin
$ Materail properties
1 30                         layer 1 to 1  Sand
1.0                          thick(1)
114.76,0.39,0.10,5.9,1.48    sk(1),ths(1),thr(1),alpha(1),rn(1)
$ output times
6                            ntimes
0.     10    1               t1,t2,tp
10.25  40    0.25
41.    60.   1.              t1,t2,tp
70.    150.  10.             t1,t2,tp
175    250   25
300  1500    50
1550
1                            ncout
30


Benchmark 3 with HYDRUS - 6x flux flux
'mcmf.flx'
'mcmf.pcp'
1.0e-6 .0001   1.0e-30           eps h1 hmin
36 1 750   0.065 0.009 0  A       mlayer nmat nkt qmax qmin iflag
$ Material properties  30 m total thickness
1 36                         layer 1 to 1  Sand
0.8243                       thick(1)
114.76,0.39,0.10,5.9,1.48    sk(1),ths(1),thr(1),alpha(1),rn(1)
$ output times
6                            ntimes
0.     10    1               t1,t2,tp
10.25  40    0.25
41.    60.   1.              t1,t2,tp
70.    150.  10.             t1,t2,tp
175    250   25
300  1500    50
1550
1
36
```

```
Benchmark with HYDRUS - 10x flux flux
'mcmf.flx'
'mcmf.pcp'
1.0e-6  .0001    1.0e-30              eps h1 hmin
48  1  750   0.15  0.009  0   A          mlayer  nmat  nkt  qmax  qmin iflag
$ Material properties  32 m total thickness
1 48                              layer 1 to 1  Sand
0.6265                                thick(1)
114.76,0.39,0.10,5.9,1.48          sk(1),ths(1),thr(1),alpha(1),rn(1)
$ output time
6                                 ntimes
0.    10     1                    t1,t2,tp
10.25  40    0.25
41.    60.   1.                         t1,t2,tp
70.   150.   10.                        t1,t2,tp
175   250    25
300  1500    50
1550
1
48
```

B-6. REFERENCES

Birchall, A., 1986, "A Microcomputer Algorithm for Solving Compartmental Models, Involving Radionuclide Transformations," *Health Physics 50*, pp. 389–397.

Rood, A. S., 1999, "A Mixing-Cell Model for Assessment of Contaminant Transport in the Unsaturated Zone Under Steady-State and Transient Flow Conditions," *Environmental Engineering Science,* 21(6).

Skrable, K. W., C. French, G Chabot, and A. Major, 1974, "A General Equation for the Kinetics of Linear First-Order Phenomena and Suggested Applications," *Health Physics 27*, 155–157.

Sullivan, T. M., 1996, *DUST Disposal Unit Source Term, Data Input Guide*, NUREG/CR-6041, BNL-NUREG-52375. Brookhaven National Laboratory, Upton, NY, 1996.