Idaho National Engineering and Environmental Laboratory

INEEL/EXT-98-00750

August 1998

GWSCREEN: A Semi-Analytical Model For Assessment Of The Groundwater Pathway From Surface Or Buried Contamination

Theory and User's Manual
Version 2.5

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Prepared for the
U.S. Department of Energy
Assistant Secretary for Environmental Management
Under DOE Idaho Operations Office
Contract DE-AC07-94ID13223

ABSTRACT

GWSCREEN was developed for assessment of the groundwater pathway from leaching of radioactive and non-radioactive substances from surface or buried sources. The code was designed for implementation in the Track I and Track II assessment of Comprehensive Environmental Response, Compensation, and Liability Act sites identified as low probability hazard at the Idaho National Engineering Laboratory.

The code calculates 1) the limiting soil concentration such that, after leaching and transport to the aquifer regulatory contaminant levels in groundwater are not exceeded, 2) peak aquifer concentration and associated human health impacts, and 3). aquifer concentrations and associated human health impacts as a function of time and space. The code uses a mass conservation approach to model three processes: contaminant release from a source volume, vertical contaminant transport in the unsaturated zone, and 2D or 3D contaminant transport in the saturated zone. The source model considers the sorptive properties and solubility of the contaminant. In Version 2.5, transport in the unsaturated zone is described by a plug flow or dispersive solution model. Transport in the saturated zone is calculated with a semi-analytical solution to the advection dispersion equation in groundwater.

Three source models are included; leaching from a surface or buried source, infiltration pond, or user-defined arbitrary release. Dispersion in the aquifer may be described by fixed dispersivity values or three, spatial-variable dispersivity functions. Version 2.5 also includes a Monte Carlo sampling routine for uncertainty/sensitivity analysis and a preprocessor to allow multiple input files and multiple contaminants to be run in a single simulation.

GWSCREEN has been validated against other codes using similar algorithms and techniques. The code was originally designed for assessment and screening of the groundwater pathway when field data are limited. It was intended to simulate relatively simple systems and may serve as a predictive tool when the system can be described as such. However, in most cases groundwater systems tend to be substantially more complex than the GWSCREEN conceptual model. Therefore, the primary function of the code has been as a screening and assessment tool.

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1. INTRODUCTION. INTRODUCTION

Multimedia exposure assessment of hazardous chemicals and radionuclides requires that all pathways of exposure be investigated. In the assessment process, limited data are often encountered, and the primary purpose for performing initial screening is to identify priority contaminants and data needs. This process is accomplished by using simplified models that make best use of the available data and conservative assumptions. The GWSCREEN model was designed to perform initial screening calculations for groundwater pathway impacts resulting from the leaching of surficial and buried contamination at Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) sites identified as low probability hazard at the Idaho National Engineering and Environmental Laboratory (INEEL) (DOE, 1992; 1994). In Version 2.0, an additional model was added to calculate impacts to groundwater from the operation of a percolation pond. The model was designed to make best use of the data that would potentially be available. These data include the area and depth of contamination, sorptive properties and solubility limit of the contaminant, depth to aquifer, and the physical properties of the aquifer (porosity, velocity, and dispersivity). For the pond model, data on effluent flow rates and operation time are required. In Version 2.4 (Rood 1994a), three-dimensional dispersion was added. Version 2.5 includes additional enhancements that include:

- a dispersive solution for transport in the unsaturated zone
- spatial-variable dispersivity functions for calculating dispersion in the aquifer
- moisture contents may be calculated internally using the van Genuchten fitting parameters
- Monte-Carlo sampling routines for sensitivity/uncertainty analysis
- preprocessor for running multiple contaminants and multiple files in a single simulation.

The modeling approach used in GWSCREEN is a mass balance approach that has its roots in the methodology presented by the Nuclear Regulatory Commission (Codell et al., 1982; Kozak et al., 1990). Similar methodologies have also been employed in a number of other assessment codes including the Remedial Action Priority System (Whelan et al., 1987) and DECHEM (Killough et al., 1991). The groundwater transport model used in GWSCREEN has been used at the INEEL for scoping and assessment purposes (Codell et al., 1982; Rood et al., 1989) and has been shown to give reasonable results when calibrated to measured data.

Model output includes the soil concentration such that, after leaching and transport to the aquifer, regulatory contaminant levels in groundwater are not exceeded. Also, groundwater concentration and health impacts as a function of time may be calculated. The model considers only drinking water consumption and does not include the transfer of contamination to food products due to irrigation with contaminated water. However, these pathways may be taken into account by adjusting the water consumption rate. Both radiological and non-radiological contaminants are considered in GWSCREEN.

GWSCREEN was not intended to be a predictive tool; rather, it was intended to provide the framework to calculate bounding impacts to groundwater from the leaching of surficial and buried contamination. The conservatism of the results are dependent on the choice of input parameters used in the evaluation.

2. METHODOLOGY. METHODOLOGY

Three primary models are employed in GWSCREEN (Figure 1): the source model, the unsaturated zone mass transport model, and the saturated zone (aquifer) mass transport model. These models are coupled together by the contaminant fluxes across the interface between source, unsaturated, and saturated zone boundaries. Three types of source release models may be employed in GWSCREEN. These are the surficial or buried source model, the percolation pond release model, and the user-defined tabulated source model. GWSCREEN calculates the source mass fluxes for the surficial or buried source model and the percolation pond release model. The user provides the source mass fluxes for the tabulated source model by generating an ASCII file containing mass flux at the source volume-unsaturated zone interface as a function of time. The unsaturated zone model uses both a simplified plug flow model and a dispersive solution, and the saturated zone model uses a semi-analytical solution to the advection-dispersion equation for transient mass flux as described by Codell et al. (1982).

2.1 Source Modeling.1 Source Modeling

2.1.1 Surface or Buried Source Model.1.1 Surface or Buried Source Model

The source volume for the surface or buried source model is defined as the zone in which contaminants have been observed or are suspected to be present. This zone, in most cases, occupies the volume bounded by the soil surface to some finite depth below the soil surface, but may also include buried waste. Release from the source volume is modeled as a first-order leaching process that accounts for decay and sorption. The contaminant is assumed to be homogeneously mixed in a finite volume, and a steady-state infiltration rate is assumed. The leaching process is described mathematically by a first-order leach-rate constant. The differential equation that describes the mass balance of contaminant in the source volume is given by

$$\frac{dM}{dt} = -(\lambda_L + \lambda_d + \lambda_o)M \tag{1}$$

where

λ_d = decay rate constant (y^{-1}),

λ_L = leach rate constant (y^{-1}),

λ_o = rate constant for other loss mechanisms (y^{-1}),

M = mass (or activity) in the source volume (mg or Ci).

The solution to Equation (1) is

$$M(t) = M_o\, e^{-(\lambda_L+\lambda_d+\lambda_o)t} \tag{2}$$

where

M_o = the initial mass or activity in the source volume (mg or Ci),

t = time (years).

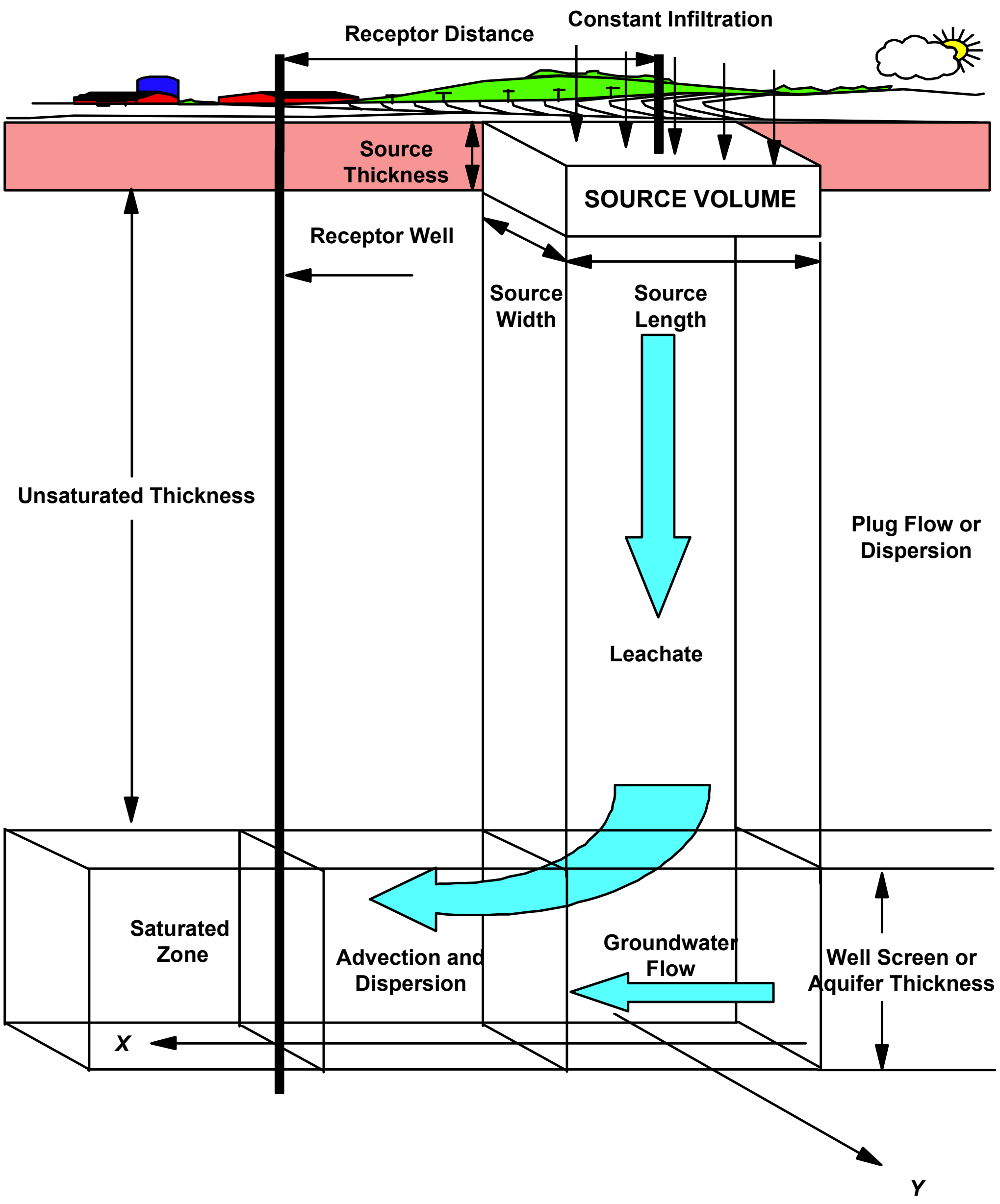

Figure 1. Conceptual model of GWSCREEN for the source volume, unsaturated zone, and aquifer.

The initial mass or activity in the source volume (M_o) is given by

$$M_o = C_o \times L \times W \times T \tag{3}$$

where

L,W,T = the length, width, and thickness of the source volume (m),
C_o = the initial concentration (Ci or mg m^{-3}) in the solid and liquid phases.

The leach rate constant (λ_L) and decay rate (λ_d) constant are given by

$$\lambda_L = \frac{P}{\theta_c R_{dc} T} \qquad \lambda_d = \frac{\text{Ln}(2)}{T_{1/2}} \tag{4}$$

where

P = the net water percolation rate (m y^{-1}),

θ_c = the volumetric moisture content in the source volume (m^3 m^{-3}),

R_{dc} = the retardation factor in the source volume,

$T_{1/2}$ = the contaminant half-life (y).

The leach rate constant was originally described by Baes and Sharp (1983). The formulation given in Equation (4) was taken from Gilbert et al. (1989).

The net water percolation rate (P) is the amount of water that enters the soil per unit time that is not lost to evapotranspiration or runoff. Under steady-state condition (no net storage), this can be approximated by

$$P = P_r - R - E \tag{5}$$

where

P_r = precipitation (m y^{-1}),

R = runoff (m y^{-1}),

E = evapotranspiration (m y^{-1}).

The value P/θ_c represents the average linear water velocity (pore velocity) in the contaminated zone and is based on the unit gradient model. Darcy's law in a one dimensional,vertically aligned, unsaturated soil column is given by

$$q_w = K(\theta)\left(\frac{\partial H}{\partial z} + \frac{\partial \psi}{\partial z}\right) \tag{6}$$

where

q_w = net water percolation rate (P) or Darcy flux (m y^{-1}),

H = elevation head (m),

ψ = suction or pressure head (m),

$K(\theta_c)$ = unsaturated hydraulic conductivity of the column (m y^{-1}),

θ = volumetric water content of the column (m m^{-3}).

Under unit gradient conditions, $\partial\psi/\partial z = 0$, $\partial H/\partial z = 1$, and $\partial\theta/\partial t = 0$. Therefore, $q_w = K(\theta_c) = P$. The unsaturated hydraulic conductivity is a function of the volumetric moisture content of the media. 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, the effective porosity is assumed equal to the total porosity.)

The relationship between hydraulic conductivity and moisture content differs for different rock types. The volumetric water content for a given material and a constant water flux is usually determined using equations that have been fitted to field data relating suction head to volumetric moisture content and hydraulic conductivity. A curve generated using the van Genuchten (1978) fitting parameters for surface sediment at the Radioactive Waste Management Complex at the INEEL is illustrated in Figures 2. These materials were characterized in detail by Bishop (1991) and McElroy and Hubbell (1990), and the van Genuchten fitting parameters, α and n, were given by Baca et al. (1992). The unsaturated hydraulic conductivity can be written in terms of the moisture content and soil fitting parameters, α and n, described in van Genuchten (1978) and given in Equations 7 and 8.

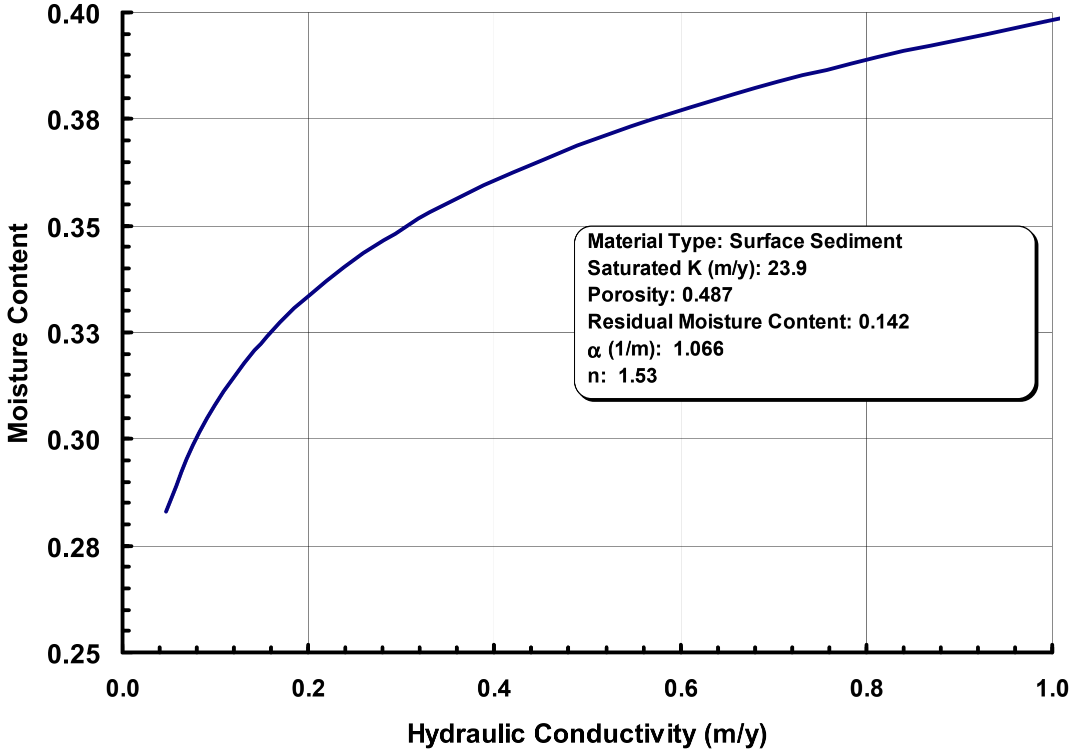

Figure 2. Volumetric moisture content verses hydraulic conductivity for surface sediment at the INEEL.

$$K(\theta) = K_{sat}\left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^{1/2}\left\{1 - \left[1 - \left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^{\frac{1}{m}}\right]^m\right\}^2 \tag{7}$$

and

$$\left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right) = \left(\frac{1}{1 + \alpha n}\right)^m \tag{8}$$

where

θ = moisture content,
θ_r = residual moisture content,
θ_s = saturated moisture content,
K_{sat} = saturated hydraulic conductivity (m y^{-1}),
α = fitting parameter (1/m),
n = fitting parameter,
$m = 1 - 1/n$.

The retardation factor in the source volume (R_{dc}) is given by

$$R_{dc} = 1 + \frac{K_{dc}\,\rho_c}{\theta_c} \tag{9}$$

where

K_{dc} = the distribution coefficient in the source volume (mL g^{-1}),
ρ_c = the bulk density of the source volume (g cm^{-3}).

For organic contaminants, the distribution coefficient is derived from the organic carbon partitioning coefficient (K_{oc}) and the fraction of organic material in the medium (f_{oc}). The distribution coefficient for organics is given by Equation (10):

$$K_d = f_{oc} K_{oc} \ . \tag{10}$$

The contaminant flux out the base of the source volume can now be calculated. The contaminant flux is given by

$$F_s(t) = \lambda_L Q(t) \tag{11}$$

where

$F_s(t)$ = the contaminant flux out the bottom of the source volume (mg or Ci y^{-1}).

The concentration of the leachate [$C_{leachate}(t)$] is given by Equation (12):

$$C_{leachate}(t) = \frac{M(t)}{L \times W \times T \times \theta_c \times R_{dc}} \tag{12}$$

For some contaminants, the initial concentration of the leachate exceeds the solubility limit of the contaminant. In this case, the concentration of the leachate and the mass flux from the source volume will be governed by the solubility limit of the contaminant. The mass balance of the contaminant in the source volume is then given by Equation (13):

$$\frac{dM}{dt} = -(\lambda_d + \lambda_o)M - R \tag{13}$$

where

$R = C_{sl} \times P \times L \times W$ (contaminant flux out bottom of source [mg y^{-1}]),
C_{sl} = the solubility limit of the contaminant (mg m^{-3}).

The solution to Equation (13) for the initial conditions $M = M_o$ at t=0 is

$$M(t) = M_o\, e^{-(\lambda_d+\lambda_o)t} - \frac{R}{\lambda_d + \lambda_o}\left(1 - e^{-(\lambda_d+\lambda_o)t}\right) . \tag{14}$$

After a period of time, the mass in the source volume is depleted sufficiently to allow for leaching to be controlled by the contaminant sorptive properties and not the solubility limit. The amount of mass in the source volume (M_{sl}) where leaching by sorptive properties takes over is given by Equation (15):

$$M_{sl} = C_{sl} \times L \times W \times T \times \theta_c \times R_{ds} \ . \tag{15}$$

When decay or other first-order loss processes are insignificant, the time required for the mass in the source volume to decrease to M_{sl} is simply $t_{sl} = (M_o - M_{sl})/R$, and the mass balance equation is $M(t) = M_o - Rt$. Decay and degradation are considered insignificant if the sum of the rate constants ($\lambda_d + \lambda_o$) is less than 6.93×10^{-11} y^{-1} (effective half time of 1×10^{10} years). If decay is significant during the release, then the solubility limited release time is given by the following:

$$t_{sl} = \frac{-\ln\left(\dfrac{M_{sl} + \dfrac{R}{\lambda_d + \lambda_o}}{M_o + \dfrac{R}{\lambda_d + \lambda_o}}\right)}{\lambda_d + \lambda_o}\ for\ \lambda_d + \lambda_o > 6.93 \times 10^{-11}$$
$$t_{sl} = \frac{M_o - M_{sl}}{R}\ for\ \lambda_d + \lambda_o < 6.93 \times 10^{-11} \ . \tag{16}$$

For radionuclides, total activity in the source volume must be converted to mass so that the quantity of the radionuclide may be related to its solubility limit. The conversion from activity to mass is given by

$$M_{(mass)} = \frac{M_{(activity)}(3.7 \times 10^{10}\ dps\ Ci^{-1})(3.1536 \times 10^{7}\ s\ y^{-1})(MW)}{\lambda_d \ \ N_A} \qquad (17)$$

where

$M_{(mass)}$ = the mass of the radionuclide in the source volume (g),
N_A = Avogadro's number (6.023×10^{23} atoms mole^{-1}),
$M_{(activity)}$ = the total activity of the radionuclide in the source volume (Ci),
dps = number of nuclear transformations per second,
MW = the molecular weight of the radionuclide (g mole^{-1}).

Solubility limited releases for radionuclides usually only affects nuclides with large half-lives since little mass is associated with nuclides with short half-lives.

Output from the source model is then given by Equation (11) for releases not controlled by the contaminant's solubility, and by the term *R* in Equations (13) and (14) for solubility limited releases. These releases provide the contaminant flux at the boundary between source volume and unsaturated zone for the surficial or buried source model.

2.1.2 Pond Release Model.1.2 Pond Release Model

The percolation pond conceptual model (Figure 3) accounts for the flow of water into the pond, the concentration of the contaminant in the pond water, sorption and decay of the contaminant in the pond sediments, and the operational lifetime of the pond. A simplified hydrologic conceptual model is used to describe flow from the pond to the aquifer. Consider the hypothetical pond illustrated in Figure 4. The flow rate into the pond is assumed to be constant, and the pond depth (h_1) is also assumed to remain constant throughout time. The pond sediments are assumed to be saturated, at least to some depth, h_2. In order for a pond to form under constant flow and steady-state conditions, the hydraulic conductivity of the pond sediments must be less than the infiltration rate. The infiltration rate into the pond sediments is given by q1. At some point below the base of the pond, unsaturated conditions may exist. This is true for conditions at the INEEL where the vadose zone consists of fractured basalt that has a measured hydraulic conductivity of around 10,000 m/y. This assumption may not be true for other sites where complete saturation may exist from the base of the pond to the aquifer. If steady state conditions exist, then q1=q2=q3.

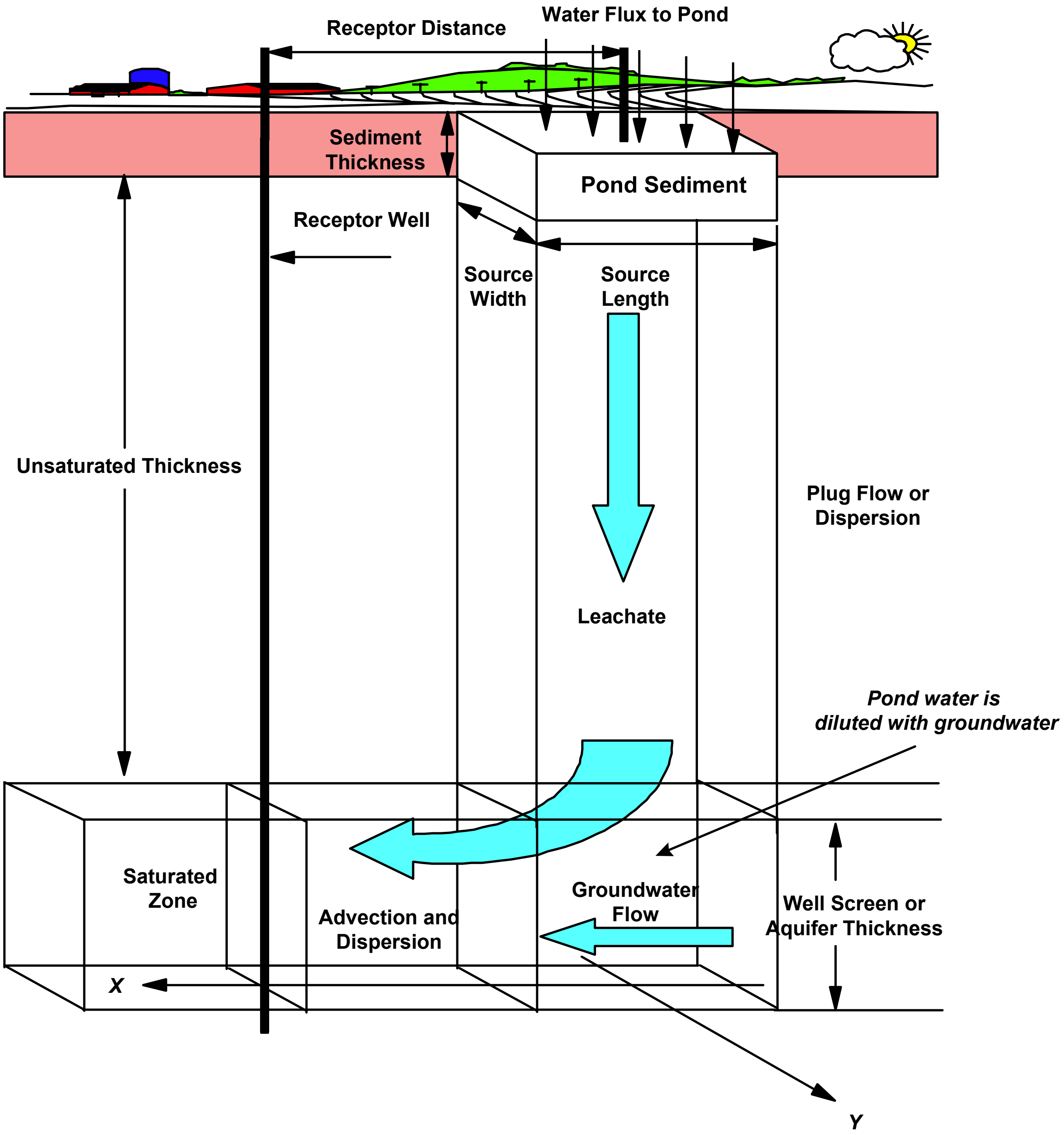

Figure 3. Conceptual model for the GWSCREEN percolation pond model.

The contaminant flux into the pond is assumed to be equal to the contaminant flux into a sediment layer underlying the pond (pond sediments). Contaminant mass balance within this sediment layer is then determined and assumed to represent a first-order process with constant input. The mass balance equation that describes the mass of contaminant in the pond sediments is given by the following:

$$\frac{dM}{dt} = R_P - (\lambda_L + \lambda_d + \lambda_E)M \tag{18}$$

where

M = mass or activity of contaminant in the pond sediments (Ci or mg),

λ_L = leach rate constant from pond sediments (y^{-1}),

λ_E = rate constant for other loss processes from the pond sediments (y^{-1}),

R_P = mass flux of the contaminant into the pond (Ci or mg y^{-1}).

The leach rate constant for pond sediments (λ_L) is given by

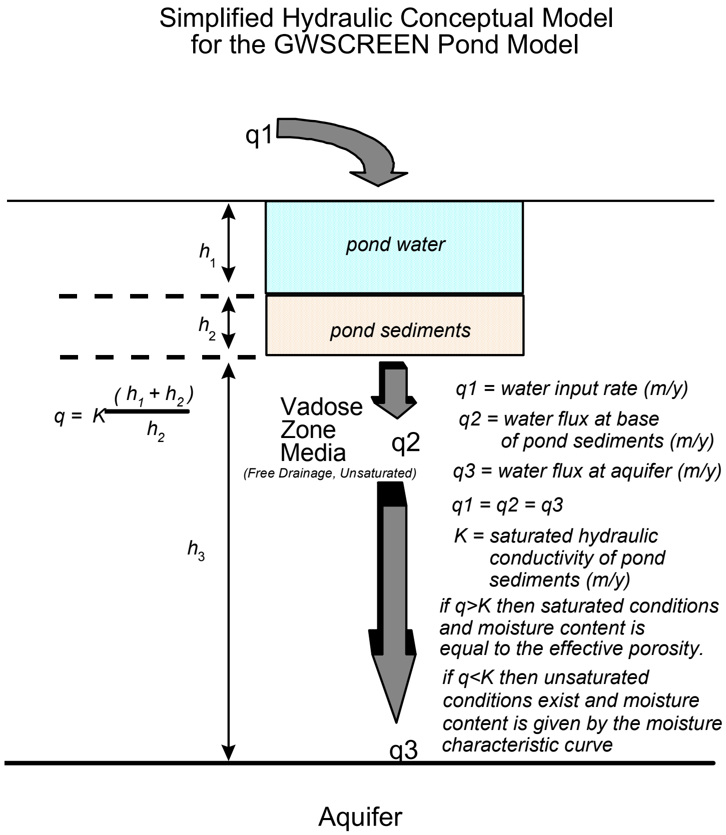

Figure 4. Simplified hydraulic conceptual model for the GWSCREEN percolation pond model.

$$\lambda_L = \frac{Q_{pond}}{\theta_p T R_{d_p} LW} \tag{19}$$

where

Q_{pond} = net water input rate into the pond ($m^3\ y^{-1}$),

θ_p = volumetric moisture content in the pond sediments ($m^3\ m^{-3}$),

R_{dp} = retardation factor in the pond sediments,

T = pond sediment thickness (m),

L,W = length and width of the pond (m).

The volumetric moisture content of the pond sediments may be estimated by the effective porosity of the pond sediments *if* a pond has formed. If a pond has formed, then the pond sediments are saturated, at least to some depth, and the volumetric moisture content is given by the effective porosity of the pond sediments. For saturated conditions, the unit gradient assumption used in the leach rate constant is violated because the hydraulic gradient in the pond sediments is no longer unity, resulting in faster water travel times through the saturated portion of the sediment. This deficiency in the model can be compensated by choosing a conservative value for the pond sediment thickness, thereby reducing the residence time of the contaminant in the pond sediment compartment.

If a pond forms periodically or exists for only part of the year, then the volumetric water content can be estimated by the hydraulic conductivity curve for the pond sediments. The infiltration rate (annual discharge rate to the pond [Q_{pond}] divided by the pond area) can be compared to the saturated hydraulic conductivity of the pond sediments. If the infiltration rate is less than the saturated hydraulic conductivity, then unsaturated conditions can be assumed, and the moisture content can be estimated by a curve similar to Figure 2 for pond sediments. The moisture content in the unsaturated zone (see Section 2.2) should be estimated in the same manner, using the infiltration rate into the pond sediments [$Q_{pond}/(L \times W)$] to determine the moisture content.

From Equation (19), it is evident that the pond sediment thickness is inversely related to the rate at which contaminants are leached from the pond sediments. Therefore, selection of the pond sediment thickness is an important factor in determining impacts of the pond. The movement of contaminants through a soil column underlying a percolation pond is transient in nature and is not treated explicitly in the pond model. Rather, a sediment layer is defined where the contaminants are free to mix, adsorb and desorb, and then leave the space. Engineered percolation ponds are not designed to retain water; rather, the hydraulic characteristics of the material underlying the pond are designed to transmit water from the pond to the underlying strata. Over time, however, the hydrologic characteristics of the pond base may change due to infilling of the pore space from fine-grained sediments suspended in the discharge water. Several approaches to estimate the pond sediment thickness are presented next. The incorporation of any of these approaches depends on site-specific considerations and available data.

The first approach makes use of any site-specific data that may exist. If characterization data indicate the presence of a sediment layer at the base of the pond that is distinctively different from the material the pond has been constructed over, then the thickness of this layer can be used as the pond sediment thickness. These data should include some estimate of the effective porosity of the pond sediments.

The second approach considers a sediment layer underlying the pond, and overlying strata that has a significantly higher conductivity. This approach is applicable when the majority of the unsaturated zone (from the base of the pond to the aquifer) is composed of materials having a higher saturated hydraulic conductivity than the pond infiltration rate ($K_{sat} > \{Q_{pond} \times L \times W\}$). In this case, unsaturated flow can be assumed in this strata. Such is the case at the INEEL where relatively thin surface sediments overlie thick sections of fractured basalt. The pond sediment thickness in this case may be assumed to be some fraction of the surface sediment thickness.

The third approach employs a default pond sediment thickness to be used when data are lacking or no defensible argument can be made to define a thickness. A value of 1.0 m is suggested as a minimum default pond sediment thickness. A sediment thickness of 1.0 m results in equilibrium conditions being established in a relatively short amount of time under most conditions except when the contaminant has a high distribution coefficient. Once equilibrium is established, contaminant flow rates in to and out of the pond sediments are equal resulting in the maximum possible release to the unsaturated zone. The 1 m default thickness was also used as a contaminant layer thickness default value in the RESRAD code (Gilbert et al., 1989).

The retardation factor for the pond sediments is given by Equation 9, substituting θ_p for θ_c. The solution to Equation (18) for the initial conditions, $M=M_o$ when t=0 is

$$M(t) = \frac{R_p}{\lambda_L + \lambda_d + \lambda_E}\left(1 - e^{-(\lambda_L+\lambda_d+\lambda_E)t}\right) + M_o\, e^{-(\lambda_L+\lambda_d+\lambda_E)t} \tag{20}$$

After operation of the pond ceases, the contaminant inventory remaining in the pond sediments are subsequently leached by percolating rainwater and snowmelt. The inventory of contaminants in the pond sediments at the end of operation is given by $M(t)$ in Equation (20), evaluated at time t_{op}, the operational lifetime of the pond. Post-pond operation leaching is evaluated using Equation (2) where $M_o = M(t_{op})$ and $\lambda_E = 0$.

The flux to the unsaturated zone (F_s) during the operation period of the pond is given by

$$F_s(t) = \lambda_L\left(\frac{R_p}{\lambda_L + \lambda_d + \lambda_E}\left(1 - e^{-(\lambda_L+\lambda_d+\lambda_E)t}\right) + M_o\, e^{-(\lambda_L+\lambda_d+\lambda_E)t}\right) \tag{21}$$

and the flux to the unsaturated zone after the operational period is given by Equation (11).

2.1.3 Dilution

The GWSCREEN conceptual model fails to account for additional water sources in the aquifer. Typically, under background infiltration conditions the volume of precipitation-derived percolating water that reaches the aquifer from the source area is insignificant compared to the volume of water flowing in the aquifer across the same area. Such may not be the case for an infiltration pond where the volume of water entering the aquifer from the source may make up a considerable fraction of the flow in the aquifer directly beneath the source. The pond model accounts for this additional water in the aquifer from percolating pond water through a dilution factor. The dilution factor takes on a value of ≤ 1.0 and represents the ratio of the aquifer flow across the cross sectional area of the contaminant plume, to the total flow across that area including water derived from surface percolation. This factor may also be calculated for any other model employed in GWSCREEN. Before proceeding with a simulation, the water flux to the aquifer should be computed and compared to the flow in the aquifer across the cross-sectional area of the source that is perpendicular to groundwater flow. For the pond model, the water flux to the aquifer is Q_{pond}. For the surface/buried source model or user defined model, the water flux is $L \times W \times P$. If the water flux to the aquifer represents a significant quantity of the aquifer flow across the cross-sectional area of the source (say within a factor of 2), then the dilution factor option in the code should be exercised. The dilution factor is given by

$$DF = \frac{\left(\varepsilon\sigma_y + w\right) b\, U\, \eta}{\left(\varepsilon\sigma_y + w\right) b\, U\, \eta + q_{total}} \tag{22}$$

where

ε = number of standard deviations of the contaminant plume perpendicular to flow from the plume center line (fixed at 2),

σ_y = standard deviation of the plume perpendicular to flow $[(2D_y\, t/R_d)^{1/2}]$ (m),

D_y = transverse dispersion coefficient in the aquifer (see aquifer model [$m^2\ y^{-1}$]),

w = width of source perpendicular to groundwater flow (m),

b = aquifer thickness (m),

U = aquifer pore velocity ($m\ y^{-1}$),

η = aquifer porosity,

q_{total} = total water flux from the source ($m^3\ y^{-1}$).

The dilution factor is multiplied by the output concentration and has the net effect of reducing the concentration. When using the pond model, or in any other source where the surface water flux is comparable to the flow in the aquifer across the cross sectional area, this option should be exercised. The approach outlined here for addressing dilution problems is somewhat different than what was used in earlier versions of GWSCREEN.

2.1.4 Tabulated Source Model.1.3 Tabulated Source Model

The user may choose to calculate a mass flux from the source volume using another model. In such cases, the user provides contaminant mass fluxes as a function of time from the source volume, and only the saturated zone and unsaturated zone model employed in GWSCREEN are used to calculate groundwater concentrations at the receptor point. The unsaturated zone model may also be ignored by setting its thickness equal to zero.

2.2 Unsaturated Zone Model.2 Unsaturated Zone Model

The unsaturated zone is defined as the zone between the base of the source volume and the top of the aquifer. The unsaturated zone is assumed to be a homogeneous, isotropic, porous media with constant, unidirectional flow in the vertical (downward) direction. The model allows for differences in the transport properties between the unsaturated zone, source volume, and saturated zone. Two different transport models are incorporated into Version 2.5; an advective dispersive solution, and a plug flow model. In the plug flow model, non-sorbing contaminants move with the vertical velocity of the water. This velocity is calculated assuming the unit gradient condition as discussed previously. For most contaminants, the plug flow model is a conservative assumption since the peak flux to the aquifer exceeds the peak flux when dispersion is considered. For contaminants with short half-lives relative to their residence time in the unsaturated zone, the plug flow assumption may not be conservative since the contaminant will arrive sooner (lower residence time in the unsaturated zone) when dispersion is considered, thereby allowing less time to decay. This observation was noted by Seitz et al. (1991) and may become a significant factor when the unsaturated transit time [see Equation (23)] is greater than 10 times the half-life of the contaminant. For these reasons, solutions to the advection-dispersion equation were implemented in the unsaturated transport model. A rule of thumb to ensure conservatism is to make sure the contaminant transit time in the unsaturated zone (T_a) does not exceed 10 times the half-life of the contaminant when the plug flow model is used; otherwise the dispersive solution should be used. If radioactive contaminants with progeny are being modeled, then other factors may also have to be considered. These factors include the half-lives and equilibrium conditions of the progeny at the time of maximum parent concentration, and the dose conversion and slope factors of the parent and progeny (see discussion in Section 3.3).

2.2.1 Plug Flow Model

The amount of decay that occurs during transit is a function of the contaminant transit time in the unsaturated zone. The transit time in the unsaturated zone (T_a) is given by the following:

$$T_a = \frac{X_u}{U_u} R_{du} \tag{23}$$

where

X_u = the distance from the base of the source volume to the top of the aquifer (m),
U_u = the unsaturated pore velocity (m y^{-1}),
R_{du} = the retardation factor in the *unsaturated* zone.

The unsaturated pore velocity (U_u) is given by

$$U_u = \frac{P}{\theta_u} \tag{24}$$

where

θ_u = the volumetric water content in the unsaturated zone ($m^3\ m^{-3}$).

Volumetric water content as a function of infiltration can be determined using a graph like illustrated in Figure 2 or Equations 7 and 8. For the pond model, P is given by $Q_{pond} \div (L \times W)$. If the pond model is being used and some of the subsurface layers have much lower hydraulic conductivity than surrounding media, then the presence of perched water should be investigated. If perched water is present, and flow is controlled by these layers, then saturated conditions may be assumed. However, a hydrogeologist should be consulted at this point because the travel time through these layers can be underestimated because of the presence of a hydraulic gradient that is greater than unity. Remember, the purpose of estimating the moisture content in the unsaturated zone is to arrive at an estimate of the pore water velocity and thereby, an estimate of the mean water travel time from the source to the aquifer. A representative moisture content that yields a water travel time that is consistent with observations can always be used instead of the methods presented in this document for estimation of moisture content. If observations and data are available, it is strongly recommended that these be incorporated into the simulation.

The retardation factor (R_{du}) in the unsaturated zone is given by

$$R_{du} = 1 + K_{du} \frac{\rho_u}{\theta_u} \tag{25}$$

where

K_{du} = the distribution coefficient in the unsaturated zone (mL g^{-1}),

ρ_u = the bulk density in the unsaturated zone (g cm^{-3}).

The fraction of mass or activity that remains after transit through the unsaturated zone (f) is given by Equation (26):

$$f = e^{-\lambda_d T_a} \tag{26}$$

The contaminant flux to the aquifer (F_a) is given by Equation (27), and it is through this term that the plug flow unsaturated zone and saturated zone models are coupled.

$$\begin{gathered} F_a = f\ \lambda_L\ Q(t)\ (leaching\ releases) \\ F_a = f\ R\ (solubility\ limited\ releases) \end{gathered} \tag{27}$$

For the pond model, the unsaturated travel time is different before and after the operational period. After discharge to the pond ceases, leaching is by rainwater or snowmelt, resulting in lower water fluxes and higher transit times in the unsaturated zone. At present, GWSCREEN ignores this difference and uses the unsaturated pore velocity computed while the pond is in operation throughout the simulation. Surface leaching from the pond sediments is reduced according to the reduction in the net infiltration before and after pond operation.

2.2.2 Dispersion Model for Unsaturated Transport

The dispersion model for unsaturated transport incorporates the same assumptions about flow as the plug flow model. Flow is assumed to be steady state, unidirectional (downward) and under unit gradient conditions. The unsaturated zone is assumed to be a homogeneous isotropic media of infinite extent. Solid and liquid contaminant phases are assumed to be in equilibrium and related by the linear distribution coefficient. The mass balance equation describing transport in one-dimension is

$$\frac{\partial C}{\partial t} + \frac{U_u}{R_{du}} \frac{\partial C}{\partial x} = \frac{D_x}{R_{du}} \frac{\partial^2 C}{\partial x^2} - \lambda_d C \tag{28}$$

where

C = concentration (mg or Ci m^{-3}),

U_u = unsaturated pore velocity (flow in the positive x direction, m y^{-1}),

D_x = dispersion coefficient in the x direction (m^2 y^{-1}),

t = time (y),

x = distance traversed parallel to direction of flow (m).

The solution to Equation 28 for an instantaneous release at x = 0 is

$$C = \frac{1}{\theta_u R_d \sqrt{4\pi D_x t / R_d}} \exp\left(\frac{\left(x - U_u t / R_d\right)^2}{4 D_x t / R_d} - \lambda_d t \right) \tag{29}$$

The contaminant flux per unit area at a distance *x* for a vertical plane source oriented perpendicular to flow is given by Equation 30.

$$F_a = \theta_u \left(U_u C - D_x \frac{\partial C}{\partial x} \right) \tag{30}$$

The total contaminant flux (mass or activity per unit time) at a distance *x* resulting from an instantaneous release of a unit quantity of contaminant at *x*=0 and *t*=0 would be (Codell et al. 1982)

$$F_a = \frac{x + \frac{U_u t}{R_{du}}}{4\sqrt{D_x \pi t^3 / R_d}} \exp\left[\frac{-\left(x - \frac{U_u t}{R_{du}} \right)}{4 D_x t / R_d} - \lambda_d t \right] \tag{31}$$

Equation 31 is formulated in terms of an instantaneous release. Solutions for arbitrary sources can be arrived at through the use of the convolution integral (Codell et al. 1982)

$$\Theta = \int_0^t F_s(\tau)\, \Theta_i(t - \tau)\, d\tau \tag{32}$$

where

Θ = the solution at time t for an arbitrary source, F_s ,

$F_s(\tau)$ = the arbitrary source release at time τ,

$\Theta_i(t-\tau)$ = the solution for an instantaneous source released at $(t-\tau)$= 0.

Equations 31 and 32 are solved using either Gauss-Legendre or Simpson rule integration. The source in Equation 32 [$F(\tau)$] is either a surface or buried source (Equation 11 and 15), infiltration pond (Equation 21), or a user defined arbitrary release. The flux (mass or activity per unit time) at time *t* is subsequently passed to the aquifer model.

2.3 Saturated Zone Model.3 Saturated Zone Model

The saturated zone model is based on an analytic solution to the advection dispersion equation for contaminants in a saturated porous media. These solutions were originally developed by Codell et al. (1982) and have been used for assessment of radionuclide transport in groundwater. These solutions apply equally as well to non-radiological contaminants. The model contains the following assumptions and limitations:

1. The model uses a Cartesian coordinate system (*x*,*y*,*z*) as a frame of reference. The positive *x* direction is in the direction of flow.

2. The flow is uniform and unidirectional. No sources or sinks are accounted for.
3. The aquifer is modeled as an isotropic, homogeneous porous media of infinite lateral extent and finite thickness.
4. Molecular diffusion is assumed to be negligible.
5. The source can be represented by a rectangular area of length L and width W and centered at the origin (0,0,0).
6. The dispersion coefficients remain constant over time.
7. Transport is limited to a single specie that may decay or degrade as a function of time. Radioactive progeny are assumed to travel at the same rate as their parent.
8. The contaminant is assumed to move as a dissolved substance. Transport in liquid organic and vapor phases are not considered.
9. Solid and liquid phases are in equilibrium and concentrations are related by the linear distribution coefficient (K_d).
10. The two-dimensional (2D) solution assumes that the contaminant is mixed vertically (z direction) in a zone defined by the length of a typical well screen for a drinking water well or the thickness of the aquifer. The three dimensional (3D) solution considers vertical dispersion in the aquifer.

Assumption 10 states that groundwater concentrations will be averaged (mixed) over the thickness of the well screen for the 2D solution. This assumption is reasonable for receptor wells close to the source since contaminants poorly mixed in the vertical direction will be diluted by water drawn over the *entire* well screen interval. For receptor wells located farther downgradient from the source, the estimated concentration will be conservative since the contaminant plume will likely extend to greater depths than the assumed well screen thickness. In these cases, a larger "mixing thickness" may be justified. The user may also select a 3D dispersion solution. Concentrations calculated using the 3D solution may be averaged over any well screen thickness, and the contaminant mass is not restricted to the mixing thickness; rather, it is restricted to the thickness of the aquifer (see Figure 5).

Calibration studies at the INEEL using the groundwater model described in this document have been performed by Codell et al. (1982) and Rood et al. (1989). Tritium plumes from the Idaho Chemical Processing Plant injection well and the Test Reactor Area percolation ponds were modeled. The predicted concentration matched measured data reasonably well considering the simplifications and assumptions of the model; however, the results were not as accurate as those made by a finite difference model (Robertson, 1974). Differences were attributed to the ability of the finite difference model to incorporate spatial differences in the flow field. This problem is reduced in simulations where the hypothetical well to be modeled is relatively close to the source (about 100 m), thereby reducing the effect of spatial variability in groundwater flow.

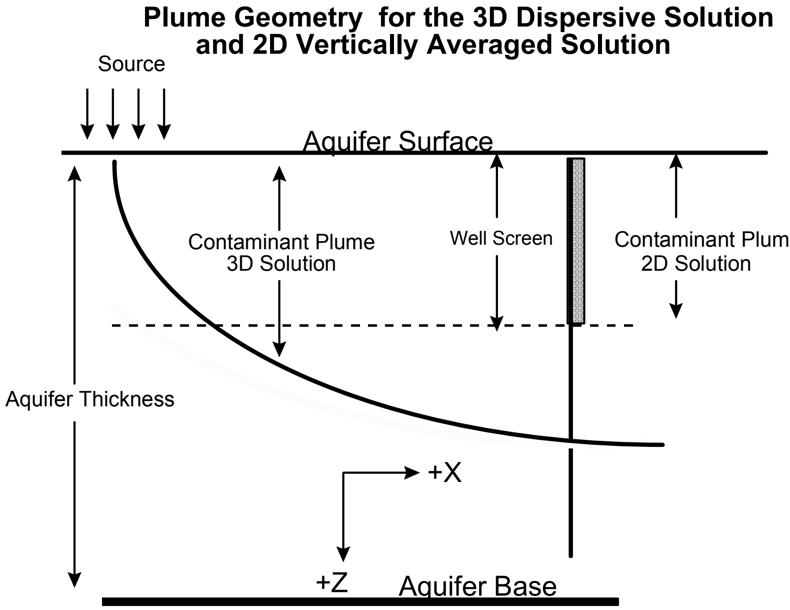

Figure 5. Plume geometry for the 3D dispersive solution and 2D vertically averaged solution. The two-dimensional solution assumes that the contaminant is mixed vertically (*z* direction) in a zone defined by the length of a typical well screen for a drinking water well or the thickness of the aquifer. The three-dimensional solution considers vertical dispersion in the aquifer.

The mass balance equation that describes contaminant transport for the stated assumptions is

$$\frac{\partial C}{\partial t}+\frac{U}{R_d}\frac{\partial C}{\partial x}=\frac{D_x}{R_d}\frac{\partial^2 C}{\partial x^2}+\frac{D_y}{R_d}\frac{\partial^2 C}{\partial y^2}+\frac{D_z}{R_d}\frac{\partial^2 C}{\partial z^2}-\lambda_d C \qquad (33)$$

where

C = concentration (mg or Ci m^{-3}),

U = average linear velocity or groundwater pore velocity (m y^{-1}),

D_x D_y D_z= dispersion coefficient in the x, y, and z direction (m^2 y^{-1}),

R_d = retardation factor in the aquifer,

t = time (y),

x = distance from center of area source to receptor parallel to groundwater flow (m),

y = distance from center of area source to receptor perpendicular to groundwater flow (m),

z = distance from the surface of the aquifer (m).

The retardation factor in the aquifer is given by

$$R_d = 1 + K_{da}\frac{\rho_a}{\eta} \qquad (34)$$

where

η = the effective porosity of the aquifer (m^3 m^{-3}),

K_{da} = the distribution coefficient in the aquifer (mL g^{-1}),

ρ_a = the bulk density in the aquifer (g cm^{-3}).

The dispersion coefficients (D_x, D_y, D_z) are given by

$$D_x = \alpha_L U \quad D_y = \alpha_T U \quad D_z = \alpha_V U \tag{35}$$

where

α_L = the longitudinal dispersivity (m),
α_T = the transverse dispersivity (m),
α_V = the vertical dispersivity (m).

The vertically averaged Green's function solution to Equation (33) for instantaneous release of mass M_a, at t = 0 at the surface of an area defined by L and W and initial concentration of zero everywhere in the model domain is given by

$$\begin{aligned} C(x,y,t) = {} & \frac{M_a}{\eta R_d} \frac{1}{2L} \frac{1}{b} \left(erf\left(\frac{x + \frac{L}{2} - \frac{Ut}{R_d}}{\sqrt{\frac{4 D_x t}{Rd}}} \right) - erf\left(\frac{x - \frac{L}{2} - \frac{Ut}{R_d}}{\sqrt{\frac{4 D_x t}{R_d}}} \right) \right) \\ & \times \frac{1}{2W} \left(erf\left(\frac{\frac{W}{2} + y}{\sqrt{\frac{4 D_y t}{R_d}}} \right) + erf\left(\frac{\frac{W}{2} - y}{\sqrt{\frac{4 D_y t}{R_d}}} \right) \right) e^{-\lambda_d t} \end{aligned} \tag{36}$$

where

b = the well screen thickness or mixing depth (m)
M_a = the initial total mass in the volume defined by L $\times$ W $\times$ b
erf = the error function
L = length of source parallel to groundwater flow (m)
W = width of source perpendicular to groundwater flow (m).

The terms L and W are identical to those defined in Equation (3). For the 3D solution, the term $1/b$ in Equation (36) is replace by Z_1.

$$Z_1 = \left(1 + 2 \sum_{m=1}^{\infty} \exp\left(\frac{m^2 \pi^2 D_Z t}{b^2 R_d} \right) \cos\left(m \pi \frac{z}{b} \right) \right) \tag{37}$$

where

z = receptor distance below the surface of the aquifer (m).

The 3D solution gives the concentration at a point specified by (x,y,z) in the aquifer. Often, the average concentration over a screened interval is more useful than concentration at a point. The average concentration over a screened well interval, b_w (from the surface of the aquifer to depth b_w), for the three-dimensional solution is given by

$$C_{3Davg}(x,y,z,t) = \frac{\int_0^{b_w} C(x,y,z,t)\,dz}{b_w} \quad . \tag{38}$$

For an arbitrary release, the concentration may be found by the convolution integral (Equation 32) replacing F_s with F_a (the flux to the aquifer). For some contaminants, the average concentration over a period of exposure is desired. If the peak concentration (maximum concentration observed at the specified receptor point) is bounded by the time periods, T_a and T_b, then the maximum average concentration is given by

$$C_{avg} = \frac{\int_{T_a}^{T_b} C(x,y,(z),t)\,dt}{T_b - T_a} \tag{39}$$

where

T_a, T_b = averaging time period (years).

Scale-Dependent Dispersivity

The scale dependent nature of hydrodynamic dispersion has been known for about 20 years (Xu and Eckstein 1996). Measurements of dispersivity in laboratory-scale experiments yield estimates that are much smaller than those measured in the field (Freeze and Cherry 1979) and field-scale experiments also often yield different dispersivity estimates when the scale of the experiment is increased from a few hundred meters to thousands of meters. Regression formulas relating dispersivity to field scale size have been proposed [Arya (1986), Neuman (1990)]. These studies used limited data in their regressions and discarded those data points that were considered unreliable. Xu and Eckstein (1996) developed regression equations based on a weighted least-squares method that incorporates all available field and experimental data. The weighting method assigns weights according to the reliability of the data. Data points were segregated into three classes; low, intermediate, and high reliability and a weight was assigned to each class. Three regression equations were formulated based on three different weighting schemes; (1:1:1), (1:1.5:2), and (1:2:3). In the weighting schemes, the first number represents the weight assigned to low reliability points, the second number represents the weight assigned to intermediate reliability points, and the third number represents the weight assigned to high reliability points. Note that the first weighing scheme assigns equal weight to all reliability data classes. The regression equations yield estimates of the longitudinal dispersivity (α_L in meters) as a function of the field scale length (L in meters) and are given by:

$$\alpha_L = 1.20\left(\log_{10} L\right)^{2.958} \; \mathit{for}\ 1{:}1{:}1\ \mathit{scheme} \tag{40}$$

$$\alpha_L = 0.94\left(\log_{10} L\right)^{2.693} \; \mathit{for}\ 1{:}1.5{:}2\ \mathit{scheme} \tag{41}$$

$$\alpha_L = 0.83\left(\log_{10} L\right)^{2.414} \; \mathit{for}\ 1{:}2{:}3\ \mathit{scheme} \tag{42}$$

The analysis reported in Xu and Eckstein shows a significant difference between the weighted and unweighted curves and further analysis indicated that increase in the longitudinal dispersivity was negligible when the scale of flow exceeds 1-km. Correlation coefficients were 0.76, 0.74, and 0.72 respectively. In GWSCREEN Version 2.5, the user may select a fixed dispersivity value or calculate longitudinal dispersivity using one of the three equations described above. If regression equations are used, then transverse and vertical dispersivity are calculated from the longitudinal dispersivity, based on a fixed ratio of the transverse (or vertical) dispersivity to the longitudinal dispersivity (i.e α_T/α_L).

2.4 Radioactive Decay and Ingrowth.4 Radioactive Decay and Ingrowth

To evaluate the movement of radioactive progeny, the model makes the simplifying assumption that radioactive progeny travel at the same rate as the parent. This assumption has been shown to be conservative (Codell et al., 1982) and greatly simplifies the calculations. The assumption is also made that no progeny exist at the time of waste emplacement. The concentration of the ith progeny in a decay chain at the receptor location is

$$C_i = C_{parent} \frac{DIF_i \, R_{d_{parent}}}{DIF_{parent} \, R_{d_i}} \tag{43}$$

where

DIF_i = decay-ingrowth factor of the ith progeny
DIF_{parent} = decay-ingrowth factor of the parent
R_{di} = retardation factor of the ith progeny
$R_{d\,parent}$ = retardation factor of the parent
C_{parent} = groundwater concentration of the parent (Ci m^{-3}).

The decay ingrowth factor is given by the following (Scrable et al., 1974):

$$DIF_i(t) = \frac{\lambda_i}{\lambda_1} \left[\left(\prod_{m=1}^{i-1} \lambda_m \right) \sum_{j=1}^{i} \frac{e^{-\lambda_j t}}{\prod_{k \neq j}^{i} \left(\lambda_k - \lambda_j \right)} \right] \tag{44}$$

where

λ_1 = decay constant for the parent (y^{-1})
λ_i = decay constant for the ith progeny (y^{-1})
t = time from waste emplacement (years).

2.5 Maximum Allowable Soil Inventory and Pond Release Limits.5 Limiting Soil Concentration

Assessment of groundwater at a contaminated site usually involves evaluation of following criteria:

- Maximum contaminant levels (MCLs) in groundwater
- Non-carcinogenic chemical toxicity from the ingestion of contaminated groundwater (non radionuclides only)

- Carcinogenic risk from the ingestion of contaminated groundwater (radionuclides and non radionuclides)
- Committed effective dose equivalent (CEDE) from the ingestion of contaminated groundwater (radionuclides only).

Maximum contaminant levels and CEDE limits are listed in 40 CFR 141 and associated amendments. At sites identified under CERCLA, maximum allowable concentrations are based on chemical toxicity or carcinogenic risk. Carcinogenic risk represents the incremental probability of an individual developing cancer over a lifetime as a result of exposure to the potential carcinogen (EPA, 1989). Chronic exposure to radionuclides are considered a carcinogenic risk. Cancer risks are calculated using a factor that relates the incremental lifetime cancer incidence risk to the level of exposure. Radiation dose from ingestion of radionuclides in groundwater is calculated using a dose conversion factor that relates the effective dose equivalent received over a period of time (usually 50 years) from the one-time ingestion of a radionuclide. Non-carcinogenic effects are evaluated based on a hazard quotient that relates an exposure level over a lifetime with a reference dose derived for a similar exposure period. Other dose and risk criteria may be implemented depending on site-specific considerations.

In GWSCREEN 2.5, the maximum allowable inventory in soil is the contaminant inventory in soil such that after leaching and transport in the unsaturated and saturated zone, MCL, radiological dose, and carcinogenic or non-carcinogenic risk limits are not exceeded. The maximum allowable inventory in soil is given by

$$M_L = M_i \frac{D_C}{D_L} \tag{45}$$

where

M_L = maximum allowable inventory in soil (Ci or mg),

M_C = inventory used in the simulation (Ci or mg),

D_C = radiological dose, carcinogenic risk, hazard quotient, or maximum contaminant concentration at the receptor well for the simulation using an inventory of M_i,

D_L = radiological dose limit, carcinogenic risk limit, hazard quotient limit, or MCL.

For the pond model, the maximum allowable effluent release rate is calculated. The maximum allowable effluent release rate is the amount of contaminant that can be discharged to the pond on an annual basis for the operational lifetime of the pond such that after leaching and transport in the unsaturated and saturated zone, MCL, radiological dose, and carcinogenic or non-carcinogenic risk limits are not exceeded. The maximum allowable pond release rate is given by replacing M_i and M_L in Equation (45) with the contaminant release rate (R in Ci or mg y^{-1}) to the pond. Maximum allowable inventories and release rates are only calculated for the built-in GWSCREEN models and are not considered for user-defined sources.

Values and units for D_L are contaminant and endpoint specific (Table 1). The value of D_C and D_L may be considered quantitative measures of the impacts to human health and D_C must be calculated for each contaminant and receptor location in a simulation.

Table 1. Suggested D_C values and units of the limiting radiological dose, carcinogenic risk, hazard quotient or maximum contaminant limit.

Contaminant Type	Human Health Endpoint	Dose or risk conversion factor units	Suggested D_c value and units
Radionuclide	Committed Effective Dose Equivalent	rem Ci^{-1}	0.004 rem y^{-1} [a]
Radionuclide	Carcinogenic risk	risk Ci^{-1}	$1 \times 10^{-6} - 1 \times 10^{-4}$ [b]
Radionuclide	Factor of the MCL	Ci m^{-3}	1.0[c]
Non-radionuclide	Carcinogenic risk	kg-d mg^{-1}	$1 \times 10^{-6} - 1 \times 10^{-4}$ [b]
Non-radionuclide	Non-carcinogenic risk (hazard quotient)	mg kg^{-1} d^{-1}	1.0[d]
Non-radionuclide	Factor of the MCL	mg m^{-3}	1.0[c]

(a) Maximum annual committed dose equivalent for the ingestion of beta-gamma emitting nuclides as reported in 40 CFR 141

(b) Range of acceptable lifetime cancer incidence risk as established by EPA (1989). The units are the number of cancers observed in a lifetime per person. For example, a value of 1×10^{-4} indicates 1 person in 10,000 will develop cancer in their lifetime or 100 persons in 1,000,000 will develop cancer in their lifetime.

(c) This factor is multiplied by the MCL to yield an acceptable groundwater concentration. A value of 1 indicates the MCL is acceptable; a value of 0.5 indicates ½ the MCL value is acceptable.

(d) See Equation (49).

2.6 Estimation of Human Heath Impacts

Human health impacts are measured in terms of radiation dose equivalent, lifetime cancer incidence risk, non-carcinogenic health effects, or ratios of predicted to acceptable levels of contamination in groundwater.

For radionuclides with a human health endpoint of CEDE (in rem), D_C is given by

$$D_C = \left(\sum_{i=1}^{n} C_i \times DCF_i \right) WI \times EF \tag{46}$$

where

C_i = groundwater concentration for the i^{th} decay chain member (Ci m^{-3}),

WI = water ingestion rate (m^3 d^{-1}),

DCF_i = ingestion dose conversion factor for the i^{th} decay chain member (rem Ci^{-1}),

EF = exposure frequency (d y^{-1}),

n = number of decay chain members.

For radionuclides with a human health endpoint of lifetime cancer incidence risk, D_C is given by

$$D_C = \left(\sum_{i=1}^{n} C_i \; SF_i \right) WI \; EF \; ED \tag{47}$$

where

C_i = average groundwater concentration over the exposure period for the i^{th} decay chain member (Ci m^{-3}),

SF_i = slope factor for the i^{th} decay chain member (risk Ci^{-1}),

ED = exposure duration (y),

n = number of decay chain members.

For radionuclides or non-radionuclides with an human health endpoint of a ratio of the predicted concentration to the MCL, D_C is simply the ratio of the predicted groundwater concentration to the MCL. A D_c value of 1.0 implies groundwater concentration at the MCL are acceptable.

For nonradioactive contaminants with an human health endpoint of lifetime cancer incidence risk, D_C is given by

$$D_C = \frac{C \times WI \times EF \times ED \times SF}{BW \times AT} \tag{48}$$

where

C = average groundwater concentration over the exposure duration (mg m^{-3}),

SF = non-radiological carcinogenic slope factor (kg- mg^{-1}),

BW = body mass (kg),

AT = averaging time (70 years × 365 days per year = 25,550 days).

For nonradioactive contaminants with an human health endpoint of noncarcinogenic risk, D_C (also known as the hazard quotient) is given by

$$D_C = \frac{C \times WI \times EF \times ED}{BW \times AT \times RfD} \tag{49}$$

where

RfD = the reference dose (mg kg^{-1} d^{-1}).

The methodology presented so far is applicable for sites that contain single contaminants. Some sites may contain multiple contaminants having the same regulatory criteria endpoint (radiological dose, carcinogenic risk, or hazard quotient). In these cases, several approaches are recommended. First, the transit time of each contaminant should be considered. If the contaminant transit times are significantly different, then the contaminants can be treated separately because concentrations will not overlap. For contaminants that have approximately the same transit time, the regulatory criteria limit can be scaled for each contaminant. The general form of the scaling equation for n number of radionuclides limited by CEDE is

$$D_{Lj} = \frac{DCF_j}{\sum_{i=1}^{n} DCF_i} \times D_L \tag{50}$$

where

D_{Lj} = CEDE limit for the j^{th} nuclide (rem y^{-1})

$\mathrm{DCF}_{\mathrm{j}}$ = dose conversion factor (DCF) for the j^{th} nuclide (rem Ci^{-1}).

The general form of the scaling equation for carcinogens is

$$D_{Lj} = \frac{SF_j}{\sum_{i=1}^{n} SF_i} \times D_L \tag{51}$$

where

D_{Lj} = the risk limit for the j^{th} contaminant (number of cancers in a lifetime per person)

SL_j = slope factor for the j^{th} contaminant $(\mathrm{mg/kg/d})^{-1}$.

In a similar manner, D_{Lj} values for mixtures of similar contaminants (i.e. all radionuclides or all chemicals with carcinogenic risk) can be calculated from Equations 50 and 51 by substituting the MCL or RfD for the DCF or SF.

3.0 CODE IMPLEMETATION. INTRODUCTION

GWSCREEN is written in FORTRAN-77 and compiled for operation on a personnel computer with an MS DOS command prompt. Non-standard extensions are mainly violations of the six-character limit used for naming variables. The FORTRAN source code is also compatible with most FORTRAN compilers on UNIX operating systems. Changes typically have to be made to the time and date system calls. A brief description of the GWSCREEN subroutines and functions are found in Table 2. A simplified schematic of the overall program flow is illustrated in Figure 6.

Table 2. A brief description of the subroutines and functions in GWSCREEN Version 2.5.

Subroutine	Called IN	Equations	Description
AREA	TRAPZD, QGAUS2	36	Function that calculates Green's function for an area source
CONTAMP	MAIN3	4, 9, 15, 16	Calculates decay constants, retardation factors, and solubility source mass and times
DECAY	MAIN3	43, 44	Calculates progeny concentrations in groundwater
DISP	MAIN3	40–42	Calculates dispersion coefficients in groundwater
DOSECAL	MAIN3	46–49	Calculates radiological dose, carcinogenic and non-carcinogenic risk, and or compares predicted concentrations to maximum contaminant levels
ERF	AREA	36	Computes error function. Includes subroutines ERRORD, GAMMP, GSER, GCF, and GAMLIN.
FLOWP	MAIN3	22	Calculates water flow parameters in the source and unsaturated zone
GOLDEN	PEAK	---	Finds maximum of function AREA using Golden Section Search
GWINT	MAIN3	39	Calculates the average groundwater concentration over the exposure duration using Gauss-Legendre integration
LICENSE	MAIN1	---	Writes GWSCREEN license information to output file
LIMITS	SIMPSON, QGAUS2, UNSAT	51	Determines integration limits for Simpson rule, and Gauss-Legendre integration routines
LINT	SOURCE	---	Linear interpolation routine for user defined source
MAIN1	none	---	Main program control unit for GWSCREEN. MAIN1 opens input and output files and determines if Monte Carlo Sampling and multiple input files are requested.
MAIN2	MAIN1	---	Program control unit for implementation of Monte Carlo sampling features
MAIN3	MAIN1 and MAIN2	---	Main program control unit for calling the computational subroutines of the code
PEAK	MAIN3	---	Determines peak search limits and calls subroutine GOLDEN (Golden Section Search) to locate maximum concentration
QGAUS2	PEAK, MAIN3	32	Determines convolution integral using Gauss-Legendre integration routine
RDK	DECAY	43, 44	Solves the decay equation for an *n* member decay chain using a matrix solution described in Birchall (1986)
READF1	MAIN2, MAIN3	---	Reads model options and site data from GWSCREEN input file
READF2	MAIN2 MAIN3	---	Reads contaminant specific data from GWSCREEN input file
READGRD	READF1	---	Reads receptor grid from external file
READSRC	READF2	---	Reads user defined source from external file
RELIM	MAIN3	45	Calculates maximum allowable contaminant inventory or release rates in soil or pond effluent
SIMPSON	MAIN3	32	Control module for Simpson rule integration routine in aquifer
SIMPSONU	UNSAT	32	Control module for Simson rule integration routine in unsaturated zone
SOURCE	TRAPZDU, UNSAT, UKERNAL	11, 14, 21	Function that calculates mass release rate from source. Includes subroutine SRCPOND that calculates releases from percolation pond

Subroutine	Called IN	Equations	Description
UNSAT	QGAUS2, SIMPSON, TRAPDZ	31	Calculates mass flux to aquifer from unsaturated zone
UTT	CONTAMP	55	Calculates mean unsaturated transit time and arrival time of leading edge of contaminant plume in unsaturated zone (includes function FUNC as a root finder)
VANG	MAIN3	7, 8	Calculates moisture content in source and unsaturated zone using the van Genuchten fitting parameters
VARCHK	MAIN2	---	Checks each model parameter to see if the user defined it as stochastic. If true, then a randomly value from the user defined distribution is returned.
WRITE1	MAIN3	---	Writes site parameters to primary output file
WRITE2	MAIN3	---	Writes calculated flow and transport parameters to primary output file
WRITE3	MAIN3	---	Writes contaminant data to primary output file
WRITE4	MAIN3	---	Writes results of transport, dose, and maximum allowable inventory calculations to primary output file
ZARG	AREA	37	Function that calculates Z term for vertical dispersivity in aquifer

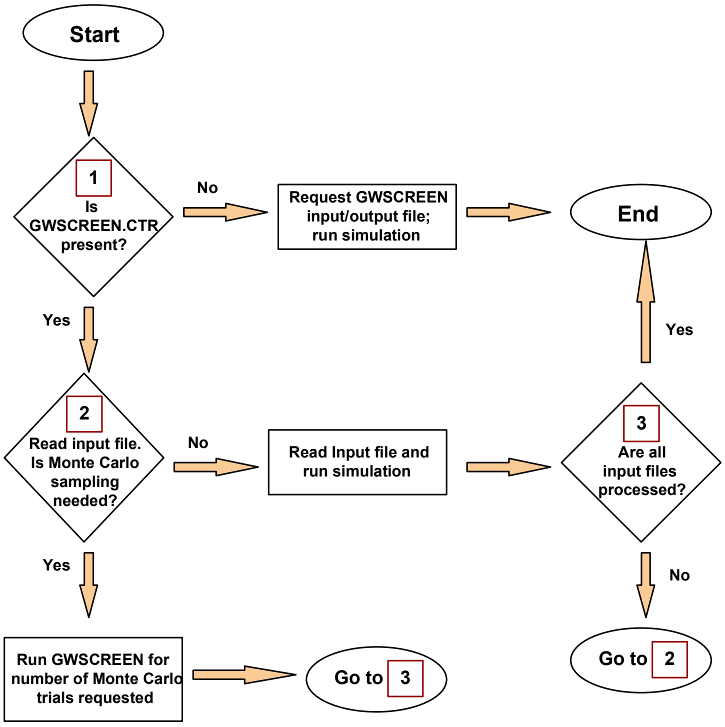

Figure 6. A simplified schematic of the overall GWSCREEN program flow and execution.

Numerical integration is required for computation of 1) the instantaneous groundwater concentration and contaminant flux [convolution integral in Equation (32)], 2) the vertically averaged groundwater concentration, and 3) the time-averaged groundwater concentration. Equation (38) for is used to vertically average the concentration across a well screen when the 3D dispersion model is employed. Equation (39) is used to time-average the concentration across the exposure duration. GWSCREEN uses two algorithms, Gauss-Legendre and Simpson's rule, to integrate Equation (32) (Press et al., 1992). Equations (38) and (39) are calculated using Gauss-Legendre only. Gauss-Legendre routines are computationally efficient for relatively smooth integrals approximated by polynomials and, if a preselected number of weight points are used, integration variables are not needed, thereby simplifying the required input for the user. For integrands that are not approximated very well by polynomials, or that are unpredictable and erratic, the Gauss-Legendre algorithms may become unstable and produce erroneous results. The Simpson rule routine, which is a more robust solver, may be used in such cases. The computational time using the Simpson's rule routine, however, is usually longer and also requires the user to input integration variables. In general, Gauss-Legendre integration should be limited to the surface and buried-source model, and Simpson rule integration should be used for the pond model. For a user-defined source, the integration routine selected should be based of the flux verses time curve relative to the time frame of interest. In general, if the mass flux to either the unsaturated zone (if dispersion is employed) or aquifer can be approximated by a pulse, then the Simpson Rule integration routine should be used. If unsure about which integration routine should be used, it is recommended that the Simpson Rule be used first and compared with the Gauss-Legendre solution. If the solutions are essentially equivalent (or within some predefined error limit) then the Gauss-Legendre integration routine can be used.

Variations of the Gauss-Legendre integration routine are found in the subroutines QGAUS2, UNSAT, and GWINT, and in the function ZARG. In GWINT and ZARG, an eight-point Gauss-Legendre routine (eight pairs of abscissas and weights) is used to integrate the instantaneous groundwater concentration over time and to vertically integrate the concentration in the aquifer. In QGAUS2 and UNSAT, a 17-point Gauss-Legendre integration routine is used to compute the convolution integral and to calculate the instantaneous groundwater concentration. The abscissas and weights for these routines were calculated using a FORTRAN routine adapted from Press et al. (1992). It was necessary to use more weight points in the QGAUS2 and UNSAT subroutine in order to achieve a stable solution to the convolution integral.

The integration limits in Equation (32) often result in values of the function $\Theta(x,t-\tau)$ that are near zero, add little to the integrand, and decrease the overall accuracy of the solution. Codell derived expressions for the integration limits, T_1 and T_2, such that for each function call of $\Theta(x,t-\tau)$, significant values to the integrand were added. These limits were presented (in Codell) for a line source with a decay term and for an area source without a decay term. The limits for an area source were modified to include a decay term in GWSCREEN. The limits (T_1, T_2) are given by

$$T_1, T_2 = t - \frac{1}{2}\left(\frac{\frac{2U(x+{}_L/2)+4D_x\gamma}{R_d}}{\left(\frac{U}{R_d}\right)^2+\frac{4Dx\lambda}{R_d}} \right)$$

$$\pm\frac{1}{2}\left(\sqrt{\left(\frac{\frac{2U(x+L/2)+4D_x\gamma}{R_d}}{\left(\frac{U}{R_d}\right)^2+\frac{4Dx\lambda}{R_d}} \right)^2 - \frac{4(x-L/2)^2}{\left(\frac{U}{R_d}\right)^2+\frac{4Dx\lambda}{R_d}}} \right) \tag{51}$$

where

T_1, , T_2 = upper and lower limits of integration (years),

γ= arbitrary value such that $e^{-\gamma} \approx 0.0$ when $T_1 < (t - \tau) < T_2$,

λ = radiological decay constant (y^{-1}).

A value of 50 was found to be adequate for γ. These limits are calculated in the subroutine LIMITS.

Equation (29) in subroutine AREA requires evaluation of error functions. The error function routine was also adapted from Numerical Recipes (Press et al., 1992) and contained in subroutines ERRORD, GAMMP, GSER, GCF, and GAMLIN.

Maximum concentration is determined in the subroutines PEAK and GOLDEN. Subroutine PEAK uses Equation (52) to calculate points that are known to lie on either side of the peak:

$$ZMIN = \frac{\left(T_{oper} + \left((x - L)\frac{R_d}{U} \right) \right)}{5} \times \frac{T_{1/2}U}{(0.1+x)R_d}$$

$$ZMAX = \left(T_{oper} + (x + L)\frac{R_d}{U} \right) 4 \tag{52}$$

where

$ZMIN$ = minimum bound (y),

$ZMAX$ = maximum bound (y),

T_{oper} = operational time of pond, $T_{oper} = 0$ if surface or buried source model is used (y).

These points, along with their midpoint, are passed to the subroutine GOLDEN (golden section routine adapted from Press et al., 1992) that calculates the maximum concentration and the time at which the maximum concentration occurred.

When dispersion is employed in the unsaturated zone, it is important to identify the arrival time of the leading edge of the plume at the aquifer-unsaturated zone interface. The arrival time of the plume leading edge may be described in terms of the standard deviation of contaminant plume at the time the plume front traverses the unsaturated thickness. Figure 7 shows plume density as a function of downgradient distance from a source for several times after release. The standard deviation of a Gaussian distributed plume (σ in meters) is given by

$$\sigma = \sqrt{\frac{2\,D_x\,t}{R_d}} \tag{53}$$

The leading edge of the plume can be defined in terms of the number of standard deviations from its center or maximum value. The mean travel time is given by Equation (23). We are interested in finding the time (t) when the plume center is located $X_u - \varepsilon\sigma$ from the source, where ε = the number of standard deviations from the mean and X_u = the unsaturated thickness. Substitution of Equation (53) into the previous equation yields

$$X_m = X_u - \varepsilon\,\sigma \tag{54}$$

where X_m = the mean distance traveled in time, t and is given by $X_m = t\,U_u/R_d$. Substitution of this expression into Equation (54) yields

$$t - \left(X_u - \varepsilon\sqrt{\frac{2D_x t}{R_d}} \right)\frac{R_d}{U_u} = 0 \qquad (55).$$

The roots to Equation (55) are solved using a bisection method described in Press et al., 1992. The value of ε has been fixed at 4 in the code.

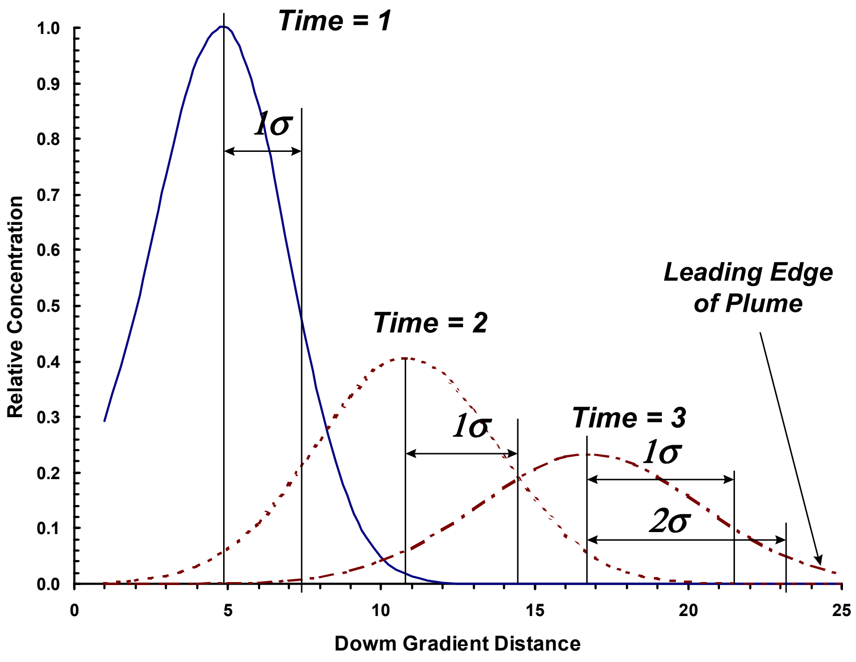

Figure 7. Longitudinal spreading of a pulse released at time = 0 showing the growth of its standard deviation with travel time and leading edge arrival time for distance of 25 units.

3.2 Input Files

Input to GWSCREEN is through several free-format ASCII files. The primary input file contains the contaminant and site-specific data and is required for execution of GWSCREEN. The second file is optional and is used control the execution of one or more input files in addition to controlling Monte Carlo sampling of selected variables. This file is named GWSCREEN.CTR and contains the name of the file to write all output, number of input files to run, and identifies the Monte Carlo variables and sampling controls. If a user defined source or spatial grid output is selected, then files containing the release rate and receptor grid must also be created.

The only required file to run GWSCREEN is the site specific input file. This file has been extensively changed from previous versions of GWSCREEN and is not backward compatible. When executing GWSCREEN, if the file GWSCREEN.CTR is not present in the default directory, then the user is prompted for a GWSCREEN input file followed by the output file name The default input file name is GWSCREEN.PAR, and the default output file name is GWSCREEN.OUT.

File format for the input files are described in Table 3 for the primary input file, Table 4 and 5 for the GWSCREEN.CTR file, and Table 6 and 7 for other external files. Additional explanation of some of the important input parameters follows.

3.2.1 Vertical Mixing Options.2.2 Vertical Mixing Options (Variables ITYPE, THICK, and Z)

The variable THICK has different meanings depending on the value of ITYPE. When ITYPE = 1, a 2D solution is employed and the contaminant is mixed within the aquifer thickness defined by the variable THICK. The value of THICK should not exceed the thickness of the aquifer. The variable Z is ignored. When ITYPE = 2 or 3, THICK represents the thickness of the aquifer. The variable Z represents the depth within the aquifer where the concentration are evaluated if ITYPE=2. If ITYPE=3, then Z represents the distance from the surface of the aquifer to a depth Z where concentrations are averaged over. This distance can be up to but not including the total aquifer thickness defined by the variable THICK.

3.2.2 Aquifer Dispersivity Options.2.2 Vertical Mixing Options (Variables IDISP, AX, AY, and AZ)

Four aquifer dispersivity options are employed in GWSCREEN Version 2.5 and are set by the value of IDISP. If IDISP = 0, then the dispersivity is fixed at the values defined for AX, AY, and AZ. If IDISP = 1, 2, or 3, then a scale dependent longitudinal dispersivity is calculated based on the regressions given in Equations 40–42. Under such conditions, the value of AY represents the ratio of transverse to longitudinal dispersivity and the value of AZ represents the ratio of vertical to longitudinal dispersivity.

3.2.3 Contaminant Type and Health Impacts.2.2 Vertical Mixing Options (Variables IMODE, DLIM, and DCF)

The type of contaminant (radionuclide or non-radionuclide) and health impacts calculated are determined by the value of IMODE. Consequently, the units of the variables DLIM and DCF are also determined by the value of IMODE. Radioactive contaminants are indicated by IMODE values from 1 to 3. Non-radioactive contaminants are indicated by IMODE values from 4 to 6. Activity units for radionuclides are Ci and mass units for non-radioactive contaminants are mg.

If the IMODE variable is 1, then committed effective dose equivalent is calculated and the DCF variable represents the ingestion dose conversion factor (rem Ci^{-1}). The variable, DLIM represents the maximum acceptable dose (in rem) from the ingestion of groundwater.

If the IMODE variable is 2, then carcinogenic risk from the ingestion of a radionuclide is calculated and the DCF variable represents the risk conversion factor (Ci^{-1}). The variable, DLIM represents the acceptable carcinogenic risk for groundwater ingestion.

If the IMODE variable is 3, then a ratio of the maximum concentration to the MCL for a radionuclide is calculated and the DCF variable represents the MCL (Ci m^{-3}). The variable, DLIM represents the acceptable ratio of the maximum (or time averaged) groundwater concentration to the MCL.

If the IMODE variable is 4, then a ratio of the maximum concentration to the MCL for a non-radionuclide is calculated and the DCF variable represents the MCL (mg m^{-3}). The variable, DLIM represents the acceptable ratio of the maximum (or time averaged) groundwater concentration to the MCL.

If the IMODE variable is 5, then carcinogenic risk from the ingestion of a carcinogenic non-radionuclide is calculated and the DCF variable represents the risk conversion factor (kg-d mg^{-1}). The variable, DLIM represents the acceptable carcinogenic risk for groundwater ingestion.

If the IMODE variable is 6, then the non-carcinogenic risk is calculated and the DCF variable represents the reference dose (mg $(kg\text{-}d)^{-1}$). The variable, DLIM represents the acceptable hazard quotient for groundwater ingestion.

3.2.4 Type of Output.2.2 Vertical Mixing Options (Variable KFLAG, INTIME, NTIMES, T1, T2, TP, and GT)

The KFLAG variable determines the type of output calculated. Maximum concentration and time of maximum are calculated by setting KFLAG to 1. The concentration is also integrated around the peak over the time defined by the variable, INTIME. For example, if the maximum concentration occurs at 300 years and the variable INTIME is equal to 30 years, then the concentration is integrated between 285 and 315 years. Typically, time-integrated groundwater concentrations are required for non-radiological carcinogenic risk calculations. In addition to maximum and time-integrated concentrations, the maximum aallowable soil inventory (IMODEL = 1) or maximum allowable effluent release rate (IMODEL = 2) are calculated when KFLAG = 1.

Setting KFLAG equal to 2 allows concentration vs. time computations. Health impacts (radiological dose, carcinogenic risk, or comparisons to reference dose or MCL) are also calculated and written to the DOSE.OUT file (see section on output files). Output time periods are determined by the array variables T1, T2 and TP (in units of years). T1 indicates the beginning time of calculation, T2 indicates the ending time of calculation, and TP indicates the print step. For example, T1, T2, and TP values of 100, 200 and 10 respectively indicate concentrations are calculated and printed beginning at year 100 and ending at year 200 and output every 10 years (100, 110, 120, 130 ... 200). The variable NTIMES determines the number of time periods to output. For example, setting NTIMES to 2 requires two sets of T1, T2, and TP values. NTIMES is limited to 10 time periods. Time is always measured from the begin time of the simulation (year 0)

Setting KFLAG to 3 allows for concentrations to be calculated on a spatial grid for a user-specified output time. A spatial grid consists of a series of X and Y coordinates. Health impacts (radiological dose, carcinogenic risk, or comparisons to reference dose or MCL) are also calculated and written to the DOSE.OUT file (see section on output files). The variable GT stores the time from the start of the simulation that concentrations are calculated at.

3.2.4 .2.2 Vertical Mixing OptionsNumerical Integration Options (ISOLVE, ISOLVEU, JSTART, JMAX, EPS)

Integration routine options are selected using the ISOLVE, and ISOLVEU variables. In general, the Simpson's rule integration routine (ISOLVE, ISOLVEU = 2) is a more robust solver than the Gauss-Legendre and is recommended for the pond model or when a user-defined release function is used; however, the routine usually requires more computational time. The variables JMAX, JSTART, and EPS are used with the Simpson's rule integration routine. The routine evaluates the integral for a variable number of points and monitors the accuracy of the solution. The accuracy is checked by computing the integral using 2^n number of middle points plus the two end points and then adding 2^{n+1} number of middle points and comparing the result with the previous evaluation. The variable JMAX defines the maximum number of iterations allowed before the integration routine is terminated. On the first iteration, the crudest approximation to the integral is performed by evaluating the function at the upper and lower limits. On each successive iteration, the number of middle points (points between the upper and lower limits of integration) evaluated are increased by a factor of 2 starting with one middle point added during the second iteration. The number of additional middle points is given by 2^{n-2} where n = the iteration number. The routine evaluates the integral for at least JSTART number iterations before the n-1 solution is checked for convergence with the n^{th} solution. For example, if the variable JSTART is set equal to 6 (its minimum allowable value) then 6 iterations are performed before convergence checking occurs. The number of middle points added on the 6th iteration is $2^{6-2} = 16$. Convergence is checked by calculating the EPS value and comparing it to the user input EPS value. The EPS variable is given by

$$EPS = \frac{|\Theta_p - \Theta_c|}{\Theta_c} \tag{56}$$

where

Θ_p = previous evaluation of the integral [Equation (32)]

Θ_c = current evaluation of the integral.

If the calculated EPS is less than the user input EPS, then the routine is terminated and the current evaluation of the integral is returned. If the calculated EPS is greater than the user input EPS, then 2^{n-2+1} number of middle points are added and a new value of the integral is calculated and checked. If convergence is not achieved in JMAX number of iterations, then the routine is terminated and the current value of the integral is returned. A message warns the user of non-convergence and the current EPS value is also printed. An adequate solution does not necessarily require convergence to be met and depends on the values of the integration variables JMAX, JSTART, and EPS. Unacceptable solutions are usually detected by observing the concentration verses time output. If there are perturbations in the concentration versus time curve that are not accounted for by the source release model, then the EPS value should be set lower and JMAX increased. In the samples problems presented in Appendix A, adequate solutions were obtained using an EPS value of 5.0×10^{-3} and a JMAX value of 12. The JSTART variable, which must be less than JMAX, was set equal to 6. Decreasing the EPS value and increasing JMAX is not without cost, however, since computational time is significantly increased when these values are changed.

3.2.5 .2.2 Vertical Mixing OptionsReceptor Coordinates (Variables X0, Y0, XREC, YREC)

The coordinate system defined by the groundwater model uses the center of the source as its origin. Groundwater flow is in the positive *X* direction. Sometimes it is convenient to define a coordinate system whose origin does not coincide with that of the model. The variables X0 and Y0 allow for translation of an external coordinate grid to that of the model coordinate system. X0 is the distance parallel to groundwater flow from the origin of the external grid to the center of the source. Y0 is the distance perpendicular to groundwater flow from the origin of the external grid to the center of the source. The receptor locations entered (XREC and YREC) are in relation to the external coordinate system.

This feature is helpful for assessing the cumulative impacts of contaminated sites that have multiple sources. An example of this type of application is illustrated in the sample problem section of this report.

3.2.6 Multiple Input Files and .2.2 Vertical Mixing OptionsMonte Carlo Sampling (File GWSCREEN.CTR)

Monte Carlo sampling and multiple file input is controlled through the file GWSCREEN.CTR (Table 4). Monte Carlo sampling is invoked when the user provides a seed value of less than 1 (SEED) *and* the sets the number of trials (NSIM) to greater than 0. When SEED is less than 1 and NSIM>0, Monte Carlo sampling is invoked and the code reads the variable NMCV on the next line immediately following the line containing the file name seed value, and number of trials to perform. This variable indicates the number of stochastic variables to evaluate in the Monte Carlo simulation. Stochastic variables are identified by their name (Table 5), distribution type, and parameters that describe the distribution. The name of the stochastic variable (in upper case) must be specified exactly as listed in Table 5. Following the stochastic variable name are four parameters that describe the distribution. Note for the normal and lognormal distributions, a minimum and maximum value is required. The minimum and maximum value allow for truncation of the distribution at its tails. If no truncation is desired, then set these values to exceed tail values.

3.2.7 .2.2 Vertical Mixing OptionsExternal Source Release Files and Receptor Grid Files

When a user-generated source function is used (IMODEL = 3), the release function, $F_S(\tau)$, in Equation (32) is linearly interpolated from the data provided by the user. Source release information is provided in a user-generated file listed on Card 14c in the main input file (Table 3). The format for this file is described in Table 6. Release rates at each time τ, are linearly interpolated from the data provided. External source release files are not tabular sources and the code linearly interpolates between the points provided by the user. The first time-flux pair should be at time 0. GWSCREEN Version 2.5 assumes a zero-flux for times greater that the last time entered in the release file. For example, if the last time entered in a release file was 100 years and concentrations are requested out to 1000 years, then zero source flux is assumed for times > 100 year. A maximum of 2000 points are allowed. When concentrations are to be calculated on a receptor grid (KFLAG=3), the receptor locations are read from a user-generated file listed on Card 12c in the main input file (Table 3). The format for this file is described in Table 7. A maximum of 2000 receptor locations may be input.

Table 3. GWSCREEN Version 2.5 Input file. Each card represents a line in the input file. Variables must be put in the same order as they are presented in the Table.

Card	Code Variable	Text Variable	Type	Description
1	TITLE	---	CHAR*80	Character title of project
2	IMODE	---	INTEGER	Defines type of impacts to be calculated and contaminant type: (1) Radiological Dose (2) Radiological Carcinogenic Risk (3) MCL for radionuclides (4) MCL for non-radionuclides (5) Carcinogenic Risk for Non-radionuclides (6) Non carcinogenic Risk for Non-radionuclides
	ITYPE	---	INTEGER	Defines type of vertical dispersion used in aquifer: (1) 2D vertically averaged solution, (2) 3D point solution, (3) 3D vertically averaged solution.
	IDISP	---	INTEGER	Defines longitudinal and transverse dispersion options: (0) Fixed dispersivity, (1-3) Spatially variable dispersivity based on 3 different algorithms (see Section 2.3.1).
	KFLAG	---	INTEGER	Defines type of output: (1) Peak concentration and maximum impacts, (2) Concentration as a function of time, (3) Concentration as a function of a spatial grid.
	IDIL		INTEGER	Computes additional dilution from infiltrating water: (1) no dilution correction, (2) dilution correction (recommended for high infiltration sources, see Section 2.1.3).
3	IMODEL	---	INTEGER	Defines type of source model: (1) surface or buried source, (2) pond source model, (3) tabulated source function.
	ISOLVE	---	INTEGER	Defines solution algorithm in aquifer: (1) Gauss-Legendre, (2) Simpsons Rule.
	ISOLVEU		INTEGER	Defines solution algorithm in unsaturated zone: (1) Gauss-Legendre, (2) Simpsons Rule.
	IMOIST	---	INTEGER	Defines how moisture content is determined in source zone: (1) user defined, (2) Calculated using van Genuchten fitting parameters.
	IMOISTU	---	INTEGER	Defines how moisture content is determined in unsaturated zone: (1) user defined, (2) Calculated using van Genuchten fitting parameters.
4	JSTART	--	INTEGER	Number of iterations to perform in the Simpson rule integration routine before convergence is checked. See discussion in Section 3.2.4.
	JMAX	---	INTEGER	Maximum number of iterations to perform for the Simpson rule integration. The maximum number of point evaluations = $[2^{jmax-1}]$. See discussion in Section 3.2.4.
	EPS	---	REAL	Convergence criteria for Simpson rule integration. See discussion in Section 3.2.4.
5	BW	BW	REAL	Body mass (weight) of receptor (kg)
	AT	AT	REAL	Averaging time (days)
	WI	I	REAL	Water intake rate (L d^{-1})
	EF	EF	REAL	Exposure frequency (d y^{-1})
	ED	ED	REAL	Exposure duration (y)

Table 3 (Continued)

Card	Code Variable	Text Variable	Type	Description
	DLIM	D_L	REAL	Acceptable level of health impacts. Units depend on the value of IMODE: (1) rem, (2) carcinogenic risk for radionuclide, (3) ratio of concentration to MCL for radionuclides, (4) ratio of concentration to MCL for non-radionuclide, (5) carcinogenic risk for non radionuclide, (6) hazard quotient.
6	X0	--	REAL	Coordinate of center of source parallel to groundwater flow relative to receptor grid coordinate system (m)
	Y0	---	REAL	Coordinate of center of source perpendicular to groundwater flow relative to receptor grid coordinate system (m)
7	L	L	REAL	Length of source parallel to groundwater flow (m)
	W	W	REAL	Width of source perpendicular to groundwater flow (m)
	PERC	P	REAL	Percolation rate through source and into unsaturated zone (m y^{-1})
8a	**Read only if IMODEL 2**			
	TOPER	t_{op}	REAL	Operation time of pond (y)
	PNDFLX	Q_{pond}	REAL	Water flux into pond (m^3 y^{-1})
	EVAP	λ_E	REAL	Evaporation of other loss rate constant from pond (y^{-1})
	THETAP	θ_p	REAL	**Read only if IMOIST = 1** Volumetric water content of pond (m^3 m^{-3})
8b	**Read only if IMODEL =1 or 2**			
	THICKS	T	REAL	Thickness of Source or pond sediment thickness (m)
	RHOS	ρ_c	REAL	Bulk density in source zone (g cm^{-3}).
8c	THETAS	θ_c	REAL	**Read only if IMOIST = 1** Volumetric water content of source or pond sediments after end of operation, (m^3 m^{-3})
8d	**Read only if IMOIST = 2**			
	ALPHA	α	REAL	van Genuchten fitting parameter for source (m^{-1})
	N	n	REAL	van Genuchten fitting parameter for source
	KSAT	K_{sat}	REAL	Saturated hydraulic conductivity for source (m y^{-1})
	PORS	θ_T	REAL	Total porosity for source (assumed to be equivalent to the effective porosity, m^3 m^{-3})
	THETAR	θ_r	REAL	Residual moisture content for source (m^3 m^{-3})
9	DEPTH	X_u	REAL	Depth from base of source to top of aquifer (unsaturated thickness) (m)
	RHOU	ρ_u	REAL	Bulk density in unsaturated zone (g cm^{-3})
	AUX	Dx	REAL	Longitudinal dispersivity in unsaturated zone (m). Set AUX = 0 for plug flow model
9a	THETAU	θ_u	REAL	**READ only if IMOISTU = 1**. Volumetric water content in unsaturated zone (m^3 m^{-3})
9b	**Read only if IMOISTU = 2**			
	ALPHAU	α	REAL	van Genuchten fitting parameter for unsaturated zone (m^{-1})
	NU	n	REAL	van Genuchten fitting parameter for unsaturated zone

Table 3 (Continued)

Card	Code Variable	Text Variable	Type	Description
	KSATU	K_{sat}	REAL	Saturated hydraulic conductivity for unsaturated zone (m y^{-1})
	PORSU	θ_T	REAL	Total porosity for unsaturated zone (assumed to be the same as effective porosity, m^3 m^{-3})
	THETARU	θ_r	REAL	Residual moisture content for unsaturated zone (m^3 m^{-3})
10	AX	α_L	REAL	Longitudinal dispersivity (m) if IDISP = 0; otherwise ignored
	AY	α_T	REAL	Transverse dispersivity (m) if IDISP = 0; otherwise the ratio of the transverse to longitudinal dispersivity
	AZ	α_V	REAL	Vertical dispersivity (m) if IDISP = 0; otherwise the ratio of the vertical to longitudinal dispersivity
	B	b	REAL	Aquifer thickness (m)
	Z	z	REAL	If ITYPE = 1 or 3, then z is the well screen thickness, else, z is the depth in the aquifer where concentrations are evaluated.
11	U	U	REAL	Darcy velocity in aquifer (m y^{-1})
	PHI	η	REAL	Porosity of aquifer (m^3 m^{-3})
	RHOA	ρ_a	REAL	Bulk density of aquifer (g cm^{-3})
12a	**Read only if KFLAG <3**			
	NRECEPT	---	INTEGER	Number of receptors
12b	**Read only if KFLAG<3; Repeat card 12b NRECEPT times**			
	XREC(I)	x	REAL	Receptor distance from center of source parallel to groundwater flow for the ith receptor (m)
	YREC(I)	y	REAL	Receptor distance from center of source perpendicular to groundwater flow for the ith receptor (m)
12c	**Read only if KFLAG=3**			
	GRIDFILE	---	CHAR*40	File name containing the x and y coordinates of each receptor (maximum 2000)
13a	**Read only if KFLAG = 2**			
	NTIMES	---	INTEGER	Number of time periods to calculate concentrations over
13b	**Read only if KFLAG = 2; Repeat card 13b NTIMES times**			
	T1(I)	---	REAL	Beginning time of the Ith time period to calculate concentration as a function of time (y)
	T2(I)	---	REAL	End time of the Ith time period to calculate concentration as a function of time (y)
	TP(I)	---	REAL	Print time step for the Ith time period (y)
13c	**Read only if KFLAG = 3**			
	GT	---	REAL	Time of concentration grid output (y)
14	NCONTAM	---	INTEGER	Number of contaminants
14a	**Repeat card 14a NCONTAM times**			
	NPROG	---	INTEGER	Number of radioactive progeny; NPROG must be less than 8. NPROG=0 for non radioactive contaminants.

Table 3 (Continued)

Card	Code Variable	Text Variable	Type	Description
	KDS	K_dc	REAL	Distribution coefficient in source zone (mL g^{-1})
	KDU	K_du	REAL	Distribution coefficient in unsaturated zone (mL g^{-1})
	ZMW	MW	REAL	Molecular weight (g mol^{-1})
	QI	M_o	REAL	Initial mass or activity (mg or Ci)
	RMI	R_p	REAL	Mass or activity input rate to pond (mg or Ci y^{-1}). Ignored if IMODEL =1 or 3.
	SL	C_{sl}	REAL	Solubility limit (mg L^{-1})
	OTHER	λ_o	REAL	Loss rate constant from source for other mechanisms (y^{-1})
14b	**Repeat card 14b NPROG+1 times for radionuclides**			
	CNAME(I,J)	---	CHAR*6	Name of the I^{th} contaminant, J^{th} decay chain member (Total decay chain members = NPROG+1)
	THALF(I,J)	---	REAL	Half life of I^{th} contaminant for J^{th} decay chain member (Total decay chain members = NPROG+1)
	KDA(I,J)	Kd_a	REAL	Distribution coefficient in aquifer for I^{th} contaminant and J^{th} decay chain member (Total decay chain members = NPROG+1)
	DCF(I,J)	---	REAL	Dose conversion factor (rem Ci^{-1}) if IMODE=1, carcinogenic slope factor for radionuclide (Ci^{-1}) if IMODE=2, MCL for radionuclide (Ci m^{-3}) if IMODE=3, MCL for non-radionuclide (mg m^{-3}) if IMODE=4, carcinogenic slope factor for non-radionuclide (kg-d mg^{-1}) if IMODE=5, reference dose for non-carcinogenic effects (mg $(kg\text{-}d)^{-1}$) if IMODE=6. for i^{th} contaminant and j^{th} decay chain member.
14c	**Read only if IMODEL = 3**			
	RELFILE	---	CHAR*40	Name of release file

Table 4. GWSCREEN Version 2.5 control file (GWSCREEN.CTR)

Card	Code Variable	Text Variable	Type	Description
1	TITLE	---	CHAR	Title of project
2	FILEOU	---	CHAR	Output file name
3	NFILES	---	INTEGER	Number of GWSCREEN input files. (maximum of 20)
4	FILEIN	---	CHAR	**Repeat card 4 NFILES times** Name of the ith input file
	NSIM	---	INTEGER	Number of Monte Carlo trials to perform. Set NSIM = 0 for deterministic calculation
	SEED	---	INTEGER	Random number seed. Set SEED $\geq$ 0 for deterministic calculations
5	**Read card 5 and 5a only if NSIM > 0 and SEED < 0**			
	NMCV	--	INTEGER	Number of stochastic variables in simulation
5a	**Read card 5a NMCV times**			
	VARNAME	---	CHAR*6	Name of stochastic variable (see below)
	DISTYPE	---	INTEGER	Type of distribution (1) normal, (2) lognormal, (3) uniform, (4) triangular
	P(i,4)	---	REAL	Four parameters that describe the distribution for the ith stochastic variable; see Table 5 for distribution descriptions

Table 5. Stochastic variables and distribution parameters allowed in GWSCREEN. (See Table 3 for variable descriptions)

Variable Name	Variable Name	Variable Name	Variable Name	Variable Name
ALPHA	KDA1[b]	KDU [b]	PORS	THETAS
ALPHAU	KDA2[b]	KSAT	PORSU	THETAU
AX[a]	KDA3 [b]	KSATU	QI	THETAU
AXU	KDA4 [b]	L	RHOA	THICKS
AY[a]	KDA5 [b]	N	RHOS	TOPER
AZ[a]	KDA6 [b]	NU	RHOU	U
B	KDA7 [b]	OTHER	RMI	W
BW	KDA8 [b]	PERC	SL	WI
DEPTH	KDA9 [b]	PHI	THETAP	Z
EVAP	KDS [b]	PNDFLX	THETAR	

Distribution Type	Parameter (1)	Parameter (2)	Parameter (3)	Parameter (4)
Normal	Mean	Standard Deviation	Minimum	Maximum
Lognormal	Geometric Mean	Geometric Standard Deviation	Minimum	Maximum
Uniform	Minimum	Maximum	ignored	ignored
Triangular	Minimum	Most Likely	Maximum	ignored

a) Ignored if IDISP $\neq$ 0

b) If one or more distribution coefficients in different media are assigned the same value, then GWSCREEN assumes a one-to-one correlation between the values. For example, if the source and unsaturated zone K_d's are assigned the same value, and the source K_d is defined as a stochastic variable, then the unsaturated K_d will also take the value of the source K_d for each Monte Carlo trial.

Table 6. File format for a user-defined release (IMODEL=3).

Card	Code Variable	Text Variable	Type	Description
1	JUNK	---	CHAR	A file header that is discarded
				Repeat Card 2 for each time and release rate entry
2	REL(1,i)	---	REAL	Time of ith release (years)
	REL(2,i)	---	REAL	Mass or activity of i^{th} release (Ci or mg y^{-1}). Maximum of 2000 individual points

Table 7. File format for a receptor grid (KFLAG=3)

Card	Code Variable	Text Variable	Type	Description
1	JUNK	---	CHAR	A file header that is discarded
				Repeat Card 2 for each X,Y receptor pair
2	X(i)	---	REAL	Receptor distance from center of source parallel to groundwater flow for the i^{th} receptor (m)
2	Y(i)	---	REAL	Receptor distance from center of source perpendicular to groundwater flow for the i^{th} receptor (m)

3.3 Output Files

The number of output files generated by GWSCREEN depends on the model options selected and whether the simulation is run using the GWSCREEN.CTR file. Primary output is written to the output file that is either identified in the GWSCREEN.CTR file or defined by the user at run-time. If a concentration time-history or receptor grid output are selected, then a file named DOSE.OUT is also generated. This file contains the heath effects calculations (radiological dose, carcinogenic risk, etc.) for each time or receptor location requested by the user in the primary input file. If Monte Carlo sampling is employed, then stochastic output is written to the file GWSCREEN.MCO and deterministic output is written to the output file identified in the GWSCREEN.CTR file.

3.3.1 Maximum Allowable Soil Inventory or Release Rate to a Pond Output.2.2 Vertical Mixing Options

When the KFLAG variable is set equal to 1 and IMODEL is ≤2, maximum allowable soil inventory and pond release rates are calculated. The maximum allowable soil inventory is defined as the contaminant inventory (in Ci or mg) in soil such that, after leaching, decay and transport to the receptor well, health impact criteria are not exceed. The maximum allowable pond release rate is the annual release quantity (in Ci or mg per year) that can be discharged to a pond facility for the operational life expectancy of the facility, such that health impact criteria at the receptor well are not exceeded. Heath impact criteria may include the maximum acceptable radiological dose or carcinogenic risk and is defined by the DLIM variable.

Limiting soil inventories for contaminants with relatively short half-lives, compared to their unsaturated transit times, are usually quite large, and often exceed the solubility limited mass

[Equation (15)]. This situation may occur even when the solubility limit is set artificially high. The user should be aware that the limiting contaminant inventory calculated under these conditions is unreasonably high and sometimes not physically possible. For radionuclides, the specific activity of the nuclide is also computed and compared to the limiting soil concentration. The specific activity is given by

$$S_p = \frac{N_A \lambda_d \ 3.1536 \times 10^7 \, s / y}{MW \ 3.7 \times 10^{10} \, dps / Ci} \ . \tag{57}$$

3.3.2 Radioactive Progeny.3.3 Radioactive Progeny

Data relating to radioactive progeny are reported to the right of the parent value in the output files. These data include the half-life, distribution coefficient, dose/risk conversion factors, groundwater concentrations, and dose/risk values.

Radionuclide specific input parameters (half-life, distribution coefficient, dose/risk conversion factor) for radioactive progeny are listed to the right of the corresponding parent value. Ground water concentrations and dose/risk values are also reported to the right of the corresponding parent value in the output file. One of the key simplifying assumptions used in GWSCREEN is that progeny travel at the same speed as their parent. Under conditions of secular equilibrium and where the parent and progeny have about the same distribution coefficient, the maximum progeny concentration at a fixed receptor point occurs about the same time as the maximum parent concentration occurs. However, even when the distribution coefficients are about the same there is no assurance that maximum progeny concentrations will occur at the same time as maximum parent concentrations. For these reasons, it is suggested that when determining maximum allowable inventories or release rates (KFLAG=1) that a run be made with KFLAG=2 so the true peak progeny concentration can be verified.

The case of "no equilibrium conditions" between parent and progeny is illustrated in example problem #8 (Figure 8). In example problem #8, the maximum ^{241}Pu concentration (parent nuclide) occurs at 319 years (compare output for sample problem #8 with Figure 8), the maximum ^{241}Am concentration occurs at 376 years, and the maximum ^{237}Np concentration occurs at 388 years. The concentrations of ^{241}Am and ^{237}Np at 319 years were 4.0×10^{-10} Ci m^{-3} and 3.4×10^{-12} Ci m^{-3} respectively. Note that these concentrations are lower than their actual maximum concentration presented in Figure 8. Also note in the output that the average concentrations for the progeny are higher than the reported maximum concentration for the progeny. This indicates that the peak progeny concentration did not occur at the same time as the peak parent concentration did. The user should be aware when non-equilibrium conditions exist and run the code in both the maximum allowable inventory and concentration versus time modes to ensure that a conservative answer has been calculated.

When concentration versus time or grid output (KFLAG=2 or 3 respectively) is designated, then concentrations and doses are identified for each member of the decay chain as “Conc Mbr 1, Conc Mbr 2, Conc Mbr 3” and so on. The parent nuclide is always the first member of the decay chain.

The ^{241}Pu flux to the aquifer and the unsaturated transit time (251 years) are also shown in Figure 8. Since the unsaturated transit time exceeds 10 times the half-life (14.4 years), then, as suggested in Section 2.2, the dispersive solution in the unsaturated zone should be used. The dispersive solution using a dispersivity of 0.5 m is shown in Figure 9. Note that the maximum Pu-241 flux to the aquifer is higher in this case compared to the flux for the no dispersion case illustrated in Figure 8. This is because the contaminant plume arrives at the aquifer sooner, allowing less time for decay.

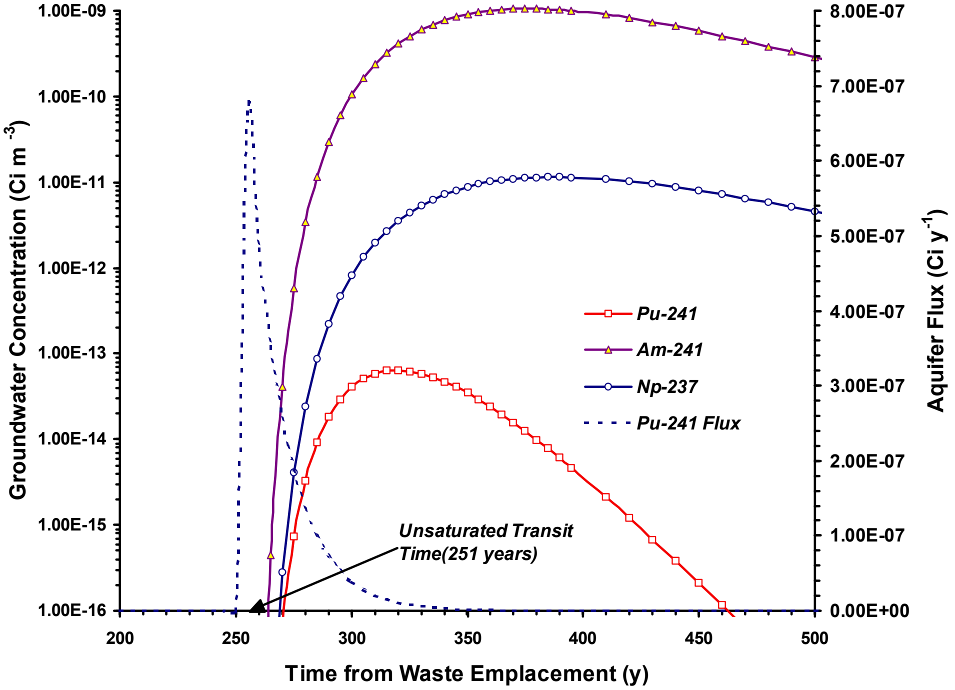

Figure 8. Concentration and flux to the aquifer (right axis) as a function of time for sample problem #8 using no dispersion in the unsaturated zone.

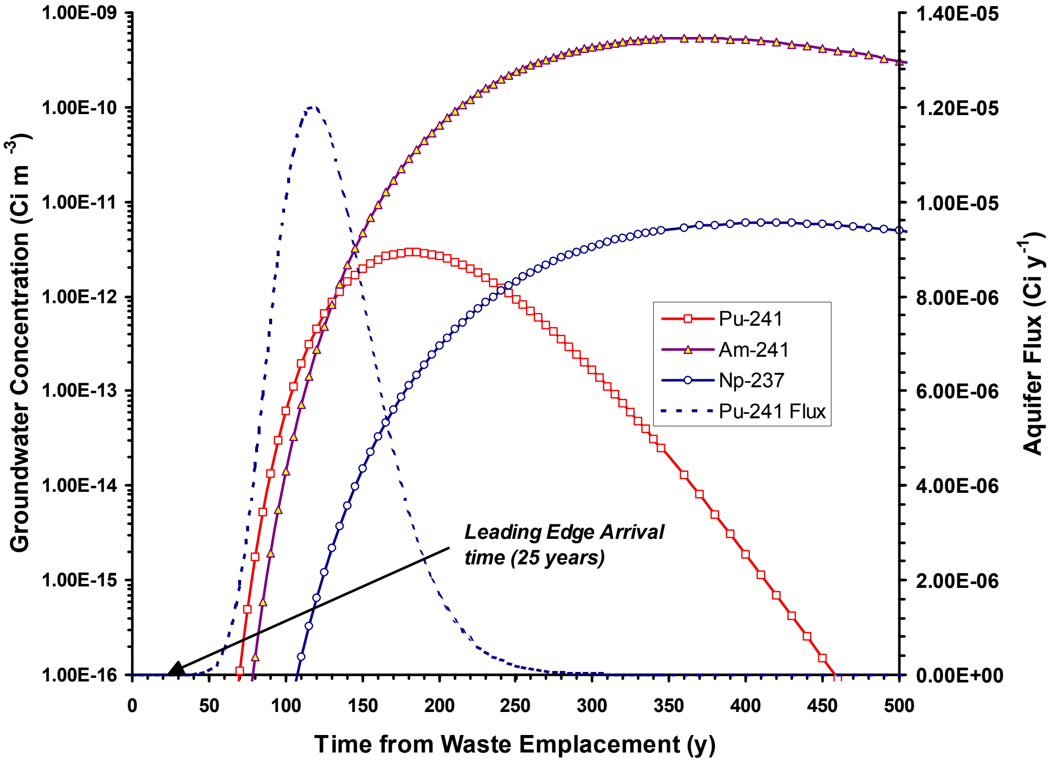

Figure 9. Concentration and flux to the aquifer (right axis) as a function of time for sample problem #8 using 0.5 m dispersion in the unsaturated zone.

3.3.3 Monte Carlo Output

Monte Carlo output is written to the file, GWSCREEN.MCO. This file echoes back the stochastic variables defined by the user and the distributions assigned to each variable. Next, output from each Monte Carlo trial is reported by time and receptor location. Output includes values of the stochastic variables for each trial. The GWSCREEN.MCO file was designed to simply store all the output from a Monte Carlo simulation. Consequently, this file has the potential to get quite large if many receptor locations and output times are selected. In order to provide more meaningful output, concentration and dose results must be extracted from the output file. The EXTRACT utility program was written for that purpose. EXTRACT is a user-interactive post processor for the Monte Carlo output file. Concentration and dose results for a user specified contaminant, receptor location, and output time may be extract from the GWSCREEN.MCO primary output file. Concentration and dose values for each simulation are written by default in EXTRACT to the GWSMC.VAL file and percentiles (in increments of 5%) are written to by default to the GWSMC.PRC file. During execution of a Monte Carlo simulation, a GWSCREEN input file named MC.PAR is written each time a trial is performed.

4.0 SAMPLE PROBLEMS. INTRODUCTION

Appendix A contains output from the eight sample problems described and used in previous versions of GWSCREEN. These sample problems are the same set used in the verification and validation of earlier versions of GWSCREEN (Rood 1993a, 1993b, 1994b, 1995) and provide documentation of the verification and validation process of Version 2.5. New features of the code are demonstrated in this section using several applications of the code to selected problems.

4.1 Multiple Source Problem

This sample problem considers the cumulative effects of multiple sources in close proximity to one another. The problem considers release of ^{14}C from the Radioactive Waste Management Complex (RWMC) at the Idaho National Engineering and Environmental Laboratory. Carbon-14 has been disposed in the facility since 1952 and the performance assessment (Maheras et al. 1994) has identified this nuclide as one of the principle dose drivers. The performance assessment only considered waste from the currently active disposal pit which opened in 1984. Concern has been expressed over the cumulative dose impacts from all ^{14}C disposed at the facility beginning in 1952. For this problem, four separate sources are considered. These sources represent different pits and trenches that are currently active or have been active in the past. Activity release rates from each source were calculated outside GWSCREEN using a model described in Rood (1994c). Sources were assigned coordinates based on their position relative to a user defined coordinate system where groundwater flow is in the positive *x* direction. For this example, the center of the first source is centered on the origin (0,0) of a Cartesian coordinate system aligned parallel to groundwater flow (Figure 10). The center of the remaining sources are defined relative to this source using the same coordinate system. Centers of sources are identified by the variables, X0 and Y0 and A separate input file is needed for each source. Each file should have the same receptor locations. Receptor locations are defined according to the user-defined coordinate system or the base grid and not actual the distance from each source.

The output times (T1, T2, and TP variables) should also be the same for each source. The input file for Source 3 is shown in Figure 11. Each source has a different user-defined activity flux to the unsaturated zone. Transport parameters were the same for each source (infiltration rate, dispersivity, depth to aquifer, etc.) but can differ from source to source.

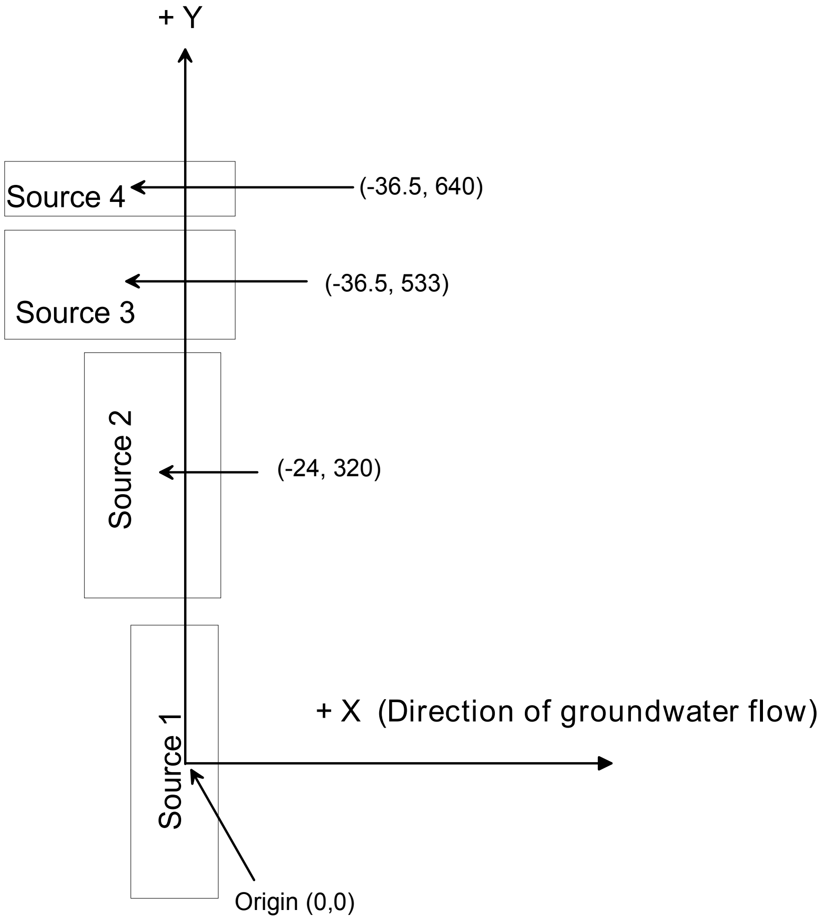

Figure 10. Configuration of area sources for a multiple source problem. Source 1 has been located at the origin of the user-defined coordinate system (in units of meters) and aligned so that the positive x direction is parallel to groundwater flow.

Concentration as a function of time at a receptor located downgradient from Source 3 are illustrated in Figure 12. The concentration considering contributions from all sources is simply the sum of the concentrations from each individual source. Note that the contribution from Source 1 is negligible compared to the contributions from the other sources because Source 1 is farthest away from the receptor.

```
GWSCREEN Sample Problem; C-14 in the RWMC  Area 3            (Card 1)
1 2 2 2 1                             (Card 2) imode,itype,idisp,kflag,idil
3 2 2 1 1                             (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.005                            (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  1.  1.0      (Card 5) bw,at,wi,ef,ed,dlim
-36.5  533.                           (Card 6) x0,y0
257.0  122.  0.1                      (Card 7) l, w, perc
11. 1.9  1.                           (Card 9) depth,rhou,axu
0.30                                  (Card 9a) thetau
9.0  3.0e-1  1.0e-1   76.  12.        (Card 10) ax,ay,az,b,z
57. 0.1  1.9                          (Card 11) u,phi,rhoa
1                                     (Card 12a) nrecept
500. 533.                             (Card 12b) xrec yrec
2                                     (Card 13a) ntimes
100.  200. 2.5                        (Card 13b)  t1 t2 tp
205.  300. 5.0                        (Card 13b)  t1 t2 tp
1                                     (Card 14) ncontam
0   0.  0.001  14. 1.0  1.0 1.0e6 0.0 (Card 14a) nprog kds kdu zmw q0 rmi sl other
C-14  5700. 0.001  2100.              (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
c14a3_a.rel
```

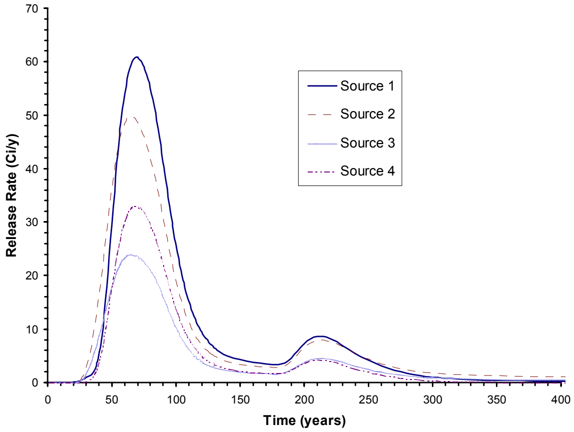

Figure 11. GWSCREEN Version 2.5 input file for the third source in the Radioactive Waste Management Complex multiple source problem. Release rates from each source are shown in the graph above this caption.

Another useful application of the multiple source model is to develop an isopleth map of concentration or dose at selected output times. Isopleth maps may be generated by using the grid output feature in GWSCREEN (set the KFLAG variable to 3) and using contour plotting software such as Surfer™ (Golden Software Inc. 1996). A grid file containing pairs of X,Y receptor points must be generated by the user and referenced by name in the GWSCREEN input files. The same grid file is used by each source (see Section 3.2.7). When presenting contoured results, one may want to overlay surface features such as land boundaries, roads, and buildings on top of the contours so the extent of the contaminant plume can be more readily visualized. Often times, the direction of groundwater flow is not north-south or east-west so the grid output results must be rotated so that they are presented according to the standard convention of north representing the top of the page. Coordinates may be rotated using the following equations.

$$\begin{aligned} X' &= X\cos(\theta) + Y\sin(\theta) \\ Y' &= X\sin(\theta) + Y\cos(\theta). \end{aligned} \tag{58}$$

where *X’* = the east west distance of the transformed coordinate, *Y’* = the north-south distance of the transformed coordinate, X = distance from the center of the source parallel to groundwater flow, Y =

distance from the center of the source perpendicular to groundwater flow, θ = the angle measured clockwise from the positive X axis of the GWSCREEN coordinate system (direction of groundwater flow) to the true direction of groundwater flow (Figure 13). In the case of the sample problem, θ = 112°. Figure 13 shows concentration isopleths at time = 100 years from the start of the simulation. Note that the direction of groundwater flow it to the southwest (S 22° W). The entire source-receptor system was then rotated 112 degrees clockwise (Figure 13) to align the GWSCREEN coordinate system with the true direction of groundwater flow.

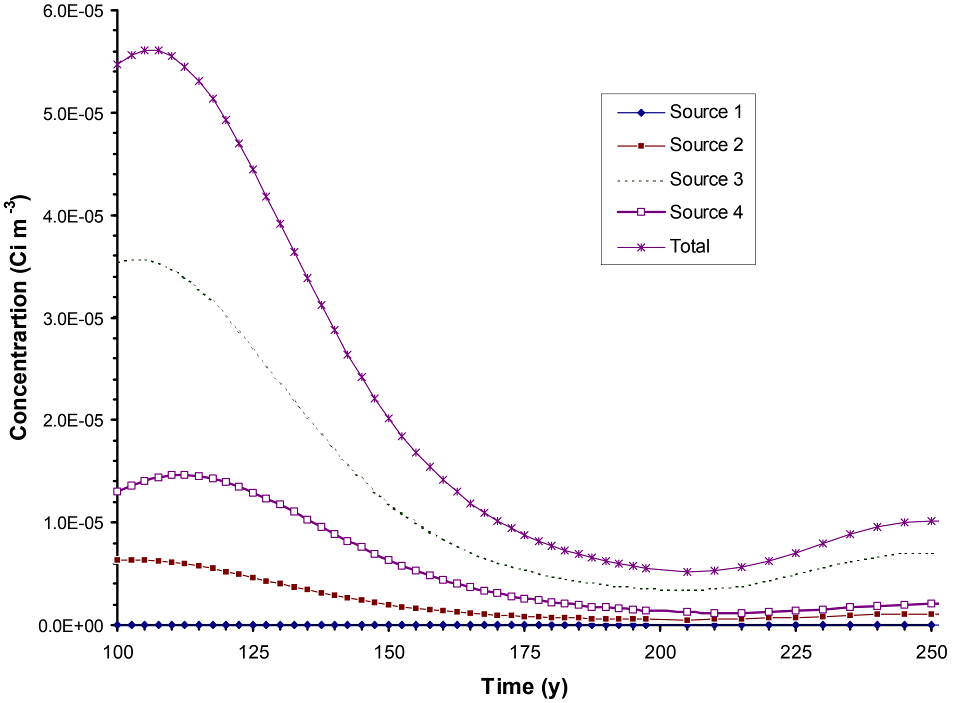

Figure 12. Carbon-14 concentration as a function of time for multiple source sample problem. The receptor was located at coordinates X=500 m and Y=533 m. Note that Source 3 has the greatest influence on the total concentration.

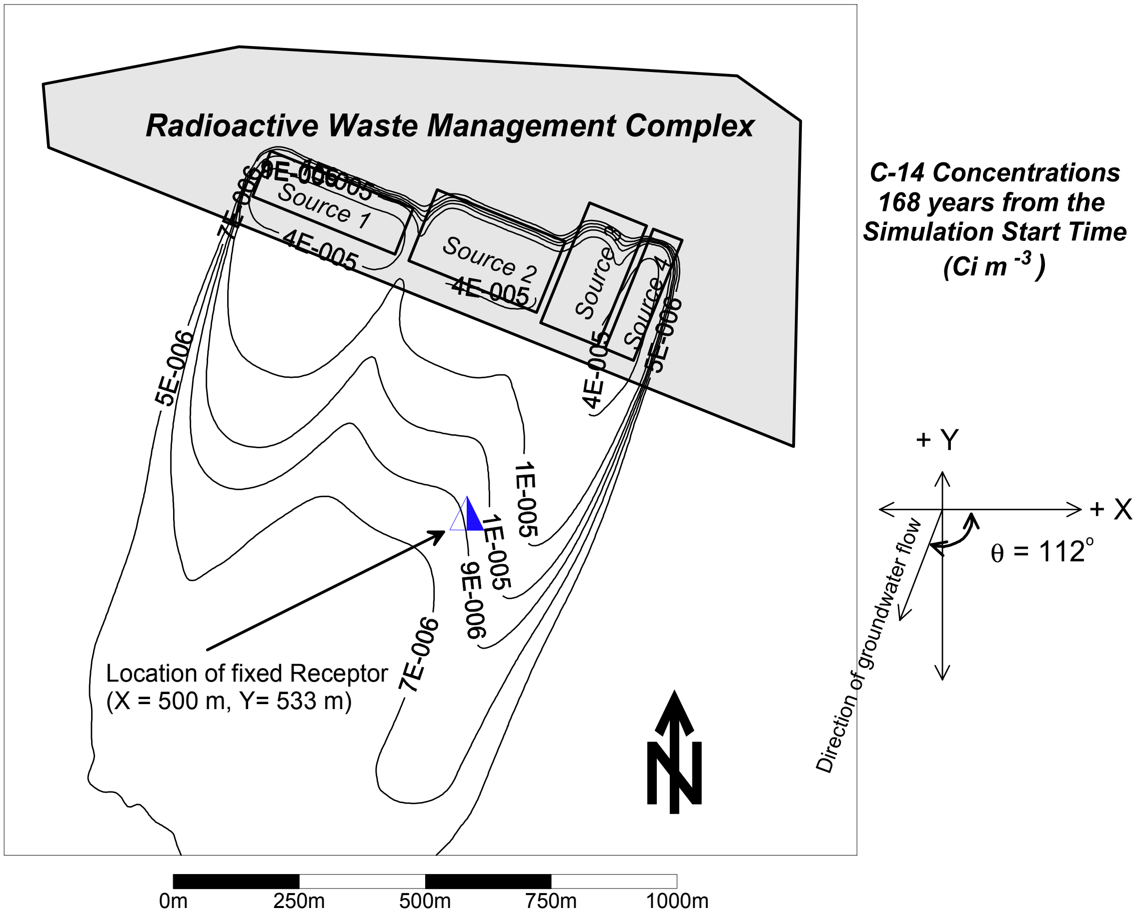

Figure 13. Isopleths of C-14 groundwater concentration at time=168 years. The fixed receptor location (triangle) is the receptor location where the time history concentration plot was calculated.

4.2 Monte Carlo Simulation

This sample problem consists of a Monte Carlo simulation using the Source 3 input file from the previous example. Instead of using the user-defined source, contaminant fluxes to the unsaturated zone were approximated using the pond model. Water percolation through the waste for the first 60-years of operation was defined by the input parameter, PNDFLX divided by the length and width of the source. Percolation after 60 years (closure of the facility) was defined by the PERC variable. A constant source of 20 Ci y^{-1} was put in the facility over a 60 year period. Seven parameters were varied according to one of the predefined distribution identified in the GWSCREEN.CTR file (Figure 14). The dose at 100 years from the start of the simulation for a receptor located at the user-coordinates X = 500 m, Y = 533 m (see previous example) was the endpoint selected for output. Five-hundred Monte Carlo trials were run.

Table 8 lists the cumulative frequency distribution percentiles of the estimated groundwater ingestion doses. The minimum dose was 0 mrem and the maximum was 41 mrem with a mean of 30 mrem and a standard deviation of 10 mrem. Percentiles were extracted from the GWSCREEN.MCO file using the EXTRACT utility program.

The output distribution reflects the overall precision of the model predictions and its validity is dependent on the choice of distributions assigned to each input parameter. It does not attempt to quantify model uncertainty. Model uncertainty is a measure of how well the model represent the processes and overall behavior of the system and is evaluated by comparing model predictions to measured values. In the sample presented here, the distributions assigned to the stochastic variables are admittedly first cut guesses and probably do not reflect our true lack of knowledge about their true, but unknown value. They are used here only to demonstrate the Monte Carlo sampling features of GWSCREEN.

The output distribution generated from the sample problem may be interpreted as follows:

- 90% of the *model predicted* doses are between 2 mrem and 39 mrem
- 5% of the *model predicted* doses are between 0 mrem and 2 mrem
- 5% of the *model predicted* doses are between 39 mrem and 41 mrem

Note that the above statements make no mention of what the true dose might be. The methods presented here only account for the uncertainty in the model predictions. The user is cautioned against using the mean, median, or any other central estimate statistic to represent the models so-called “best estimate”. The probability is the same for any value within the distribution and selecting the mean or median makes about as much sense as selecting the 5th or 95th percentile. There is no “best estimate”, rather the answer is the distribution itself, of which all values within the distribution have equal probability of occurrence. Note however that for a given percentile range, there is less spread in the distribution near the median or mean value compared to values near the tails (see Table 8)

Sensitivity of ingestion dose equivalent to input parameter values is given in Table 9. Sensitivities were calculated by computing the rank correlation coefficient between each stochastic variable and the resulting dose. Sensitivity may also be expressed in terms of the percentage contribution to the variance in the dose. Percent contribution to the variance in dose was *approximated* by squaring the rank correlation coefficients and normalizing then to 100%. For this example, the dose was most sensitive to the percolation rate followed by the depth of the unsaturated zone. The percolation rate is proportional to the mass flux of C-14 reaching the aquifer. Model output was more sensitive to the PERC variable compared to the PNDFLX variable because PERC was assigned a broader distribution compared to PNDFLX.

The distribution coefficient is typically a very sensitive parameter. However, in this example the distribution of K_d’s contained relatively small values resulting in relatively constant retardation factors and thus, low sensitivity. Also note that GWSCREEN assumes K_d values are correlated between media (source, unsaturated, and saturated zones) when identical K_d values are assigned to any two media. For example, if the source and unsaturated zone have the same K_d value and the source K_d is defined as a stochastic variable, then GWSCREEN also treats the unsaturated K_d as stochastic and assigns it the same value as the source.

GWSCREEN.CTR File

```
Monte Carlo Simulation - area 3 RWMC
area3mc.out
1
area3.par         500    -20
6
KDS     2   .001      2.5    0.000001  10.      (lognormal)
KDA1    2   0.0001    3.0    0.0000001 1.0      (lognormal)
PERC    1   0.1       0.05   0.01      1.0      (normal)
DEPTH   4   8.       11.0   14.0       0.       (triangular)
THICKS  3   5.        7.0    0.0       0.       (uniform)
PNDFLX  3   2500.  3600.     0.0       0.0      (uniform)
```

area3mc.par file

```
GWSCREEN Sample Problem 2; Monte Carlo Sim C-14 in the RWMC  Area 3            (Card 1)
1 2 2 2 1                             (Card 2) imode,itype,idisp,kflag,idil
2 2 2 2 2                             (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.005                            (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  1.  1.0      (Card 5) bw,at,wi,ef,ed,dlim
-36.5  533.                           (Card 6) x0,y0
257.0  122.  0.1                      (Card 7) l, w, perc
60. 3.098e3  0.0                      (Card 8a) toper pndflx evap thetap
6.  1.5                               (Card 8b) thicks rhos
1.066 1.523 23.9 0.478  0.142         (Card 8d) alpha n ksat pors thetar
11. 1.9  1.                           (Card 9) depth,rhou,axu
1.066 1.523 23.9 0.478  0.142         (Card 9d) alphau nu ksatu porsu thetaru
9.0  3.0e-1  1.0e-1   76.  12.        (Card 10) ax,ay,az,b,z
57. 0.1  1.9                          (Card 11) u,phi,rhoa
1                                     (Card 12a) nrecept
500. 533.                             (Card 12b) xrec yrec
1                                     (Card 13a) ntimes
100. 102.  2.                         (Card 13b) t1,t2,tp
1                                     (Card 14) ncontam
0. 0.001 0.001 14. 1.0 20.0 1.0e6 0.0 (Card 14a) nprog kds kdu zmw q0 rmi sl other
C-14  5700. 0.00  2100.               (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

Figure 14. GWSCREEN.CTR file for Monte Carlo simulation (top) and area3.par input file.

Table 8. Percentiles of ingestion dose for the sample Monte Carlo simulation using a ^{14}C release from Source 3 (described in the previous problem) and 500 trials. Percentile results were extracted from the GWSCREEN.MCO file using the EXTRACT utility.

Percentile	Dose (rem)
0%	0.000
5%	0.002
10%	0.014
15%	0.022
20%	0.025
25%	0.028
30%	0.029
35%	0.030
40%	0.032
45%	0.033
50%	0.034
55%	0.034
60%	0.035
65%	0.035
70%	0.036
75%	0.037
80%	0.037
85%	0.038
90%	0.038
95%	0.039
100%	0.041

Table 9 Sensitivity analysis results for the sample Monte Carlo simulation using a ^{14}C release from Source 3 (described in the previous problem) and 500 trials.

	KDS	KDA	PERC	THICKS	DEPTH	PNDFLX
Correlation Coefficient (r)	0.020	0.025	0.398	0.006	0.067	-0.068
% Contribution to Variance	0.23%	0.36%	94.0%	0.02%	2.64	2.77%

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APPENDIX A: GWSCREEN Sample Problems

The input and output files for nine sample problems are presented in this appendix. These are the same sample problems presented in the earlier versions of GWSCREEN (Rood, 1994) and are presented here to illustrate that GWSCREEN Version 2.5 gives identical results. Exceptions are noted. Each sample problem was intended to demonstrate a different aspect of the GWSCREEN code. The sample problems were run on an Dell® GXMX 5166 personal computer. Code execution time was less than or equal to 1 second for each sample problem. Results for sample problems 3 and 6 that were limited by the solubility of the contaminant have somewhat different answers than those generated using earlier versions of GWSCREEN. These differences are noted in the brief description of each problem that follows.

Sample Problem 1:

Maximum allowable inventory for ^{239}Pu in a 50 m x 50 m x 2.5 m source volume located in an environment similar to eastern Idaho and using the default transport parameters presented in DOE/ID-1-340(92), Revision 1. The maximum allowable groundwater concentration was based on a carcinogenic target risk of 1×10^{-6} and was given by

$$C_{\max} = \frac{1 \times 10^{-6}}{SF \times I \times ED \times EF}$$

where

C_{max} = maximum allowable groundwater concentration averaged over the consumption period (Ci L^{-1})
SF = slope factor (Ci^{-1})
I= water consumption rate (2 L d^{-1})
ED = exposure duration (30 years)
EF = exposure frequency (350 d y^{-1}).

The slope factor for ^{239}Pu is 31 Ci^{-1} therefore the maximum allowable groundwater concentration is

$$\frac{1 \times 10^{-6}}{31\,\mathrm{Ci} \times 2\ \mathrm{L/d} \times 350\ \mathrm{d/y}\ 30\ \mathrm{y}} = 1.5\,\mathrm{Ci} \times 10^{-12}\ \mathrm{L}^{-1}$$

When performing these calculations for radionuclides that decay to other radionuclides (progeny), the risks due to the progeny must also be considered. Plutonium 239 decays to ^{235}U with a half-life of 2.41×10^{4} years. Uranium 235 has a long half-life (7.04×10^{8} years) and therefore little of this isotope will decay during the time period of interest. For this example, only the ^{235}U decay chain member will be considered. The maximum allowable groundwater concentration for ^{235}U based on carcinogenic risk (slope factor = 130 Ci^{-1}) is 3.7×10^{-13} Ci L^{-1}. The maximum parent groundwater concentration adjusted for *n* number of decay chain members is given by the following.

$$C_L = \frac{CA_{parent}}{\sum_{i=1}^{n} \frac{CA_i}{MCL_i}}$$

where

MCL_i = maximum contaminant limit for i^{th} member of the decay chain (Ci L^{-1})
CA_{parent} = maximum parent groundwater concentration averaged over the consumption period (Ci L^{-1})
CA_i = maximum groundwater concentration for the i^{th} decay chain member averaged over the consumption period (Ci L^{-1})
I = water intake rate (L d^{-1})
C_L = maximum allowable *parent* groundwater concentration for progeny (Ci L^{-1}).

This value was printed in earlier versions of GWSCREEN but is not printed in GWSCREEN version 2.5. Maximum allowable inventory is instead calculated by simply summing the ratio of the modeled concentration to the limiting groundwater concentrations and adjusting it so the sum of the ratios is less than 1.0 The ^{235}U progeny had little impact on the results since very little activity is generated during the period of transit from the source to receptor.

Sample Problem 2: Maximum Permissible Concentration .

Maximum allowable inventory in soil for Sr-90 in a 25 m × 25 m × 1.0 m source volume located in an environment similar to eastern Idaho and using the default parameters presented in DOE/ID-1-340(92), Revision 1. The maximum allowable soil inventory was based on the maximum permissible concentration in a community drinking water systems described in 40 CFR 141, Subpart B, Table A, of 8 pCi L^{-1}.

Sample Problem 3a.

Maximum allowable inventory in soil for mercury carbonate (Hg_2CO_3) in a 25 m × 25 m × 1.0 m source volume located in an environment similar to eastern Idaho and using the default parameters presented in DOE/ID-1-340(92), Revision 1. The maximum allowable inventory in soil was based on subchronic noncarcinogenic toxicity (1 year exposure period) using an RfD value of 3.0×10^{-4} mg/kg/day. Sample problem 3 (and 6) illustrates the solubility release model in GWSCREEN version 2.5. The solubility limit used in the simulation was based on the carbonate form of mercury and was obtained from the CRC Handbook of Chemistry and Physics. When run in the “backwards” direction (setting the KFLAG variable to 1), version 2.5 calculates impacts from solubility-limited contaminant releases differently than earlier versions of the code. In previous versions, maximum groundwater concentration and maximum allowable contaminant inventory in soil were calculated ignoring the effects of solubility. The pore water concentration of the maximum allowable inventory was then compared to the solubility limit of the contaminant. If the pore water concentration exceeded the solubility limit, then a warning was printed in the output file.

In version 2.5, the maximum groundwater concentration and maximum allowable inventory in soil are calculated based on the solubility limit of the contaminant in the source and the user defined (specified in the input file) initial inventory in the source volume. Two warning flags are then printed depending on the results of the calculation.

1. If the pore water concentration of the maximum allowable inventory exceeds the solubility limit of the contaminant, then the statement

```
WARNING: PORE WATER CONCENTRATION OF THE MAXIMUM ALLOWABLE INVENTORY
           EXCEEDS THE SOLUBILITY LIMIT OF THE CONTAMINANT
```

   is printed to the output file.

2. If the pore water concentration of the user-defined inventory (specified in the input file) exceeds the solubility limit of the contaminant, then the statement

```
WARNING: THE SOLUBILITY LIMIT OF THE CONTAMINANT WAS EXCEEDED IN THE SOURCE
```

   is printed to the output file.

These warning statements indicate that soil inventories greater than the solubility limited mass of 4.23 kg (reported earlier in the output file) will not result in proportional increases in groundwater concentrations at the receptor. A maximum allowable soil mass of 8100 kg was calculated for this example and the pore water concentration for this mass exceeded the solubility limit (0.045 mg L^{-1}) of the mercury compound. The pore water concentration (given by Equation 12) is

$$8.1 \times 10^9 \text{ mg}/(25 \text{ m} \times 25 \text{ m} \times 1 \text{ m} \times 0.4 \times [1+ \{100 \text{ mL/g } 1.5 \text{ g/cm}^3\}/0.4]) = 86 \text{ mg/L}$$

which is substantially higher than the solubility limit of the contaminant. The user input mass (281 kg) also results in a pore water concentration (2.9 mg/L) that exceeds the solubility limit of the compound.

<u>Sample Problem 3b.</u>

Concentration verses time for the 281 kg mercury carbonate source described in problem 3a. Note that the contaminant mass, QI, exceeds the solubility limited mass calculated in sample problem 3a and reported in the output file. Therefore, the release is solubility limited controlled. Contaminant flux to the unsaturated zone is constant until the source mass is depleted to the solubility limited mass of 4.23×10^6 mg. After that, release from the source volume occurs by first order leaching. The solubility limited release time was 9841 years.

In this example, concentration as a function of time is printed to the output file. The first column in the concentration output lists the time from the start of waste emplacement. In the second column, the aquifer flux at each specified output time is printed. The third column reports the aquifer concentration for each specified output time. If a radioactive species with progeny are modeled, then progeny concentrations are reported to the right of the parent concentration. The "DOSE.OUT" file is also generated. In this file, the health effects (hazard quotients in this case) are output for each time period specified by the input file. Note that the maximum aquifer concentration is the same as calculated in problem 3a (KFLAG=1). Both aquifer concentrations and aquifer flux are constant until the solubility limited release time (plus transit time in the vadose zone and aquifer) is exceeded; Concentrations and fluxes then decrease exponentially.

Sample Problem 4a.

Maximum allowable inventory in soil for 2,3,7,8-tetrachlorodibenzo-p-dioxine (TCDD) in a remediated storage site in Biloxi, Mississippi. The maximum allowable soil inventory was based on a carcinogenic slope factor of 1.5E5 $(mg/kg/day)^{-1}$. In this example, the optional loss rate constant for the source was employed. Research has indicated (Schaum, 1984) that TCDD degrades in soil with a half life of around 100 years and near the surface with a half life of 12 years. Degradation rates of TCDD in groundwater were unknown. Degradation only affects TCDD in the source compartment (soil) and it was assumed that the surface soil was clean. Therefore, a half life of 100 years was used to calculate the degradation rate constant (variable RC2 in GWSCREEN) for the source volume. This degradation rate was only applied to TCDD in the source volume; TCDD outside the source was assumed to have an infinite half life. The K_d value used in the example was based on an organic partitioning coefficient (K_{oc}) of 3.3×10^6 mL g^{-1} and a fraction of organic carbon of 5.0×10^{-4}. A well screen thickness of 5 m was selected.

Sample Problem 4b

Maximum allowable inventory in soil for 2,3,7,8-tetrachlorodibenzo-p-dioxine (TCDD) in a remediated storage site in Biloxi, Mississippi for a 5 m well screen thickness in a 25 m thick aquifer. This problem illustrates the 3D vertically averaged solution (ITYPE=2). Note that average concentration is less than what was calculated in problem 4a because the contaminant is allowed to disperse in the *total* thickness of the aquifer. In problem 4a, the contaminant is only allowed to disperse in the first 5 m of the aquifer.

Sample Problem 5

Maximum allowable ^{226}Ra inventory in soil for a hypothetical uranium mill tailings pile containing an average ^{226}Ra concentration of 500 pCi g^{-1} . The maximum allowable inventory was based on the proposed maximum contaminant limit (MCL) for ^{226}Ra in groundwater of 20 pCi L^{-1} (40 CRF 141) and 1.0 pCi L^{-1} for ^{210}Pb. Note that the ratio of the peak concentration to

MCL was greatest for ^{210}Pb compared (1.23) to ^{226}Ra (0.121). A peak concentration/MCL ratio greater than 1 indicates groundwater concentrations exceeded MCLs. Maximum allowable inventory was controlled by the ^{210}Pb daughter product an not the ^{226}Ra parent.

Sample Problem 6a

Maximum allowable ^{59}Ni activity inventory in soil at a hypothetical site. Maximum allowable ^{59}Ni inventories in soil were based on a annual committed dose equivalent of 4 mrem y^{-1}. Sample problem 6 (and 3) illustrates the solubility release model in GWSCREEN version 2.5. When run in the "backwards" direction (setting the KFLAG variable to 1), version 2.5 calculates impacts from solubility-limited contaminant releases differently than earlier versions of the code. In previous versions, maximum concentration and maximum allowable soil inventory were calculated ignoring the effects of solubility. The pore water concentration of the maximum allowable inventory was then compared to the solubility limit of the contaminant. If the pore water concentration exceeded the solubility limit, then a warning was printed in the output file.

In version 2.5, the maximum groundwater concentration and maximum allowable inventory in soil are calculated based on the solubility limit of the contaminant and the user defined (specified in the input file) initial inventory in the source volume. Two warning flags are then printed depending on the results of the calculation.

1. If the pore water concentration of the maximum allowable inventory exceeds the solubility limit of the contaminant, then the statement

```
WARNING: PORE WATER CONCENTRATION OF THE MAXIMUM ALLOWABLE INVENTORY
         EXCEEDS THE SOLUBILITY LIMIT OF THE CONTAMINANT
```

   is printed to the output file.

2. If the pore water concentration of the user-defined inventory (specified in the input file) exceeds the solubility limit of the contaminant, then the statement

```
WARNING: THE SOLUBILITY LIMIT OF THE CONTAMINANT WAS EXCEEDED IN THE SOURCE
```

   is printed to the output file.

These warning statements indicate that soil inventories greater than the solubility limited mass of 82,800 mg (reported earlier in the output file) will not result in proportional increases in groundwater concentrations at the receptor. A maximum allowable activity inventory in soil of 4,400 Ci (54.8 kg) was calculated for this nuclide. The pore water concentration in the source volume for this mass exceeded the solubility limit (0.0036 mg L^{-1}) of Ni and therefore, the first warning statement was printed. The user-input activity of 1,000 Ci (12.4 kg) also results in pore water concentrations that exceed the solubility limit of the nuclide. Therefore, the second warning statement was printed.

Sample Problem 6b

Concentration versus time for a 1000 Ci inventory (11 nCi g^{-1}) Ni-59 source at a hypothetical site. The release is solubility limited for the time given by Equation 16. The maximum dose can be computed from the maximum concentration (6.5×10^{-9} Ci L^{-1}) by multiplying by an annual water ingestion rate and dose conversion factor.

Dose = 6.5E-9 Ci/L × 730 L/y × 200 rem/Ci × 1000 mrem/rem = 0.95 mrem/y.

This value is computed and printed in the DOSE.OUT file. Since this value is below the 4 mrem y^{-1} criteria, then the hypothetical inventory would be considered acceptable in terms of groundwater protection.

Sample Problem 7a

Maximum allowable release rate to a hypothetical percolation pond receiving 4000 m^3 y^{-1} of liquid effluent containing 0.25 μCi L^{-1} of ^{90}Sr. In this example, the unsaturated thickness was set very thin so that the pond effluent essentially goes directly into the aquifer. Additional dilution in the aquifer from pond effluent was not calculated in this sample problem so that results would be comparable to earlier versions of GWSCREEN that did not include this option. Including additional dilution from pond effluent by setting the IDIL variable to 2 results in about a 7% decrease in the peak concentration for this problem.

Sample Problem 7b

Concentration as a function of time for the pond described in problem 7a. In this example, the tabulated source function was used. The mass flux from the pond as a function of time was calculated using Equation 21 for time periods less than 30 years and Equation 11 for time periods > 30 years. These releases rates were calculated on a spreadsheet and exported to the file, PB-7.REL. This file was then referenced in the problem 7b input file. Note that the flux to the aquifer at 30 years (95.7 Ci y^{-1}) does not equal the mass input rate to the pond (100 Ci y^{-1}) indicating that the pond sediment compartment did not equilibrated during the 30-year operational period. The aquifer flux after 30 years drops to 1.8 Ci y^{-1} and then decreases exponentially. The large drop following 30 years is due to the change in net infiltration during and after operation of the pond.

Sample Problem 7c

Maximum allowable release rate to a hypothetical percolation pond receiving 4000 m^3 y^{-1} liquid effluent containing 0.25 μCi L^{-1} of ^{90}Sr. This is basically the same problem as described in problem 7a however, the maximum allowable release rate was based on carcinogenic risk instead of radiological dose and the vertically averaged 3D solution was used instead of the 2D solution.

In this example, the aquifer thickness and the well screen thickness were set equal to one another. Under these conditions, the concentration calculated with the vertically averaged 3D solution should be the same as the concentration calculated using the 2D vertically averaged solution. The GWSCREEN output reports maximum concentrations and average concentrations. Average concentrations were not comparable because the averaging times used in sample problem 7a and 7c were different. Maximum concentrations are comparable and these values were the same for problem 7a and 7c.

Sample Problem 8

Maximum allowable inventory in soil ^{241}Pu in an environment similar to eastern Idaho. The limiting soil concentration is based carcinogenic risk. This example shows the importance of including radioactive progeny in the assessment. The risk resulting from ^{241}Pu alone is insignificant (6.0E-12). However the risk from the progeny, ^{241}Am (2.4E-6) is within what EPA defines at the “point of departure for acceptable risk (1×10^{-4} to 1×10^{-6})”. Also note the discussion in Section 3.3.2 of this document concerning this example.

Sample Problem 9

Maximum allowable inventory in soil for a 25 m × 15 m hydrocarbon spill containing benzene. The optional loss rate constant (λ_o) was used to model volatilization losses from the source volume. Volatilization losses from groundwater were not accounted for. The volatilization rate constant (0.0113 y^{-1}) and the degradation half life (0.95 years) were calculated using a methodology and data obtained in Ünlü (1992). Maximum allowable inventories in soil were based on the carcinogenic risk associated with benzene exposure. Sorption coefficients were based on a K_{oc} value of 83 mL g^{-1} and a foc of 0.003.

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GWSCREEN.CTR File

```
GWSCREEN Version 2.5 - Test Problems                 (Card 1)
```

```
test.out                                              (Card 2)
14                                                     (Card 3)
PB-1.PAR            0   0          (Card 4) file nsim seed
PB-2.PAR            0   0
PB-3A.PAR           0   0
PB-3B.PAR           0   0
PB-4A.PAR           0   0
PB-4B.PAR           0   0
PB-5.PAR            0   0
PB-6A.PAR           0   0
PB-6B.PAR           0   0
PB-7A.PAR           0   0
PB-7B.PAR           0   0
PB-7C.PAR           0   0
PB-8.PAR            0   0
PB-9.PAR            0   0
```

GWSCREEN Input Files

PB-1.PAR

```
Example Problem #1 Pu-239 for GWSCREEN Ver 2.5             (Card 1)
3 1 0 1 1                              (Card 2) imode,itype,idisp,kflag idil
1 1 1 1 1                              (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.001                             (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  1.  1.0       (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                 (Card 6) x0,y0
50.  50.  1.0                          (Card 7) l,w,perc
2.5 1.5                                (Card 8b) thicks,rhos
0.35                                   (Card 8c) thetas
50. 1.9  0                             (Card 9) depth,rhou,axu
0.090                                  (Card 9a) thetau
1.0e-3  5.0e-4  5.0e-4   76.  15.      (Card 10) ax,ay,az,b,z
57. 0.1  1.9                           (Card 11) u,phi,rhoa
1                                      (Card 12a nrecept
0.  0.                                 (Card 12b) xrec(i) yrec(i)
1                                      (Card 14) ncontam
1   22.  22.  239. 1.0  1.0 1.0e6 0.0 (Card 14a) nprog kds kdu zmw q0 rmi sl other
Pu-239 2.41E4 22. 1.5E-09              (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
U-235  7.04E8 6.  3.7E-10              (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

PB-2.PAR

```
Example Problem #2 Sr-90 limit based on 1.44 pCi/L for GWSCREEN Ver 2.5  (Card 1)
3 1 0 1 1                               (Card 2) imode,itype,idisp,kflag idil
1 1 1 1 1                              (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.001                             (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  30.  1.0      (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                 (Card 6) x0,y0
25.  25.  1.0                          (Card 7) l,w,perc
1.0 1.5                                (Card 8b) thicks,rhos
0.35                                   (Card 8c) thetas
5. 1.9  0                              (Card 9) depth,rhou,axu
0.090                                  (Card 9a) thetau
1.0e-3  5.0e-4  5.0e-4   76.  15.      (Card 10) ax,ay,az,b,z
57. 0.1  2.0                           (Card 11) u,phi,rhoa
1                                      (Card 12a nrecept
0.  0.                                 (Card 12b) xrec(i) yrec(i)
1                                      (Card 14) ncontam
0   24.  24.  90. 1.0  1.0 1.0e6 0.0  (Card 14a) nprog kds kdu zmw q0 rmi sl other
Sr-90  2.85E1 24. 1.44E-9              (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

PB-3A.PAR

```
Example Problem #3a Hg (Hg2CO3) 30 year chronic exposure GWSCREEN Ver 2.5  (Card 1)
6 1 0 1 1                               (Card 2) imode,itype,idisp,kflag idil
1 1 1 1 1                              (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.001                             (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  30.  1.0      (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                 (Card 6) x0,y0
25.  25.  1.0                          (Card 7) l,w,perc
1.0 1.5                                (Card 8b) thicks,rhos
0.40                                   (Card 8c) thetas
50. 1.9  0.                            (Card 9) depth,rhou,axu
0.40                                   (Card 9a) thetau
9.0  4.0  5.0e-4   76.  15.            (Card 10) ax,ay,az,b,z
57. 0.1  1.9                           (Card 11) u,phi,rhoa
```

```
1                                     (Card 12a nrecept
12.5  0.                              (Card 12b) xrec(i) yrec(i)
1                                     (Card 14) ncontam
0 100. 100. 461. 2.81E8 1.0 4.5e-2 0. (Card 14a) nprog kds kdu zmw q0 rmi sl other
Hg2CO3   1.0E9  100. 3.0E-4           (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

PB-3B.PAR

```
Example Problem #3b Hg (Hg2CO3) 30 year chronic exposure GWSCREEN Ver 2.5  (Card 1)
6 1 0 2 1                              (Card 2) imode,itype,idisp,kflag idil
1 1 1 1 1                             (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.001                            (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  30.  1.0     (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                (Card 6) x0,y0
25.  25.  1.0                         (Card 7) l,w,perc
1.0 1.5                               (Card 8b) thicks,rhos
0.40                                  (Card 8c) thetas
50. 1.9  0.                           (Card 9) depth,rhou,axu
0.40                                  (Card 9a) thetau
9.0  4.0  5.0e-4   76.  15.           (Card 10) ax,ay,az,b,z
57. 0.1  1.9                          (Card 11) u,phi,rhoa
1                                     (Card 12a nrecept
12.5  0.                              (Card 12b) xrec(i) yrec(i)
1                                     (Card 13a) ntimes
19000.  1.952e4  10.                  (Card 13b) t1(i) t2(i) tp(i)
1                                     (Card 14) ncontam
0 100. 100. 461. 2.81E8 1.0 4.5e-2 0. (Card 14a) nprog kds kdu zmw q0 rmi sl other
Hg2CO3   1.0E9  100. 3.0E-4           (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

PB-4A.PAR

```
Example Problem #4a TCDD dioxin storage at Biloxi GWSCREEN Ver 2.5  (Card 1)
5 1 0 1 1                                      (Card 2) imode,itype,idisp,kflag idil
1 1 1 1 1                                     (Card 3)
imodel,isolve,isolveu,imoist,imoistu
6 12 0.001                                    (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  30.  1.0E-6          (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                        (Card 6) x0,y0
250. 250. 0.58                                (Card 7) l,w,perc
0.61 2.0                                      (Card 8b) thicks,rhos
0.125                                         (Card 8c) thetas
1. 2.0  0                                     (Card 9) depth,rhou,axu
0.125                                         (Card 9a) thetau
30.9  9.0   5.0e-4   5.  5.                   (Card 10) ax,ay,az,b,z
12.65 0.25 2.0                                (Card 11) u,phi,rhoa
2                                             (Card 12a nrecept
152.  0.                                      (Card 12b) xrec(i) yrec(i)
3000. 0.
1                                             (Card 14) ncontam
0  1650. 1650. 322. 7.6e4  1.0 2.0e-4 0.00693 (Card 14a) nprog kds kdu zmw q0 rmi sl other
TCDD  1.E9 1650.  1.5E+5                      (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

PB-4B.PAR

```
Example Problem #4B TCDD at Biloxi GWSCREEN Ver 2.5 25 m vert avg source   (Card 1)
5 3 0 1 1                                     (Card 2) imode,itype,idisp,kflag idil
1 1 1 1 1                                     (Card 3)
imodel,isolve,isolveu,imoist,imoistu
6 12 0.001                                    (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  30.  1.0E-6          (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                        (Card 6) x0,y0
250. 250. 0.58                                (Card 7) l,w,perc
0.61 2.0                                      (Card 8b) thicks,rhos
0.125                                         (Card 8c) thetas
1. 2.0  0                                     (Card 9) depth,rhou,axu
0.125                                         (Card 9a) thetau
30.9  9.0   9.0  25.  5.                      (Card 10) ax,ay,az,b,z
12.65 0.25 2.0                                (Card 11) u,phi,rhoa
1                                             (Card 12a nrecept
152.  0.                                      (Card 12b) xrec(i) yrec(i)
1                                             (Card 14) ncontam
0  1650. 1650. 322. 7.6e4  1.0 2.0e-4 0.00693 (Card 14a) nprog kds kdu zmw q0 rmi sl other
TCDD  1.E9 1650.  1.5E+5                      (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

PB-5.PAR

```
Example Problem #5 Ra-226 limiting soil conc Including Pb-210 GWSCREEN Ver 2.5   (Card 1)
```

```
3 1 0 1 1                              (Card 2) imode,itype,idisp,kflag idil
1 1 1 1 1                             (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.001                            (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350. 1. 1.00       (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                (Card 6) x0,y0
100.  100. 0.1                        (Card 7) l,w,perc
5.0 1.8                               (Card 8b) thicks,rhos
0.10                                  (Card 8c) thetas
25. 2.0  0                            (Card 9) depth,rhou,axu
0.15                                  (Card 9a) thetau
1.0e+1 1.0  5.0e-4   5.  5.           (Card 10) ax,ay,az,b,z
90. 0.3  2.0                          (Card 11) u,phi,rhoa
1                                     (Card 12a nrecept
50.  0.                               (Card 12b) xrec(i) yrec(i)
1                                     (Card 14) ncontam
1   100.  10.  226. 9.0  1.0 1.0  0.0 (Card 14a) nprog kds kdu zmw q0 rmi sl other
Ra-226  1600. 10. 2.00E-08             (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
Pb-210  22.3  20.  1.0E-09             (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

PB-6A.PAR

```
Example Problem #6a Ni-59 Solubility Limited Release GWSCREEN Ver 2.5  (Card 1)
1 1 0 1 1                             (Card 2) imode,itype,idisp,kflag idil
1 1 1 1 1                             (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.001                            (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  1.  4.0E-3   (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                (Card 6) x0,y0
100.  100.  0.1                       (Card 7) l,w,perc
5.0 1.8                               (Card 8b) thicks,rhos
0.10                                  (Card 8c) thetas
0.5 2.0  0                            (Card 9) depth,rhou,axu
0.150                                 (Card 9a) thetau
1.0e+1  1.0e-0  5.0e-4   5.  5.0      (Card 10) ax,ay,az,b,z
90. 0.3  2.0                          (Card 11) u,phi,rhoa
1                                     (Card 12a nrecept
50. 0.                                (Card 12b) xrec(i) yrec(i)
1                                     (Card 14) ncontam
0. 0.2  8.0  59. 1000. 1.0 3.6e-3 0.0 (Card 14a) nprog kds kdu zmw q0 rmi sl other
Ni-59  7.5E4 10. 200.                 (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

PB-6B.PAR

```
Example Problem #6B Ni-59 Solubility Limited Release GWSCREEN Ver 2.5  (Card 1)
1 1 0 2 1                             (Card 2) imode,itype,idisp,kflag idil
1 1 1 1 1                             (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.001                            (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  1.  4.0E-3   (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                (Card 6) x0,y0
100.  100.  0.1                       (Card 7) l,w,perc
5.0 1.8                               (Card 8b) thicks,rhos
0.10                                  (Card 8c) thetas
0.5 2.0  0                            (Card 9) depth,rhou,axu
0.150                                 (Card 9a) thetau
1.0e+1  1.0e-0  5.0e-4   5.  5.0      (Card 10) ax,ay,az,b,z
90. 0.3  2.0                          (Card 11) u,phi,rhoa
1                                     (Card 12a nrecept
50. 0.                                (Card 12b) xrec(i) yrec(i)
5                                     (Card 13a) ntimes
100. 130. 3.                          (Card 13b) t1(i) t2(i) tp(i)
130. 160. 3.                          (Card 13b) t1(i) t2(i) tp(i)
160. 190. 3.                          (Card 13b) t1(i) t2(i) tp(i)
210. 3000. 200.                       (Card 13b) t1(i) t2(i) tp(i)
3075. 5000. 75.                       (Card 13b) t1(i) t2(i) tp(i)
1                                     (Card 14) ncontam
0. 0.2  8.0  59. 1000. 1.0 3.6e-3 0.0 (Card 14a) nprog kds kdu zmw q0 rmi sl other
Ni-59  7.5E4 10. 200.                 (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

PB-7A.PAR

```
Example Problem #7a Sr-90 Release to a Pond GWSCREEN Ver 2.5  (Card 1)
1 1 0 1 1                             (Card 2) imode,itype,idisp,kflag idil
2 2 1 1 1                             (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.001                            (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  1.  4.0E-3   (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                (Card 6) x0,y0
20.  20.    0.2                       (Card 7) l,w,perc
30. 4000. 0.0  0.4                    (Card 8a) toper, pndflx,evap,thetap
0.5 1.5                               (Card 8b) thicks,rhos
```

```
0.36                                   (Card 8c) thetas
5.0e-5 1.9  0                          (Card 9) depth,rhou,axu
0.120                                  (Card 9a) thetau
9.0e+0  4.0e-0  5.0e-4   15.  15.      (Card 10) ax,ay,az,b,z
57. 0.1  1.9                           (Card 11) u,phi,rhoa
1                                      (Card 12a nrecept
100. 0.                                (Card 12b) xrec(i) yrec(i)
1                                      (Card 14) ncontam
0. 24. 24.0  90. 0. 100. 1.0  0.0      (Card 14a) nprog kds kdu zmw q0 rmi sl other
Sr-90  28.5 22. 1.3e5                  (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

PB-7B.PAR

```
Example Problem #7a Sr-90 Release to a Pond GWSCREEN Ver 2.5  (Card 1)
1 1 0 2 1                              (Card 2) imode,itype,idisp,kflag idil
3 2 1 1 1                              (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.001                             (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  1.  4.0E-3    (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                 (Card 6) x0,y0
20.  20.    0.2                        (Card 7) l,w,perc
5.0e-5 1.9  0                          (Card 9) depth,rhou,axu
0.120                                  (Card 9a) thetau
9.0e+0  4.0e-0  5.0e-4   15.  15.      (Card 10) ax,ay,az,b,z
57. 0.1  1.9                           (Card 11) u,phi,rhoa
1                                      (Card 12a nrecept
100. 0.                                (Card 12b) xrec(i) yrec(i)
3                                      (Card 13a) ntimes
0.0 30.0  2.0                          (Card 13b) t1(i) t2(i) tp(i)
32. 62.0  2.0                          (Card 13b) t1(i) t2(i) tp(i)
64. 94.0  1.0                          (Card 13b) t1(i) t2(i) tp(i)
1                                      (Card 14) ncontam
0. 24. 24.0  90. 0. 1.0 1.0  0.0       (Card 14a) nprog kds kdu zmw q0 rmi sl other
Sr-90  28.5 22. 1.3e5                  (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
pb-7.rel                               (Card 14c) relfile
```

PB-7.REL

```
   year          flux (Ci/y)     Pb-7.rel
   0.0000E+00    0.0000E+00
   1.0000E+00    4.1808E+01
   2.0000E+00    6.5364E+01
   3.0000E+00    7.8636E+01
   4.0000E+00    8.6113E+01
   5.0000E+00    9.0325E+01
   6.0000E+00    9.2699E+01
   7.0000E+00    9.4036E+01
   8.0000E+00    9.4789E+01
   9.0000E+00    9.5213E+01
   1.0000E+01    9.5453E+01
   1.1000E+01    9.5587E+01
   1.2000E+01    9.5663E+01
   1.3000E+01    9.5706E+01
   1.4000E+01    9.5730E+01
   1.5000E+01    9.5744E+01
   1.6000E+01    9.5751E+01
   1.7000E+01    9.5756E+01
   1.8000E+01    9.5758E+01
   1.9000E+01    9.5759E+01
   2.0000E+01    9.5760E+01
   2.1000E+01    9.5761E+01
   2.2000E+01    9.5761E+01
   2.3000E+01    9.5761E+01
   2.4000E+01    9.5761E+01
   2.5000E+01    9.5761E+01
   2.6000E+01    9.5761E+01
   2.7000E+01    9.5761E+01
   2.8000E+01    9.5761E+01
   2.9000E+01    9.5761E+01
   3.0000E+01    9.5761E+01
   3.2000E+01    1.7866E+00
   3.3000E+01    1.7246E+00
   3.4000E+01    1.6647E+00
   3.5000E+01    1.6069E+00
   3.6000E+01    1.5512E+00
   3.7000E+01    1.4973E+00
   3.8000E+01    1.4454E+00
```

```
   3.9000E+01    1.3952E+00
   4.0000E+01    1.3468E+00
   4.1000E+01    1.3000E+00
   4.2000E+01    1.2549E+00
   4.3000E+01    1.2114E+00
   4.4000E+01    1.1693E+00
   4.5000E+01    1.1287E+00
   4.6000E+01    1.0896E+00
   4.7000E+01    1.0518E+00
   4.8000E+01    1.0153E+00
   4.9000E+01    9.8002E-01
   5.0000E+01    9.4601E-01
   5.1000E+01    9.1317E-01
   5.2000E+01    8.8148E-01
   5.3000E+01    8.5089E-01
   5.4000E+01    8.2136E-01
   5.5000E+01    7.9285E-01
   5.6000E+01    7.6534E-01
   5.7000E+01    7.3878E-01
   5.8000E+01    7.1314E-01
   5.9000E+01    6.8839E-01
   6.0000E+01    6.6450E-01
   6.1000E+01    6.4143E-01
   6.2000E+01    6.1917E-01
   6.4000E+01    5.7694E-01
   6.6000E+01    5.3759E-01
   6.8000E+01    5.0092E-01
   7.0000E+01    4.6676E-01
   7.2000E+01    4.3492E-01
   7.4000E+01    4.0526E-01
   7.6000E+01    3.7762E-01
   7.8000E+01    3.5186E-01
   8.0000E+01    3.2786E-01
   8.2000E+01    3.0550E-01
   8.4000E+01    2.8466E-01
   8.6000E+01    2.6525E-01
   8.8000E+01    2.4715E-01
   9.0000E+01    2.3030E-01
   9.2000E+01    2.1459E-01
   9.4000E+01    1.9995E-01
```

PB-7C.PAR

```
Example Problem #7c Sr-90 Release to a Pond 3D Vert Avg sol GWSCREEN Ver 2.5  (Card 1)
2 3 0 1 1                             (Card 2) imode,itype,idisp,kflag idil
2 2 1 1 1                             (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.01                             (Card 4) jstart jmax eps
70. 2.555E+04 2.0  365. 30.  1.0E-6   (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                (Card 6) x0,y0
20.  20.    0.2                       (Card 7) l,w,perc
30. 4000. 0.0  0.4                    (Card 8a) toper, pndflx,evap,thetap
0.5 1.5                               (Card 8b) thicks,rhos
0.36                                  (Card 8c) thetas
5.0e-5 1.9  0                         (Card 9) depth,rhou,axu
0.120                                 (Card 9a) thetau
9.0e+0  4.0e-0  4.0e-0   15.  14.999  (Card 10) ax,ay,az,b,z
57. 0.1  1.9                          (Card 11) u,phi,rhoa
1                                     (Card 12a nrecept
100. 0.                               (Card 12b) xrec(i) yrec(i)
1                                     (Card 14) ncontam
0. 24. 24.0  90. 0. 100. 1.0  0.0      (Card 14a) nprog kds kdu zmw q0 rmi sl other
Sr-90  28.5 22. 36.                   (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

PB-8.PAR

```
Example Problem #8 Pu-241, Am-241 & Np-237 Carcin Risk GWSCREEN Ver 2.5  (Card 1)
2 1 0 1 1                             (Card 2) imode,itype,idisp,kflag idil
1 1 1 1 1                             (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.001                            (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  30.  1.0E-6  (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                (Card 6) x0,y0
70.  30.  1.0                         (Card 7) l,w,perc
2.0 1.5                               (Card 8b) thicks,rhos
0.35                                  (Card 8c) thetas
6. 1.9  0                             (Card 9) depth,rhou,axu
0.090                                 (Card 9a) thetau
```

```
9.0  4.0  5.0e-4   76.   15.          (Card 10) ax,ay,az,b,z
57. 0.1  1.9                          (Card 11) u,phi,rhoa
1                                     (Card 12a nrecept
135.  0.                              (Card 12b) xrec(i) yrec(i)
1                                     (Card 14) ncontam
2. 22. 22. 241. 10.0 1.0 7.11e6 0.0   (Card 14a) nprog kds kdu zmw q0 rmi sl other
Pu-241 1.44E1 22. 4.8                 (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
Am-241 432.2 340. 310.                (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
Np-237 2.10E6 5.  270                 (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

PB-9.PAR

```
Example Problem #9 Hydrocarbon Benzene Spill with Vapor Loss GWSCREEN Ver 2.5  (Card 1)
5 1 0 1 1                                   (Card 2) imode,itype,idisp,kflag idil
1 1 1 1 1                                   (Card 3) imodel,isolve,isolveu,imoist,imoistu
6 12 0.001                                  (Card 4) jstart jmax eps
70. 2.555E+04 2.0  350.  30.  1.0E-6        (Card 5) bw,at,wi,ef,ed,dlim
0.  0.                                      (Card 6) x0,y0
15.  25.  0.1                               (Card 7) l,w,perc
2.0 1.5                                     (Card 8b) thicks,rhos
0.30                                        (Card 8c) thetas
0.1 1.9  0                                  (Card 9) depth,rhou,axu
0.090                                       (Card 9a) thetau
9.0   4.0   5.0e-4   76.  15.               (Card 10) ax,ay,az,b,z
57. 0.1  1.9                                (Card 11) u,phi,rhoa
1                                           (Card 12a nrecept
25.  0.                                     (Card 12b) xrec(i) yrec(i)
1                                           (Card 14) ncontam
0 0.25 0.25 78.1 5.62e8 1.0 1.78e3 1.13e-2  (Card 14a) nprog kds kdu zmw q0 rmi sl other
Benzene 0.95  0.25 5.2e-2                   (Card 14b) cname(i),thalf(i),kda(i),dcf(i)
```

GWSCREEN Output File

```
GWSCREEN Version 2.5 - Test Problems                 (Card 1)
TIME OF RUN: 16:53:13.89  DATE OF RUN: 08/13/98
  **************************************************
  *                                                *
  *     This output was produced by the model:     *
  *                                                *
  *                   GWSCREEN                     *
  *                  Version 2.5                   *
  *    A semi-analytical model for the assessment  *
  *    of the groundwater pathway from the leaching *
  *    of surficial and buried contamination and   *
  *  release of contaminants from percolation ponds *
  *                   08/13/98                     *
  *                 Arthur S. Rood                 *
  * Idaho National Engineering and Environmental   *
  *  Laboratory, Lockheed Martin Idaho Technologies *
  *   Company, Integrated Earth Sciences Unit      *
  *                  PO Box 1625                   *
  *            Idaho Falls, Idaho 83415            *
  **************************************************
 ===========================================================================
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                  LIMITATION OF LIABILITY

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 ==========================================================================

OUTPUT FILE NAME: test.out
INPUT FILE NAME: PB-1.PAR
Title: Example Problem #1 Pu-239 for GWSCREEN Ver 2.5            (Card 1)
----------------------------------------------------------------------------
Model Run Options
----------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                             3
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                     1
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:           0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:            1
IDIL (1) No dilution factor (2) Include Dilution Factor:        1
IMOIST Source Moisture Content Option:                          1
IMOISTU Unsaturated Moisture Content Option:                    1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:            1
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)      1
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
```

```
Health Effects: Ratio of groundwater concentration to radionuclide MCL
Output mass/activity units:   Ci
Output concentration units:   Ci/m**3
Dose/Risk Conversion Units:   Ci/m**3
Output health effects units:  Ratio of Cp/Cmcl
Cp = Peak groundwater concentration, Cmcl = Maximum contaminant limit
-----------------------------------------------------------------------------
Exposure Parameters
-----------------------------------------------------------------------------
Body Mass (kg):              70.       Averaging Time (days):      25550.
Water Ingestion (L/d):       2.000E+00 Exposure Freq (day/year):   3.500E+02
Exposure Duration (y):       1.000E+00 Limiting Dose:              1.000E+00
-----------------------------------------------------------------------------
Site Parameters
-----------------------------------------------------------------------------
X Coordinate:                0.000E+00  Y Coordinate:               0.000E+00
Source Length (m):           5.000E+01  Source Width (m):           5.000E+01
Percolation Rate (m/y):      1.000E+00
Source Thickness (m):        2.500E+00  Src Bulk Density (g/cc):    1.500E+00
Source Moisture Content:     3.500E-01
-----------------------------------------------------------------------------
Unsaturated Zone Parameters
-----------------------------------------------------------------------------
Unsat Zone Thickness (m):    5.000E+01  Unsat Bulk Density:         1.900E+00
Unsat Dispersivity (m):      0.000E+00  Unsat Moisture Content:     9.000E-02
-----------------------------------------------------------------------------
Aquifer Zone Parameters
-----------------------------------------------------------------------------
Longitudinal Disp (m):       1.000E-03  Transverse Disp (m):        5.000E-04
Aquifer Thickness (m):       7.600E+01  Well Screen Thickness (m):  1.500E+01
Darcy Velocity (m/y):        5.700E+01  Aquifer Porosity:           1.000E-01
Bulk Density (g/cc):         1.900E+00
-----------------------------------------------------------------------------
Calculated Flow Parameters
-----------------------------------------------------------------------------
Percolation Water Flux (m3/y):  2.5000E+03
Unsat Pore Velocity (m/y):      1.1111E+01
Aquifer Pore Velocity (m/y):    5.7000E+02
Longitudinal Disp (m**2/y):     5.7000E-01
Transverse Disp (m**2/y):       2.8500E-01
-----------------------------------------------------------------------------
Contaminant Data
-----------------------------------------------------------------------------
Contaminant Name:              Pu-239
Number of Progeny:              1
Progeny Names:                 U-235
Half Life (y):                  2.410E+04 7.040E+08
Other Source Loss Rate (1/y):   0.000E+00
Kd Source (ml/g):               2.200E+01
Solubility Limit (mg/L):        1.000E+06
Molecular Weight (mg/L):        2.390E+02
Initial mass/activity:          1.000E+00
Kd Unsat (ml/g):                2.200E+01
Kd Aquifer (ml/g):              2.200E+01 6.000E+00
Risk/Dose Conversion Factor     1.500E-09 3.700E-10
-----------------------------------------------------------------------------
Calculated Contaminant Values
-----------------------------------------------------------------------------
Decay Constants (1/y):          2.8761E-05 9.8458E-10
Leach Rate Constant (1/y):      1.1994E-02
Solubility Limited Mass (mg):   2.0844E+14
Solubility Limited Act (Ci):    1.2948E+10
Unsat Retardation Factor:       4.6544E+02
Mean Unsat Transit Time (y):    2.0945E+03
Aquifer Retardation Factor:     4.190E+02 1.150E+02
Minimum Peak Window Time (y):   2.0945E+03
Maximum Peak Window Time (y):   4.1897E+03
-----------------------------------------------------------------------------
Results for Receptor X =  0.00000E+00 Y = 0.00000E+00
-----------------------------------------------------------------------------
Peak Concentration (Ci/m**3):          1.177E-07  9.198E-13
Time of Peak (y):                      2.1128E+03
Maximum Dose:                          7.847E+01  2.486E-03
Total Dose (all members):              7.848E+01
Maximum Allowable Inventory (Ci):      1.274E-02
Execution Time (Seconds):    0

INPUT FILE NAME: PB-2.PAR
Title: Example Problem #2 Sr-90 limit based on 1.44 pCi/L for GWSCREEN Ver 2.5  (Card 1
-----------------------------------------------------------------------------
Model Run Options
-----------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                             3
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                     1
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:           0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:            1
IDIL (1) No dilution factor (2) Include Dilution Factor:        1
IMOIST Source Moisture Content Option:                          1
IMOISTU Unsaturated Moisture Content Option:                    1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:            1
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)      1
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
Health Effects: Ratio of groundwater concentration to radionuclide MCL
Output mass/activity units:   Ci
Output concentration units:   Ci/m**3
Dose/Risk Conversion Units:   Ci/m**3
Output health effects units:  Ratio of Cp/Cmcl
Cp = Peak groundwater concentration, Cmcl = Maximum contaminant limit
-----------------------------------------------------------------------------
Exposure Parameters
-----------------------------------------------------------------------------
```

```
Body Mass (kg):              70.       Averaging Time (days):      25550.
Water Ingestion (L/d):       2.000E+00 Exposure Freq (day/year):   3.500E+02
Exposure Duration (y):       3.000E+01 Limiting Dose:              1.000E+00
-----------------------------------------------------------------------------
Site Parameters
-----------------------------------------------------------------------------
X Coordinate:                0.000E+00  Y Coordinate:              0.000E+00
Source Length (m):           2.500E+01  Source Width (m):          2.500E+01
Percolation Rate (m/y):      1.000E+00
Source Thickness (m):        1.000E+00  Src Bulk Density (g/cc):    1.500E+00
Source Moisture Content:     3.500E-01
-----------------------------------------------------------------------------
Unsaturated Zone Parameters
-----------------------------------------------------------------------------
Unsat Zone Thickness (m):    5.000E+00  Unsat Bulk Density:         1.900E+00
Unsat Dispersivity (m):      0.000E+00  Unsat Moisture Content:     9.000E-02
-----------------------------------------------------------------------------
Aquifer Zone Parameters
-----------------------------------------------------------------------------
Longitudinal Disp (m):       1.000E-03  Transverse Disp (m):        5.000E-04
Aquifer Thickness (m):       7.600E+01  Well Screen Thickness (m):  1.500E+01
Darcy Velocity (m/y):        5.700E+01  Aquifer Porosity:           1.000E-01
Bulk Density (g/cc):         2.000E+00
-----------------------------------------------------------------------------
Calculated Flow Parameters
-----------------------------------------------------------------------------
Percolation Water Flux (m3/y):  6.2500E+02
Unsat Pore Velocity (m/y):      1.1111E+01
Aquifer Pore Velocity (m/y):    5.7000E+02
Longitudinal Disp (m**2/y):     5.7000E-01
Transverse Disp (m**2/y):       2.8500E-01
-----------------------------------------------------------------------------
Contaminant Data
-----------------------------------------------------------------------------
Contaminant Name:              Sr-90
Number of Progeny:              0
Half Life (y):                  2.850E+01
Other Source Loss Rate (1/y):   0.000E+00
Kd Source (ml/g):               2.400E+01
Solubility Limit (mg/L):        1.000E+06
Molecular Weight (mg/L):        9.000E+01
Initial mass/activity:          1.000E+00
Kd Unsat (ml/g):                2.400E+01
Kd Aquifer (ml/g):              2.400E+01
Risk/Dose Conversion Factor     1.440E-09
-----------------------------------------------------------------------------
Calculated Contaminant Values
-----------------------------------------------------------------------------
Decay Constants (1/y):          2.4321E-02
Leach Rate Constant (1/y):      2.7510E-02
Solubility Limited Mass (mg):   2.2719E+13
Solubility Limited Act (Ci):    3.1690E+12
Unsat Retardation Factor:       5.0767E+02
Mean Unsat Transit Time (y):    2.2845E+02
Aquifer Retardation Factor:     4.810E+02
Minimum Peak Window Time (y):   2.2845E+02
Maximum Peak Window Time (y):   4.5774E+02
-----------------------------------------------------------------------------
Results for Receptor X =  0.00000E+00 Y = 0.00000E+00
-----------------------------------------------------------------------------
Peak Concentration (Ci/m**3):          1.660E-09
Time of Peak (y):                      2.3901E+02
Concentrations Averaged Between:       2.2845E+02 and  2.5845E+02 years
Average Concentration (Ci/m**3):       1.021E-09
Maximum Dose:                          7.087E-01
Maximum Allowable Inventory (Ci):      1.411E+00
Execution Time (Seconds):    0

INPUT FILE NAME: PB-3A.PAR
Title: Example Problem #3a Hg (Hg2CO3) 30 year chronic exposure GWSCREEN Ver 2.5  (Card
-----------------------------------------------------------------------------
Model Run Options
-----------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                             6
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                     1
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:           0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:            1
IDIL (1) No dilution factor (2) Include Dilution Factor:        1
IMOIST Source Moisture Content Option:                          1
IMOISTU Unsaturated Moisture Content Option:                    1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:            1
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)      1
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
Health Effects: Non-carcinogenic effects for non-radiological contaminants
Output mass/activity units:   mg
Output concentration units:   mg/m**3
Dose/Risk Conversion Units:   mg-g/kg
Output health effects units:  hazard quotient
-----------------------------------------------------------------------------
Exposure Parameters
-----------------------------------------------------------------------------
Body Mass (kg):              70.       Averaging Time (days):      25550.
Water Ingestion (L/d):       2.000E+00 Exposure Freq (day/year):   3.500E+02
Exposure Duration (y):       3.000E+01 Limiting Dose:              1.000E+00
-----------------------------------------------------------------------------
Site Parameters
-----------------------------------------------------------------------------
X Coordinate:                0.000E+00  Y Coordinate:              0.000E+00
Source Length (m):           2.500E+01  Source Width (m):          2.500E+01
Percolation Rate (m/y):      1.000E+00
Source Thickness (m):        1.000E+00  Src Bulk Density (g/cc):    1.500E+00
```

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Source Moisture Content:     4.000E-01
-----------------------------------------------------------------------------
Unsaturated Zone Parameters
-----------------------------------------------------------------------------
Unsat Zone Thickness (m):    5.000E+01  Unsat Bulk Density:         1.900E+00
Unsat Dispersivity (m):      0.000E+00  Unsat Moisture Content:     4.000E-01
-----------------------------------------------------------------------------
Aquifer Zone Parameters
-----------------------------------------------------------------------------
Longitudinal Disp (m):       9.000E+00  Transverse Disp (m):        4.000E+00
Aquifer Thickness (m):       7.600E+01  Well Screen Thickness (m):  1.500E+01
Darcy Velocity (m/y):        5.700E+01  Aquifer Porosity:           1.000E-01
Bulk Density (g/cc):         1.900E+00
-----------------------------------------------------------------------------
Calculated Flow Parameters
-----------------------------------------------------------------------------
Percolation Water Flux (m3/y):  6.2500E+02
Unsat Pore Velocity (m/y):      2.5000E+00
Aquifer Pore Velocity (m/y):    5.7000E+02
Longitudinal Disp (m**2/y):     5.1300E+03
Transverse Disp (m**2/y):       2.2800E+03
-----------------------------------------------------------------------------
Contaminant Data
-----------------------------------------------------------------------------
Contaminant Name:              Hg2CO3
Half Life (y):                  1.000E+09
Other Source Loss Rate (1/y):   0.000E+00
Kd Source (ml/g):               1.000E+02
Solubility Limit (mg/L):        4.500E-02
Molecular Weight (mg/L):        4.610E+02
Initial mass/activity:          2.810E+08
Kd Unsat (ml/g):                1.000E+02
Kd Aquifer (ml/g):              1.000E+02
Risk/Dose Conversion Factor     3.000E-04
-----------------------------------------------------------------------------
Calculated Contaminant Values
-----------------------------------------------------------------------------
Decay Constants (1/y):          6.9315E-10
Leach Rate Constant (1/y):      6.6489E-03
Solubility Limited Mass (mg):   4.2300E+06
Solubility Limited Time (y):    9.8407E+03
Unsat Retardation Factor:       4.7600E+02
Mean Unsat Transit Time (y):    9.5200E+03
Aquifer Retardation Factor:     1.901E+03
Minimum Peak Window Time (y):   9.5200E+03
Maximum Peak Window Time (y):   2.8967E+04
-----------------------------------------------------------------------------
Results for Receptor X =  1.25000E+01 Y = 0.00000E+00
-----------------------------------------------------------------------------
Peak Concentration (mg/m**3):          8.872E-01
Time of Peak (y):                      1.1887E+04
Concentrations Averaged Between:       1.1872E+04 and  1.1902E+04 years
Average Concentration (mg/m**3):       8.871E-01
Maximum Dose:                          3.472E-02
Maximum Allowable Inventory (mg):      8.093E+09
WARNING: PORE WATER CONCENTRATION OF THE MAXIMUM ALLOWABLE INVENTORY
         EXCEEDS THE SOLUBILITY LIMIT OF THE CONTAMINANT
WARNING: THE SOLUBILITY LIMIT OF THE CONTAMINANT WAS EXCEEDED IN THE SOURCE
Execution Time (Seconds):    0

INPUT FILE NAME: PB-3B.PAR
Title: Example Problem #3b Hg (Hg2CO3) 30 year chronic exposure GWSCREEN Ver 2.5  (Card
-----------------------------------------------------------------------------
Model Run Options
-----------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                             6
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                     1
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:           0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:            2
IDIL (1) No dilution factor (2) Include Dilution Factor:        1
IMOIST Source Moisture Content Option:                          1
IMOISTU Unsaturated Moisture Content Option:                    1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:            1
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)      1
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
Health Effects: Non-carcinogenic effects for non-radiological contaminants
Output mass/activity units:   mg
Output concentration units:   mg/m**3
Dose/Risk Conversion Units:   mg-g/kg
Output health effects units:  hazard quotient
-----------------------------------------------------------------------------
Exposure Parameters
-----------------------------------------------------------------------------
Body Mass (kg):              70.       Averaging Time (days):      25550.
Water Ingestion (L/d):       2.000E+00 Exposure Freq (day/year):   3.500E+02
Exposure Duration (y):       3.000E+01 Limiting Dose:              1.000E+00
-----------------------------------------------------------------------------
Site Parameters
-----------------------------------------------------------------------------
X Coordinate:                0.000E+00  Y Coordinate:               0.000E+00
Source Length (m):           2.500E+01  Source Width (m):           2.500E+01
Percolation Rate (m/y):      1.000E+00
Source Thickness (m):        1.000E+00  Src Bulk Density (g/cc):    1.500E+00
Source Moisture Content:     4.000E-01
-----------------------------------------------------------------------------
Unsaturated Zone Parameters
-----------------------------------------------------------------------------
Unsat Zone Thickness (m):    5.000E+01  Unsat Bulk Density:         1.900E+00
Unsat Dispersivity (m):      0.000E+00  Unsat Moisture Content:     4.000E-01
-----------------------------------------------------------------------------
Aquifer Zone Parameters
```

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-----------------------------------------------------------------------------
Longitudinal Disp (m):       9.000E+00  Transverse Disp (m):        4.000E+00
Aquifer Thickness (m):       7.600E+01  Well Screen Thickness (m):  1.500E+01
Darcy Velocity (m/y):        5.700E+01  Aquifer Porosity:           1.000E-01
Bulk Density (g/cc):         1.900E+00
-----------------------------------------------------------------------------
Calculated Flow Parameters
-----------------------------------------------------------------------------
Percolation Water Flux (m3/y):  6.2500E+02
Unsat Pore Velocity (m/y):      2.5000E+00
Aquifer Pore Velocity (m/y):    5.7000E+02
Longitudinal Disp (m**2/y):     5.1300E+03
Transverse Disp (m**2/y):       2.2800E+03
-----------------------------------------------------------------------------
Contaminant Data
-----------------------------------------------------------------------------
Contaminant Name:              Hg2CO3
Half Life (y):                  1.000E+09
Other Source Loss Rate (1/y):   0.000E+00
Kd Source (ml/g):               1.000E+02
Solubility Limit (mg/L):        4.500E-02
Molecular Weight (mg/L):        4.610E+02
Initial mass/activity:          2.810E+08
Kd Unsat (ml/g):                1.000E+02
Kd Aquifer (ml/g):              1.000E+02
Risk/Dose Conversion Factor     3.000E-04
-----------------------------------------------------------------------------
Calculated Contaminant Values
-----------------------------------------------------------------------------
Decay Constants (1/y):          6.9315E-10
Leach Rate Constant (1/y):      6.6489E-03
Solubility Limited Mass (mg):   4.2300E+06
Solubility Limited Time (y):    9.8407E+03
Unsat Retardation Factor:       4.7600E+02
Mean Unsat Transit Time (y):    9.5200E+03
Aquifer Retardation Factor:     1.901E+03
-----------------------------------------------------------------------------
Concentration vs Time Results for Receptor X =  1.25000E+01 Y = 0.00000E+00
-----------------------------------------------------------------------------
   Time        Flux     Conc Mbr 1
 (years)  (mg or Ci/y) (mg or Ci per cubic meter)
-----------------------------------------------------------------------------
 1.9000E+04  2.812E+04  8.850E-01
 1.9010E+04  2.812E+04  8.850E-01
 1.9020E+04  2.812E+04  8.850E-01
 1.9030E+04  2.812E+04  8.850E-01
 1.9040E+04  2.812E+04  8.850E-01
 1.9050E+04  2.812E+04  8.850E-01
 1.9060E+04  2.812E+04  8.850E-01
 1.9070E+04  2.812E+04  8.850E-01
 1.9080E+04  2.812E+04  8.850E-01
 1.9090E+04  2.812E+04  8.850E-01
 1.9100E+04  2.812E+04  8.850E-01
 1.9110E+04  2.812E+04  8.850E-01
 1.9120E+04  2.812E+04  8.850E-01
 1.9130E+04  2.812E+04  8.850E-01
 1.9140E+04  2.812E+04  8.850E-01
 1.9150E+04  2.812E+04  8.850E-01
 1.9160E+04  2.812E+04  8.850E-01
 1.9170E+04  2.812E+04  8.850E-01
 1.9180E+04  2.812E+04  8.850E-01
 1.9190E+04  2.812E+04  8.850E-01
 1.9200E+04  2.812E+04  8.850E-01
 1.9210E+04  2.812E+04  8.850E-01
 1.9220E+04  2.812E+04  8.850E-01
 1.9230E+04  2.812E+04  8.850E-01
 1.9240E+04  2.812E+04  8.850E-01
 1.9250E+04  2.812E+04  8.850E-01
 1.9260E+04  2.812E+04  8.850E-01
 1.9270E+04  2.812E+04  8.850E-01
 1.9280E+04  2.812E+04  8.850E-01
 1.9290E+04  2.812E+04  8.850E-01
 1.9300E+04  2.812E+04  8.850E-01
 1.9310E+04  2.812E+04  8.850E-01
 1.9320E+04  2.812E+04  8.850E-01
 1.9330E+04  2.812E+04  8.850E-01
 1.9340E+04  2.812E+04  8.850E-01
 1.9350E+04  2.812E+04  8.850E-01
 1.9360E+04  2.812E+04  8.850E-01
 1.9370E+04  2.643E+04  8.827E-01
 1.9380E+04  2.473E+04  8.704E-01
 1.9390E+04  2.314E+04  8.590E-01
 1.9400E+04  2.165E+04  8.483E-01
 1.9410E+04  2.026E+04  8.163E-01
 1.9420E+04  1.896E+04  7.863E-01
 1.9430E+04  1.774E+04  7.582E-01
 1.9440E+04  1.660E+04  7.319E-01
 1.9450E+04  1.553E+04  7.073E-01
 1.9460E+04  1.453E+04  6.804E-01
 1.9470E+04  1.360E+04  6.454E-01
 1.9480E+04  1.272E+04  6.127E-01
 1.9490E+04  1.190E+04  5.820E-01
 1.9500E+04  1.114E+04  5.534E-01
 1.9510E+04  1.042E+04  5.266E-01
Maximum Concentration and Time for Member #1:  8.850E-01  1.900E+04
Average Concentration Between 1.8985E+04 and 1.9015E+04 years: 8.850E-01
Execution Time (Seconds):    0

INPUT FILE NAME: PB-4A.PAR
Title: Example Problem #4a TCDD dioxin storage at Biloxi GWSCREEN Ver 2.5  (Card 1)
-----------------------------------------------------------------------------
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Model Run Options
-----------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                             5
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                     1
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:           0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:            1
IDIL (1) No dilution factor (2) Include Dilution Factor:        1
IMOIST Source Moisture Content Option:                          1
IMOISTU Unsaturated Moisture Content Option:                    1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:            1
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)      1
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
Health Effects: Carcinogenic incidence risk for non-radiological contaminants
Output mass/activity units:   mg
Output concentration units:   mg/m**3
Dose/Risk Conversion Units:   kg-d/mg
Output health effects units:  carcinogenic risk
-----------------------------------------------------------------------------
Exposure Parameters
-----------------------------------------------------------------------------
Body Mass (kg):              70.       Averaging Time (days):      25550.
Water Ingestion (L/d):       2.000E+00 Exposure Freq (day/year):   3.500E+02
Exposure Duration (y):       3.000E+01 Limiting Dose:              1.000E-06
-----------------------------------------------------------------------------
Site Parameters
-----------------------------------------------------------------------------
X Coordinate:                0.000E+00  Y Coordinate:               0.000E+00
Source Length (m):           2.500E+02  Source Width (m):           2.500E+02
Percolation Rate (m/y):      5.800E-01
Source Thickness (m):        6.100E-01  Src Bulk Density (g/cc):    2.000E+00
Source Moisture Content:     1.250E-01
-----------------------------------------------------------------------------
Unsaturated Zone Parameters
-----------------------------------------------------------------------------
Unsat Zone Thickness (m):    1.000E+00  Unsat Bulk Density:         2.000E+00
Unsat Dispersivity (m):      0.000E+00  Unsat Moisture Content:     1.250E-01
-----------------------------------------------------------------------------
Aquifer Zone Parameters
-----------------------------------------------------------------------------
Longitudinal Disp (m):       3.090E+01  Transverse Disp (m):        9.000E+00
Aquifer Thickness (m):       5.000E+00  Well Screen Thickness (m):  5.000E+00
Darcy Velocity (m/y):        1.265E+01  Aquifer Porosity:           2.500E-01
Bulk Density (g/cc):         2.000E+00
-----------------------------------------------------------------------------
Calculated Flow Parameters
-----------------------------------------------------------------------------
Percolation Water Flux (m3/y):  3.6250E+04
Unsat Pore Velocity (m/y):      4.6400E+00
Aquifer Pore Velocity (m/y):    5.0600E+01
Longitudinal Disp (m**2/y):     1.5635E+03
Transverse Disp (m**2/y):       4.5540E+02
-----------------------------------------------------------------------------
Contaminant Data
-----------------------------------------------------------------------------
Contaminant Name:             TCDD
Half Life (y):                  1.000E+09
Other Source Loss Rate (1/y):   6.930E-03
Kd Source (ml/g):               1.650E+03
Solubility Limit (mg/L):        2.000E-04
Molecular Weight (mg/L):        3.220E+02
Initial mass/activity:          7.600E+04
Kd Unsat (ml/g):                1.650E+03
Kd Aquifer (ml/g):              1.650E+03
Risk/Dose Conversion Factor     1.500E+05
-----------------------------------------------------------------------------
Calculated Contaminant Values
-----------------------------------------------------------------------------
Decay Constants (1/y):          6.9315E-10
Leach Rate Constant (1/y):      2.8812E-04
Solubility Limited Mass (mg):   2.5163E+07
Unsat Retardation Factor:       2.6401E+04
Mean Unsat Transit Time (y):    5.6899E+03
Aquifer Retardation Factor:     1.320E+04
Minimum Peak Window Time (y):   7.0987E+03
Maximum Peak Window Time (y):   9.0951E+04
-----------------------------------------------------------------------------
Results for Receptor X =  1.52000E+02 Y = 0.00000E+00
-----------------------------------------------------------------------------
Peak Concentration (mg/m**3):          2.411E-06
Time of Peak (y):                      3.6822E+04
Concentrations Averaged Between:       3.6807E+04 and  3.6837E+04 years
Average Concentration (mg/m**3):       2.411E-06
Maximum Dose:                          4.247E-06
Maximum Allowable Inventory (mg):      1.789E+04
Minimum Peak Window Time (y):   1.5570E+05
Maximum Peak Window Time (y):   1.5770E+06
-----------------------------------------------------------------------------
Results for Receptor X =  3.00000E+03 Y = 0.00000E+00
-----------------------------------------------------------------------------
Peak Concentration (mg/m**3):          1.820E-08
Time of Peak (y):                      6.9910E+05
Concentrations Averaged Between:       6.9909E+05 and  6.9912E+05 years
Average Concentration (mg/m**3):       1.820E-08
Maximum Dose:                          3.205E-08
Maximum Allowable Inventory (mg):      2.371E+06
Execution Time (Seconds):    0

INPUT FILE NAME: PB-4B.PAR
Title: Example Problem #4B TCDD at Biloxi GWSCREEN Ver 2.5 25 m vert avg source   (Card
-----------------------------------------------------------------------------
Model Run Options
```

```
----------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                             5
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                     3
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:           0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:            1
IDIL (1) No dilution factor (2) Include Dilution Factor:        1
IMOIST Source Moisture Content Option:                          1
IMOISTU Unsaturated Moisture Content Option:                    1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:            1
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)      1
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
Health Effects: Carcinogenic incidence risk for non-radiological contaminants
Output mass/activity units:   mg
Output concentration units:   mg/m**3
Dose/Risk Conversion Units:   kg-d/mg
Output health effects units:  carcinogenic risk
----------------------------------------------------------------------------
Exposure Parameters
----------------------------------------------------------------------------
Body Mass (kg):              70.       Averaging Time (days):      25550.
Water Ingestion (L/d):       2.000E+00 Exposure Freq (day/year):   3.500E+02
Exposure Duration (y):       3.000E+01 Limiting Dose:              1.000E-06
----------------------------------------------------------------------------
Site Parameters
----------------------------------------------------------------------------
X Coordinate:                0.000E+00  Y Coordinate:              0.000E+00
Source Length (m):           2.500E+02  Source Width (m):          2.500E+02
Percolation Rate (m/y):      5.800E-01
Source Thickness (m):        6.100E-01  Src Bulk Density (g/cc):   2.000E+00
Source Moisture Content:     1.250E-01
----------------------------------------------------------------------------
Unsaturated Zone Parameters
----------------------------------------------------------------------------
Unsat Zone Thickness (m):    1.000E+00  Unsat Bulk Density:        2.000E+00
Unsat Dispersivity (m):      0.000E+00  Unsat Moisture Content:    1.250E-01
----------------------------------------------------------------------------
Aquifer Zone Parameters
----------------------------------------------------------------------------
Longitudinal Disp (m):       3.090E+01  Transverse Disp (m):       9.000E+00
Vertical Dispersivity (m):   9.000E+00
Aquifer Thickness (m):       2.500E+01  Well Screen Thickness (m): 5.000E+00
Darcy Velocity (m/y):        1.265E+01  Aquifer Porosity:          2.500E-01
Bulk Density (g/cc):         2.000E+00
----------------------------------------------------------------------------
Calculated Flow Parameters
----------------------------------------------------------------------------
Percolation Water Flux (m3/y):  3.6250E+04
Unsat Pore Velocity (m/y):      4.6400E+00
Aquifer Pore Velocity (m/y):    5.0600E+01
Longitudinal Disp (m**2/y):     1.5635E+03
Transverse Disp (m**2/y):       4.5540E+02
Vertical Disp (m**2/y):         4.5540E+02
----------------------------------------------------------------------------
Contaminant Data
----------------------------------------------------------------------------
Contaminant Name:              TCDD
Half Life (y):                  1.000E+09
Other Source Loss Rate (1/y):   6.930E-03
Kd Source (ml/g):               1.650E+03
Solubility Limit (mg/L):        2.000E-04
Molecular Weight (mg/L):        3.220E+02
Initial mass/activity:          7.600E+04
Kd Unsat (ml/g):                1.650E+03
Kd Aquifer (ml/g):              1.650E+03
Risk/Dose Conversion Factor     1.500E+05
----------------------------------------------------------------------------
Calculated Contaminant Values
----------------------------------------------------------------------------
Decay Constants (1/y):          6.9315E-10
Leach Rate Constant (1/y):      2.8812E-04
Solubility Limited Mass (mg):   2.5163E+07
Unsat Retardation Factor:       2.6401E+04
Mean Unsat Transit Time (y):    5.6899E+03
Aquifer Retardation Factor:     1.320E+04
Minimum Peak Window Time (y):   7.0987E+03
Maximum Peak Window Time (y):   9.0951E+04
----------------------------------------------------------------------------
Results for Receptor X =  1.52000E+02 Y = 0.00000E+00
----------------------------------------------------------------------------
Peak Concentration (mg/m**3):          4.823E-07
Time of Peak (y):                      3.6822E+04
Concentrations Averaged Between:       3.6807E+04 and  3.6837E+04 years
Average Concentration (mg/m**3):       4.823E-07
Maximum Dose:                          8.494E-07
Maximum Allowable Inventory (mg):      8.947E+04
Execution Time (Seconds):    0

INPUT FILE NAME: PB-5.PAR
Title: Example Problem #5 Ra-226 limiting soil conc Including Pb-210 GWSCREEN Ver 2.5
----------------------------------------------------------------------------
Model Run Options
----------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                             3
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                     1
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:           0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:            1
IDIL (1) No dilution factor (2) Include Dilution Factor:        1
IMOIST Source Moisture Content Option:                          1
IMOISTU Unsaturated Moisture Content Option:                    1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:            1
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)      1
```

```
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
Health Effects: Ratio of groundwater concentration to radionuclide MCL
Output mass/activity units:   Ci
Output concentration units:   Ci/m**3
Dose/Risk Conversion Units:   Ci/m**3
Output health effects units:  Ratio of Cp/Cmcl
Cp = Peak groundwater concentration, Cmcl = Maximum contaminant limit
-----------------------------------------------------------------------------
Exposure Parameters
-----------------------------------------------------------------------------
Body Mass (kg):              70.       Averaging Time (days):      25550.
Water Ingestion (L/d):       2.000E+00 Exposure Freq (day/year):   3.500E+02
Exposure Duration (y):       1.000E+00 Limiting Dose:              1.000E+00
-----------------------------------------------------------------------------
Site Parameters
-----------------------------------------------------------------------------
X Coordinate:                0.000E+00  Y Coordinate:               0.000E+00
Source Length (m):           1.000E+02  Source Width (m):           1.000E+02
Percolation Rate (m/y):      1.000E-01
Source Thickness (m):        5.000E+00  Src Bulk Density (g/cc):    1.800E+00
Source Moisture Content:     1.000E-01
-----------------------------------------------------------------------------
Unsaturated Zone Parameters
-----------------------------------------------------------------------------
Unsat Zone Thickness (m):    2.500E+01  Unsat Bulk Density:         2.000E+00
Unsat Dispersivity (m):      0.000E+00  Unsat Moisture Content:     1.500E-01
-----------------------------------------------------------------------------
Aquifer Zone Parameters
-----------------------------------------------------------------------------
Longitudinal Disp (m):       1.000E+01  Transverse Disp (m):        1.000E+00
Aquifer Thickness (m):       5.000E+00  Well Screen Thickness (m):  5.000E+00
Darcy Velocity (m/y):        9.000E+01  Aquifer Porosity:           3.000E-01
Bulk Density (g/cc):         2.000E+00
-----------------------------------------------------------------------------
Calculated Flow Parameters
-----------------------------------------------------------------------------
Percolation Water Flux (m3/y):  1.0000E+03
Unsat Pore Velocity (m/y):      6.6667E-01
Aquifer Pore Velocity (m/y):    3.0000E+02
Longitudinal Disp (m**2/y):     3.0000E+03
Transverse Disp (m**2/y):       3.0000E+02
-----------------------------------------------------------------------------
Contaminant Data
-----------------------------------------------------------------------------
Contaminant Name:              Ra-226
Number of Progeny:              1
Progeny Names:                 Pb-210
Half Life (y):                  1.600E+03 2.230E+01
Other Source Loss Rate (1/y):   0.000E+00
Kd Source (ml/g):               1.000E+02
Solubility Limit (mg/L):        1.000E+00
Molecular Weight (mg/L):        2.260E+02
Initial mass/activity:          9.000E+00
Kd Unsat (ml/g):                1.000E+01
Kd Aquifer (ml/g):              1.000E+01 2.000E+01
Risk/Dose Conversion Factor     2.000E-08 1.000E-09
-----------------------------------------------------------------------------
Calculated Contaminant Values
-----------------------------------------------------------------------------
Decay Constants (1/y):          4.3322E-04 3.1083E-02
Leach Rate Constant (1/y):      1.1105E-04
Solubility Limited Mass (mg):   9.0050E+09
Solubility Limited Act (Ci):    8.9102E+06
Unsat Retardation Factor:       1.3433E+02
Mean Unsat Transit Time (y):    5.0375E+03
Aquifer Retardation Factor:     6.767E+01 1.343E+02
Minimum Peak Window Time (y):   5.0375E+03
Maximum Peak Window Time (y):   1.0098E+04
-----------------------------------------------------------------------------
Results for Receptor X =  5.00000E+01 Y = 0.00000E+00
-----------------------------------------------------------------------------
Peak Concentration (Ci/m**3):          2.415E-09  1.234E-09
Time of Peak (y):                      5.0962E+03
Maximum Dose:                          1.208E-01  1.234E+00
Total Dose (all members):              1.355E+00
Maximum Allowable Inventory (Ci):      6.644E+00
Execution Time (Seconds):    0

INPUT FILE NAME: PB-6A.PAR
Title: Example Problem #6a Ni-59 Solubility Limited Release GWSCREEN Ver 2.5  (Card 1)
-----------------------------------------------------------------------------
Model Run Options
-----------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                            1
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                    1
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:          0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:           1
IDIL (1) No dilution factor (2) Include Dilution Factor:       1
IMOIST Source Moisture Content Option:                         1
IMOISTU Unsaturated Moisture Content Option:                   1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:           1
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)     1
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
Health Effects: Committed effective dose equivalent calculation
Output mass/activity units:   Ci
Output concentration units:   Ci/m**3
Dose/Risk Conversion Units:   rem/Ci
Output health effects units:  rem
-----------------------------------------------------------------------------
Exposure Parameters
-----------------------------------------------------------------------------
```

```
Body Mass (kg):              70.       Averaging Time (days):      25550.
Water Ingestion (L/d):       2.000E+00 Exposure Freq (day/year):   3.500E+02
Exposure Duration (y):       1.000E+00 Limiting Dose:              4.000E-03
-----------------------------------------------------------------------------
Site Parameters
-----------------------------------------------------------------------------
X Coordinate:                0.000E+00  Y Coordinate:              0.000E+00
Source Length (m):           1.000E+02  Source Width (m):          1.000E+02
Percolation Rate (m/y):      1.000E-01
Source Thickness (m):        5.000E+00  Src Bulk Density (g/cc):   1.800E+00
Source Moisture Content:     1.000E-01
-----------------------------------------------------------------------------
Unsaturated Zone Parameters
-----------------------------------------------------------------------------
Unsat Zone Thickness (m):    5.000E-01  Unsat Bulk Density:        2.000E+00
Unsat Dispersivity (m):      0.000E+00  Unsat Moisture Content:    1.500E-01
-----------------------------------------------------------------------------
Aquifer Zone Parameters
-----------------------------------------------------------------------------
Longitudinal Disp (m):       1.000E+01  Transverse Disp (m):       1.000E+00
Aquifer Thickness (m):       5.000E+00  Well Screen Thickness (m): 5.000E+00
Darcy Velocity (m/y):        9.000E+01  Aquifer Porosity:          3.000E-01
Bulk Density (g/cc):         2.000E+00
-----------------------------------------------------------------------------
Calculated Flow Parameters
-----------------------------------------------------------------------------
Percolation Water Flux (m3/y):  1.0000E+03
Unsat Pore Velocity (m/y):      6.6667E-01
Aquifer Pore Velocity (m/y):    3.0000E+02
Longitudinal Disp (m**2/y):     3.0000E+03
Transverse Disp (m**2/y):       3.0000E+02
-----------------------------------------------------------------------------
Contaminant Data
-----------------------------------------------------------------------------
Contaminant Name:              Ni-59
Number of Progeny:              0
Half Life (y):                  7.500E+04
Other Source Loss Rate (1/y):   0.000E+00
Kd Source (ml/g):               2.000E-01
Solubility Limit (mg/L):        3.600E-03
Molecular Weight (mg/L):        5.900E+01
Initial mass/activity:          1.000E+03
Kd Unsat (ml/g):                8.000E+00
Kd Aquifer (ml/g):              1.000E+01
Risk/Dose Conversion Factor     2.000E+02
-----------------------------------------------------------------------------
Calculated Contaminant Values
-----------------------------------------------------------------------------
Decay Constants (1/y):          9.2420E-06
Leach Rate Constant (1/y):      4.3478E-02
Solubility Limited Mass (mg):   8.2800E+04
Solubility Limited Act (Ci):    6.6949E+00
Solubility Limited Time (y):    3.3590E+03
Unsat Retardation Factor:       1.0767E+02
Mean Unsat Transit Time (y):    8.0750E+01
Aquifer Retardation Factor:     6.767E+01
Minimum Peak Window Time (y):   8.0750E+01
Maximum Peak Window Time (y):   3.5433E+03
-----------------------------------------------------------------------------
Results for Receptor X =  5.00000E+01 Y = 0.00000E+00
-----------------------------------------------------------------------------
Peak Concentration (Ci/m**3):          6.457E-06
Time of Peak (y):                      2.7909E+03
Maximum Dose:                          9.039E-04
Maximum Allowable Inventory (Ci):      4.425E+03
WARNING: PORE WATER CONCENTRATION OF THE MAXIMUM ALLOWABLE INVENTORY
         EXCEEDS THE SOLUBILITY LIMIT OF THE CONTAMINANT
WARNING: THE SOLUBILITY LIMIT OF THE CONTAMINANT WAS EXCEEDED IN THE SOURCE
Execution Time (Seconds):    0

INPUT FILE NAME: PB-6B.PAR
Title: Example Problem #6B Ni-59 Solubility Limited Release GWSCREEN Ver 2.5  (Card 1)
-----------------------------------------------------------------------------
Model Run Options
-----------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                             1
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                     1
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:           0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:            2
IDIL (1) No dilution factor (2) Include Dilution Factor:        1
IMOIST Source Moisture Content Option:                          1
IMOISTU Unsaturated Moisture Content Option:                    1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:            1
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)      1
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
Health Effects: Committed effective dose equivalent calculation
Output mass/activity units:   Ci
Output concentration units:   Ci/m**3
Dose/Risk Conversion Units:   rem/Ci
Output health effects units:  rem
-----------------------------------------------------------------------------
Exposure Parameters
-----------------------------------------------------------------------------
Body Mass (kg):              70.       Averaging Time (days):      25550.
Water Ingestion (L/d):       2.000E+00 Exposure Freq (day/year):   3.500E+02
Exposure Duration (y):       1.000E+00 Limiting Dose:              4.000E-03
-----------------------------------------------------------------------------
Site Parameters
-----------------------------------------------------------------------------
X Coordinate:                0.000E+00  Y Coordinate:              0.000E+00
Source Length (m):           1.000E+02  Source Width (m):          1.000E+02
```

```
Percolation Rate (m/y):      1.000E-01
Source Thickness (m):        5.000E+00  Src Bulk Density (g/cc):    1.800E+00
Source Moisture Content:     1.000E-01
-----------------------------------------------------------------------------
Unsaturated Zone Parameters
-----------------------------------------------------------------------------
Unsat Zone Thickness (m):    5.000E-01  Unsat Bulk Density:         2.000E+00
Unsat Dispersivity (m):      0.000E+00  Unsat Moisture Content:     1.500E-01
-----------------------------------------------------------------------------
Aquifer Zone Parameters
-----------------------------------------------------------------------------
Longitudinal Disp (m):       1.000E+01  Transverse Disp (m):        1.000E+00
Aquifer Thickness (m):       5.000E+00  Well Screen Thickness (m):  5.000E+00
Darcy Velocity (m/y):        9.000E+01  Aquifer Porosity:           3.000E-01
Bulk Density (g/cc):         2.000E+00
-----------------------------------------------------------------------------
Calculated Flow Parameters
-----------------------------------------------------------------------------
Percolation Water Flux (m3/y):  1.0000E+03
Unsat Pore Velocity (m/y):      6.6667E-01
Aquifer Pore Velocity (m/y):    3.0000E+02
Longitudinal Disp (m**2/y):     3.0000E+03
Transverse Disp (m**2/y):       3.0000E+02
-----------------------------------------------------------------------------
Contaminant Data
-----------------------------------------------------------------------------
Contaminant Name:              Ni-59
Number of Progeny:              0
Half Life (y):                  7.500E+04
Other Source Loss Rate (1/y):   0.000E+00
Kd Source (ml/g):               2.000E-01
Solubility Limit (mg/L):        3.600E-03
Molecular Weight (mg/L):        5.900E+01
Initial mass/activity:          1.000E+03
Kd Unsat (ml/g):                8.000E+00
Kd Aquifer (ml/g):              1.000E+01
Risk/Dose Conversion Factor     2.000E+02
-----------------------------------------------------------------------------
Calculated Contaminant Values
-----------------------------------------------------------------------------
Decay Constants (1/y):          9.2420E-06
Leach Rate Constant (1/y):      4.3478E-02
Solubility Limited Mass (mg):   8.2800E+04
Solubility Limited Act (Ci):    6.6949E+00
Solubility Limited Time (y):    3.3590E+03
Unsat Retardation Factor:       1.0767E+02
Mean Unsat Transit Time (y):    8.0750E+01
Aquifer Retardation Factor:     6.767E+01
-----------------------------------------------------------------------------
Concentration vs Time Results for Receptor X =  5.00000E+01 Y = 0.00000E+00
-----------------------------------------------------------------------------
   Time        Flux     Conc Mbr 1
 (years)  (mg or Ci/y) (mg or Ci per cubic meter)
-----------------------------------------------------------------------------
 1.0000E+02  2.909E-01  4.437E-06
 1.0300E+02  2.909E-01  4.917E-06
 1.0600E+02  2.909E-01  5.298E-06
 1.0900E+02  2.909E-01  5.594E-06
 1.1200E+02  2.909E-01  5.820E-06
 1.1500E+02  2.909E-01  5.989E-06
 1.1800E+02  2.909E-01  6.115E-06
 1.2100E+02  2.909E-01  6.209E-06
 1.2400E+02  2.909E-01  6.277E-06
 1.2700E+02  2.909E-01  6.327E-06
 1.3000E+02  2.909E-01  6.363E-06
 1.3300E+02  2.909E-01  6.389E-06
 1.3600E+02  2.909E-01  6.408E-06
 1.3900E+02  2.909E-01  6.421E-06
 1.4200E+02  2.909E-01  6.431E-06
 1.4500E+02  2.909E-01  6.438E-06
 1.4800E+02  2.909E-01  6.443E-06
 1.5100E+02  2.909E-01  6.446E-06
 1.5400E+02  2.909E-01  6.449E-06
 1.5700E+02  2.909E-01  6.451E-06
 1.6000E+02  2.909E-01  6.452E-06
 1.6300E+02  2.909E-01  6.453E-06
 1.6600E+02  2.909E-01  6.454E-06
 1.6900E+02  2.909E-01  6.454E-06
 1.7200E+02  2.909E-01  6.455E-06
 1.7500E+02  2.909E-01  6.455E-06
 1.7800E+02  2.909E-01  6.455E-06
 1.8100E+02  2.909E-01  6.455E-06
 1.8400E+02  2.909E-01  6.455E-06
 1.8700E+02  2.909E-01  6.455E-06
 2.1000E+02  2.909E-01  6.455E-06
 4.1000E+02  2.909E-01  6.456E-06
 6.1000E+02  2.909E-01  6.457E-06
 8.1000E+02  2.909E-01  6.457E-06
 1.0100E+03  2.909E-01  6.457E-06
 1.2100E+03  2.909E-01  6.457E-06
 1.4100E+03  2.909E-01  6.457E-06
 1.6100E+03  2.909E-01  6.457E-06
 1.8100E+03  2.909E-01  6.457E-06
 2.0100E+03  2.909E-01  6.457E-06
 2.2100E+03  2.909E-01  6.457E-06
 2.4100E+03  2.909E-01  6.457E-06
 2.6100E+03  2.909E-01  6.457E-06
 3.0750E+03  2.909E-01  6.457E-06
 3.1500E+03  2.909E-01  6.457E-06
 3.2250E+03  2.909E-01  6.457E-06
 3.3000E+03  2.909E-01  6.457E-06
```

```
 3.3750E+03  2.909E-01  6.457E-06
 3.4500E+03  1.864E-01  5.996E-06
 3.5250E+03  7.145E-03  3.687E-07
 3.6000E+03  2.739E-04  1.417E-08
 3.6750E+03  1.050E-05  5.433E-10
 3.7500E+03  4.023E-07  2.082E-11
 3.8250E+03  1.542E-08  7.981E-13
 3.9000E+03  5.910E-10  3.059E-14
 3.9750E+03  2.265E-11  1.172E-15
 4.0500E+03  8.683E-13  4.494E-17
 4.1250E+03  3.328E-14  1.722E-18
 4.2000E+03  1.276E-15  6.602E-20
 4.2750E+03  4.889E-17  2.530E-21
 4.3500E+03  1.874E-18  9.698E-23
 4.4250E+03  7.182E-20  3.717E-24
 4.5000E+03  2.753E-21  1.425E-25
 4.5750E+03  1.055E-22  5.461E-27
 4.6500E+03  4.044E-24  2.093E-28
 4.7250E+03  1.550E-25  8.022E-30
 4.8000E+03  5.941E-27  3.075E-31
 4.8750E+03  2.277E-28  1.179E-32
Maximum Concentration and Time for Member #1:  6.457E-06  1.210E+03
Execution Time (Seconds):    0

INPUT FILE NAME: PB-7A.PAR
Title: Example Problem #7a Sr-90 Release to a Pond GWSCREEN Ver 2.5  (Card 1)
------------------------------------------------------------------------------
Model Run Options
------------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                              1
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                      1
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:            0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:             1
IDIL (1) No dilution factor (2) Include Dilution Factor:         1
IMOIST Source Moisture Content Option:                           1
IMOISTU Unsaturated Moisture Content Option:                     1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:             2
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)       2
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
JSTART:   6
JMAX  :  12
EPS   :  1.000E-03
Health Effects: Committed effective dose equivalent calculation
Output mass/activity units:   Ci
Output concentration units:   Ci/m**3
Dose/Risk Conversion Units:   rem/Ci
Output health effects units:  rem
------------------------------------------------------------------------------
Exposure Parameters
------------------------------------------------------------------------------
Body Mass (kg):               70.       Averaging Time (days):      25550.
Water Ingestion (L/d):        2.000E+00 Exposure Freq (day/year):   3.500E+02
Exposure Duration (y):        1.000E+00 Limiting Dose:              4.000E-03
------------------------------------------------------------------------------
Site Parameters
------------------------------------------------------------------------------
X Coordinate:                 0.000E+00  Y Coordinate:               0.000E+00
Source Length (m):            2.000E+01  Source Width (m):           2.000E+01
Percolation Rate (m/y):       2.000E-01
Pond Operation Time (y):      3.000E+01  Water Input Rate (m3/y):    4.000E+03
Evap Rate Constant (1/y):     0.000E+00  Pond Moisture Content:      4.000E-01
Source Thickness (m):         5.000E-01  Src Bulk Density (g/cc):    1.500E+00
Source Moisture Content:      3.600E-01
------------------------------------------------------------------------------
Unsaturated Zone Parameters
------------------------------------------------------------------------------
Unsat Zone Thickness (m):     5.000E-05  Unsat Bulk Density:         1.900E+00
Unsat Dispersivity (m):       0.000E+00  Unsat Moisture Content:     1.200E-01
------------------------------------------------------------------------------
Aquifer Zone Parameters
------------------------------------------------------------------------------
Longitudinal Disp (m):        9.000E+00  Transverse Disp (m):        4.000E+00
Aquifer Thickness (m):        1.500E+01  Well Screen Thickness (m):  1.500E+01
Darcy Velocity (m/y):         5.700E+01  Aquifer Porosity:           1.000E-01
Bulk Density (g/cc):          1.900E+00
------------------------------------------------------------------------------
Calculated Flow Parameters
------------------------------------------------------------------------------
Percolation Water Flux (m3/y):  8.0000E+01
Total Water Flux (m3/y):        4.0800E+03
Unsat Pore Velocity (m/y):      1.6667E+00
Aquifer Pore Velocity (m/y):    5.7000E+02
Longitudinal Disp (m**2/y):     5.1300E+03
Transverse Disp (m**2/y):       2.2800E+03
------------------------------------------------------------------------------
Contaminant Data
------------------------------------------------------------------------------
Contaminant Name:              Sr-90
Number of Progeny:              0
Half Life (y):                  2.850E+01
Other Source Loss Rate (1/y):   0.000E+00
Kd Source (ml/g):               2.400E+01
Solubility Limit (mg/L):        1.000E+00
Molecular Weight (mg/L):        9.000E+01
Initial mass/activity:          0.000E+00
Mass/act input (mg or Ci/y):    1.000E+02
Kd Unsat (ml/g):                2.400E+01
Kd Aquifer (ml/g):              2.200E+01
Risk/Dose Conversion Factor     1.300E+05
------------------------------------------------------------------------------
Calculated Contaminant Values
```

```
-----------------------------------------------------------------------------
Decay Constants (1/y):          2.4321E-02
Leach Rate Constant (1/y):      1.1001E-02
Pnd Leach Rate Constant (1/y):  5.4945E-01
Solubility Limited Mass (mg):   0.0000E+00
Solubility Limited Act (Ci):    0.0000E+00
Unsat Retardation Factor:       3.8100E+02
Mean Unsat Transit Time (y):    1.1430E-02
Aquifer Retardation Factor:     4.190E+02
Minimum Peak Window Time (y):   5.1363E+00
Maximum Peak Window Time (y):   1.7778E+02
-----------------------------------------------------------------------------
Results for Receptor X =  1.00000E+02 Y = 0.00000E+00
-----------------------------------------------------------------------------
Peak Concentration (Ci/m**3):          1.456E-04
Time of Peak (y):                      6.8106E+01
Maximum Dose:                          1.325E+01
Maximum Allowable Release Rate (Ci/y): 3.020E-02
Execution Time (Seconds):    1

INPUT FILE NAME: PB-7B.PAR
Title: Example Problem #7B Sr-90 Release to a Pond GWSCREEN Ver 2.5  (Card 1)
-----------------------------------------------------------------------------
Model Run Options
-----------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                           1
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                   1
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:         0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:          2
IDIL (1) No dilution factor (2) Include Dilution Factor:      1
IMOIST Source Moisture Content Option:                        1
IMOISTU Unsaturated Moisture Content Option:                  1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:          3
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)    2
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
JSTART:   6
JMAX  :  12
EPS   :  1.000E-03
Health Effects: Committed effective dose equivalent calculation
Output mass/activity units:   Ci
Output concentration units:   Ci/m**3
Dose/Risk Conversion Units:   rem/Ci
Output health effects units:  rem
-----------------------------------------------------------------------------
Exposure Parameters
-----------------------------------------------------------------------------
Body Mass (kg):              70.       Averaging Time (days):      25550.
Water Ingestion (L/d):       2.000E+00 Exposure Freq (day/year):   3.500E+02
Exposure Duration (y):       1.000E+00 Limiting Dose:              4.000E-03
-----------------------------------------------------------------------------
Site Parameters
-----------------------------------------------------------------------------
X Coordinate:                0.000E+00  Y Coordinate:               0.000E+00
Source Length (m):           2.000E+01  Source Width (m):           2.000E+01
Percolation Rate (m/y):      2.000E-01
-----------------------------------------------------------------------------
Unsaturated Zone Parameters
-----------------------------------------------------------------------------
Unsat Zone Thickness (m):    5.000E-05  Unsat Bulk Density:         1.900E+00
Unsat Dispersivity (m):      0.000E+00  Unsat Moisture Content:     1.200E-01
-----------------------------------------------------------------------------
Aquifer Zone Parameters
-----------------------------------------------------------------------------
Longitudinal Disp (m):       9.000E+00  Transverse Disp (m):        4.000E+00
Aquifer Thickness (m):       1.500E+01  Well Screen Thickness (m):  1.500E+01
Darcy Velocity (m/y):        5.700E+01  Aquifer Porosity:           1.000E-01
Bulk Density (g/cc):         1.900E+00
-----------------------------------------------------------------------------
Calculated Flow Parameters
-----------------------------------------------------------------------------
Percolation Water Flux (m3/y):  8.0000E+01
Unsat Pore Velocity (m/y):      1.6667E+00
Aquifer Pore Velocity (m/y):    5.7000E+02
Longitudinal Disp (m**2/y):     5.1300E+03
Transverse Disp (m**2/y):       2.2800E+03
-----------------------------------------------------------------------------
Contaminant Data
-----------------------------------------------------------------------------
Contaminant Name:              Sr-90
Number of Progeny:              0
Half Life (y):                  2.850E+01
Other Source Loss Rate (1/y):   0.000E+00
Release File Name:             pb-7.rel
Kd Unsat (ml/g):                2.400E+01
Kd Aquifer (ml/g):              2.200E+01
Risk/Dose Conversion Factor     1.300E+05
-----------------------------------------------------------------------------
Release File Contents
-----------------------------------------------------------------------------
  Year      Flux Ci/y
 0.000E+00  0.000E+00
 1.000E+00  4.181E+01
 2.000E+00  6.536E+01
 3.000E+00  7.864E+01
 4.000E+00  8.611E+01
 5.000E+00  9.033E+01
 6.000E+00  9.270E+01
 7.000E+00  9.404E+01
 8.000E+00  9.479E+01
 9.000E+00  9.521E+01
 1.000E+01  9.545E+01
```

```
 1.100E+01  9.559E+01
 1.200E+01  9.566E+01
 1.300E+01  9.571E+01
 1.400E+01  9.573E+01
 1.500E+01  9.574E+01
 1.600E+01  9.575E+01
 1.700E+01  9.576E+01
 1.800E+01  9.576E+01
 1.900E+01  9.576E+01
 2.000E+01  9.576E+01
 2.100E+01  9.576E+01
 2.200E+01  9.576E+01
 2.300E+01  9.576E+01
 2.400E+01  9.576E+01
 2.500E+01  9.576E+01
 2.600E+01  9.576E+01
 2.700E+01  9.576E+01
 2.800E+01  9.576E+01
 2.900E+01  9.576E+01
 3.000E+01  9.576E+01
 3.200E+01  1.787E+00
 3.300E+01  1.725E+00
 3.400E+01  1.665E+00
 3.500E+01  1.607E+00
 3.600E+01  1.551E+00
 3.700E+01  1.497E+00
 3.800E+01  1.445E+00
 3.900E+01  1.395E+00
 4.000E+01  1.347E+00
 4.100E+01  1.300E+00
 4.200E+01  1.255E+00
 4.300E+01  1.211E+00
 4.400E+01  1.169E+00
 4.500E+01  1.129E+00
 4.600E+01  1.090E+00
 4.700E+01  1.052E+00
 4.800E+01  1.015E+00
 4.900E+01  9.800E-01
 5.000E+01  9.460E-01
 5.100E+01  9.132E-01
 5.200E+01  8.815E-01
 5.300E+01  8.509E-01
 5.400E+01  8.214E-01
 5.500E+01  7.929E-01
 5.600E+01  7.653E-01
 5.700E+01  7.388E-01
 5.800E+01  7.131E-01
 5.900E+01  6.884E-01
 6.000E+01  6.645E-01
 6.100E+01  6.414E-01
 6.200E+01  6.192E-01
 6.400E+01  5.769E-01
 6.600E+01  5.376E-01
 6.800E+01  5.009E-01
 7.000E+01  4.668E-01
 7.200E+01  4.349E-01
 7.400E+01  4.053E-01
 7.600E+01  3.776E-01
 7.800E+01  3.519E-01
 8.000E+01  3.279E-01
 8.200E+01  3.055E-01
 8.400E+01  2.847E-01
 8.600E+01  2.652E-01
 8.800E+01  2.472E-01
 9.000E+01  2.303E-01
 9.200E+01  2.146E-01
 9.400E+01  1.999E-01
------------------------------------------------------------------------------
Calculated Contaminant Values
------------------------------------------------------------------------------
Decay Constants (1/y):          2.4321E-02
Unsat Retardation Factor:       3.8100E+02
Mean Unsat Transit Time (y):    1.1430E-02
Aquifer Retardation Factor:     4.190E+02
------------------------------------------------------------------------------
Concentration vs Time Results for Receptor X =  1.00000E+02 Y = 0.00000E+00
------------------------------------------------------------------------------
   Time        Flux     Conc Mbr 1
 (years)  (mg or Ci/y) (mg or Ci per cubic meter)
------------------------------------------------------------------------------
 0.0000E+00  0.000E+00  0.000E+00
 2.0000E+00  6.508E+01  0.000E+00
 4.0000E+00  8.600E+01  0.000E+00
 6.0000E+00  9.265E+01  3.025E-17
 8.0000E+00  9.475E+01  8.679E-14
 1.0000E+01  9.542E+01  1.160E-11
 1.2000E+01  9.564E+01  3.222E-10
 1.4000E+01  9.570E+01  3.570E-09
 1.6000E+01  9.572E+01  2.203E-08
 1.8000E+01  9.573E+01  9.137E-08
 2.0000E+01  9.573E+01  2.854E-07
 2.2000E+01  9.573E+01  7.244E-07
 2.4000E+01  9.573E+01  1.565E-06
 2.6000E+01  9.573E+01  2.990E-06
 2.8000E+01  9.573E+01  5.178E-06
 3.2000E+01  2.323E+00  1.242E-05
 3.4000E+01  1.665E+00  1.765E-05
 3.6000E+01  1.551E+00  2.399E-05
 3.8000E+01  1.446E+00  3.137E-05
 4.0000E+01  1.347E+00  3.971E-05
 4.2000E+01  1.255E+00  4.889E-05
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 4.4000E+01  1.169E+00  5.875E-05
 4.6000E+01  1.090E+00  6.915E-05
 4.8000E+01  1.015E+00  7.988E-05
 5.0000E+01  9.461E-01  9.069E-05
 5.2000E+01  8.816E-01  1.014E-04
 5.4000E+01  8.215E-01  1.115E-04
 5.6000E+01  7.654E-01  1.209E-04
 5.8000E+01  7.132E-01  1.293E-04
 6.0000E+01  6.646E-01  1.362E-04
 6.4000E+01  5.770E-01  1.459E-04
 6.5000E+01  5.573E-01  1.473E-04
 6.6000E+01  5.377E-01  1.485E-04
 6.7000E+01  5.193E-01  1.491E-04
 6.8000E+01  5.010E-01  1.493E-04
 6.9000E+01  4.839E-01  1.493E-04
 7.0000E+01  4.668E-01  1.490E-04
 7.1000E+01  4.509E-01  1.482E-04
 7.2000E+01  4.350E-01  1.472E-04
 7.3000E+01  4.201E-01  1.459E-04
 7.4000E+01  4.053E-01  1.443E-04
 7.5000E+01  3.915E-01  1.425E-04
 7.6000E+01  3.777E-01  1.405E-04
 7.7000E+01  3.648E-01  1.382E-04
 7.8000E+01  3.519E-01  1.358E-04
 7.9000E+01  3.399E-01  1.332E-04
 8.0000E+01  3.279E-01  1.304E-04
 8.1000E+01  3.167E-01  1.275E-04
 8.2000E+01  3.055E-01  1.246E-04
 8.3000E+01  2.951E-01  1.215E-04
 8.4000E+01  2.847E-01  1.184E-04
 8.5000E+01  2.750E-01  1.153E-04
 8.6000E+01  2.653E-01  1.120E-04
 8.7000E+01  2.562E-01  1.087E-04
 8.8000E+01  2.472E-01  1.054E-04
 8.9000E+01  2.388E-01  1.021E-04
 9.0000E+01  2.303E-01  9.883E-05
 9.1000E+01  2.225E-01  9.557E-05
 9.2000E+01  2.146E-01  9.228E-05
 9.3000E+01  2.073E-01  8.917E-05
Maximum Concentration and Time for Member #1:  1.493E-04  6.800E+01
Execution Time (Seconds):    0

INPUT FILE NAME: PB-7C.PAR
Title: Example Problem #7c Sr-90 Release to a Pond 3D Vert Avg sol GWSCREEN Ver 2.5  (C
-----------------------------------------------------------------------------
Model Run Options
-----------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                             2
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                     3
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:           0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:            1
IDIL (1) No dilution factor (2) Include Dilution Factor:        1
IMOIST Source Moisture Content Option:                          1
IMOISTU Unsaturated Moisture Content Option:                    1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:            2
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)      2
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
JSTART:   6
JMAX  :  12
EPS   :  1.000E-02
Health Effects: Carcinogenic incidence risk for radionuclides
Output mass/activity units:   Ci
Output concentration units:   Ci/m**3
Dose/Risk Conversion Units:   1/Ci
Output health effects units:  carcinogenic risk
-----------------------------------------------------------------------------
Exposure Parameters
-----------------------------------------------------------------------------
Body Mass (kg):              70.       Averaging Time (days):      25550.
Water Ingestion (L/d):       2.000E+00 Exposure Freq (day/year):   3.650E+02
Exposure Duration (y):       3.000E+01 Limiting Dose:              1.000E-06
-----------------------------------------------------------------------------
Site Parameters
-----------------------------------------------------------------------------
X Coordinate:                0.000E+00  Y Coordinate:               0.000E+00
Source Length (m):           2.000E+01  Source Width (m):           2.000E+01
Percolation Rate (m/y):      2.000E-01
Pond Operation Time (y):     3.000E+01  Water Input Rate (m3/y):    4.000E+03
Evap Rate Constant (1/y):    0.000E+00  Pond Moisture Content:      4.000E-01
Source Thickness (m):        5.000E-01  Src Bulk Density (g/cc):    1.500E+00
Source Moisture Content:     3.600E-01
-----------------------------------------------------------------------------
Unsaturated Zone Parameters
-----------------------------------------------------------------------------
Unsat Zone Thickness (m):    5.000E-05  Unsat Bulk Density:         1.900E+00
Unsat Dispersivity (m):      0.000E+00  Unsat Moisture Content:     1.200E-01
-----------------------------------------------------------------------------
Aquifer Zone Parameters
-----------------------------------------------------------------------------
Longitudinal Disp (m):       9.000E+00  Transverse Disp (m):        4.000E+00
Vertical Dispersivity (m):   4.000E+00
Aquifer Thickness (m):       1.500E+01  Well Screen Thickness (m):  1.500E+01
Darcy Velocity (m/y):        5.700E+01  Aquifer Porosity:           1.000E-01
Bulk Density (g/cc):         1.900E+00
-----------------------------------------------------------------------------
Calculated Flow Parameters
-----------------------------------------------------------------------------
Percolation Water Flux (m3/y):  8.0000E+01
Total Water Flux (m3/y):        4.0800E+03
Unsat Pore Velocity (m/y):      1.6667E+00
Aquifer Pore Velocity (m/y):    5.7000E+02
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Longitudinal Disp (m**2/y):     5.1300E+03
Transverse Disp (m**2/y):       2.2800E+03
Vertical Disp (m**2/y):         2.2800E+03
-----------------------------------------------------------------------------
Contaminant Data
-----------------------------------------------------------------------------
Contaminant Name:              Sr-90
Number of Progeny:              0
Half Life (y):                  2.850E+01
Other Source Loss Rate (1/y):   0.000E+00
Kd Source (ml/g):               2.400E+01
Solubility Limit (mg/L):        1.000E+00
Molecular Weight (mg/L):        9.000E+01
Initial mass/activity:          0.000E+00
Mass/act input (mg or Ci/y):    1.000E+02
Kd Unsat (ml/g):                2.400E+01
Kd Aquifer (ml/g):              2.200E+01
Risk/Dose Conversion Factor     3.600E+01
-----------------------------------------------------------------------------
Calculated Contaminant Values
-----------------------------------------------------------------------------
Decay Constants (1/y):          2.4321E-02
Leach Rate Constant (1/y):      1.1001E-02
Pnd Leach Rate Constant (1/y):  5.4945E-01
Solubility Limited Mass (mg):   0.0000E+00
Solubility Limited Act (Ci):    0.0000E+00
Unsat Retardation Factor:       3.8100E+02
Mean Unsat Transit Time (y):    1.1430E-02
Aquifer Retardation Factor:     4.190E+02
Minimum Peak Window Time (y):   5.1363E+00
Maximum Peak Window Time (y):   1.7778E+02
-----------------------------------------------------------------------------
Results for Receptor X =  1.00000E+02 Y = 0.00000E+00
-----------------------------------------------------------------------------
Peak Concentration (Ci/m**3):          1.463E-04
Time of Peak (y):                      6.9802E+01
Concentrations Averaged Between:       5.4802E+01 and  8.4802E+01 years
Average Concentration (Ci/m**3):       1.336E-04
Maximum Dose:                          1.053E-01
Maximum Allowable Release Rate (Ci/y): 9.495E-04
Execution Time (Seconds):    0

INPUT FILE NAME: PB-8.PAR
Title: Example Problem #8 Pu-241, Am-241 & Np-237 Carcin Risk GWSCREEN Ver 2.5  (Card 1
-----------------------------------------------------------------------------
Model Run Options
-----------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                             2
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                     1
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:           0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:            1
IDIL (1) No dilution factor (2) Include Dilution Factor:        1
IMOIST Source Moisture Content Option:                          1
IMOISTU Unsaturated Moisture Content Option:                    1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:            1
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)      1
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
Health Effects: Carcinogenic incidence risk for radionuclides
Output mass/activity units:   Ci
Output concentration units:   Ci/m**3
Dose/Risk Conversion Units:   1/Ci
Output health effects units:  carcinogenic risk
-----------------------------------------------------------------------------
Exposure Parameters
-----------------------------------------------------------------------------
Body Mass (kg):              70.       Averaging Time (days):      25550.
Water Ingestion (L/d):       2.000E+00 Exposure Freq (day/year):   3.500E+02
Exposure Duration (y):       3.000E+01 Limiting Dose:              1.000E-06
-----------------------------------------------------------------------------
Site Parameters
-----------------------------------------------------------------------------
X Coordinate:                0.000E+00  Y Coordinate:               0.000E+00
Source Length (m):           7.000E+01  Source Width (m):           3.000E+01
Percolation Rate (m/y):      1.000E+00
Source Thickness (m):        2.000E+00  Src Bulk Density (g/cc):    1.500E+00
Source Moisture Content:     3.500E-01
-----------------------------------------------------------------------------
Unsaturated Zone Parameters
-----------------------------------------------------------------------------
Unsat Zone Thickness (m):    6.000E+00  Unsat Bulk Density:         1.900E+00
Unsat Dispersivity (m):      0.000E+00  Unsat Moisture Content:     9.000E-02
-----------------------------------------------------------------------------
Aquifer Zone Parameters
-----------------------------------------------------------------------------
Longitudinal Disp (m):       9.000E+00  Transverse Disp (m):        4.000E+00
Aquifer Thickness (m):       7.600E+01  Well Screen Thickness (m):  1.500E+01
Darcy Velocity (m/y):        5.700E+01  Aquifer Porosity:           1.000E-01
Bulk Density (g/cc):         1.900E+00
-----------------------------------------------------------------------------
Calculated Flow Parameters
-----------------------------------------------------------------------------
Percolation Water Flux (m3/y):  2.1000E+03
Unsat Pore Velocity (m/y):      1.1111E+01
Aquifer Pore Velocity (m/y):    5.7000E+02
Longitudinal Disp (m**2/y):     5.1300E+03
Transverse Disp (m**2/y):       2.2800E+03
-----------------------------------------------------------------------------
Contaminant Data
-----------------------------------------------------------------------------
Contaminant Name:              Pu-241
Number of Progeny:              2
```

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Progeny Names:                 Am-241       Np-237
Half Life (y):                  1.440E+01 4.322E+02 2.100E+06
Other Source Loss Rate (1/y):   0.000E+00
Kd Source (ml/g):               2.200E+01
Solubility Limit (mg/L):        7.110E+06
Molecular Weight (mg/L):        2.410E+02
Initial mass/activity:          1.000E+01
Kd Unsat (ml/g):                2.200E+01
Kd Aquifer (ml/g):              2.200E+01 3.400E+02 5.000E+00
Risk/Dose Conversion Factor     4.800E+00 3.100E+02 2.700E+02
------------------------------------------------------------------------------
Calculated Contaminant Values
------------------------------------------------------------------------------
Decay Constants (1/y):          4.8135E-02 1.6038E-03 3.3007E-07
Leach Rate Constant (1/y):      1.4993E-02
Solubility Limited Mass (mg):   9.9590E+14
Solubility Limited Act (Ci):    1.0268E+14
Unsat Retardation Factor:       4.6544E+02
Mean Unsat Transit Time (y):    2.5134E+02
Aquifer Retardation Factor:     4.190E+02 6.461E+03 9.600E+01
Minimum Peak Window Time (y):   2.5347E+02
Maximum Peak Window Time (y):   7.3189E+02
------------------------------------------------------------------------------
Results for Receptor X =  1.35000E+02 Y = 0.00000E+00
------------------------------------------------------------------------------
NOTE: Concentrations and Doses Reported in Order of the Decay Chain
NOTE: Progeny Concentrations are Reported at the Time of the Maximum Parent Concentration
Peak Concentration (Ci/m**3):          6.360E-14  3.993E-10  3.388E-12
Time of Peak (y):                      3.1910E+02
Concentrations Averaged Between:       3.0410E+02 and  3.3410E+02 years
Average Concentration (Ci/m**3):       5.951E-14  4.052E-10  3.487E-12
Maximum Dose:                          5.999E-12  2.638E-06  1.977E-08
Total Dose (all members):              2.657E-06
Maximum Allowable Inventory (Ci):      3.763E+00
Execution Time (Seconds):    0

INPUT FILE NAME: PB-9.PAR
Title: Example Problem #9 Hydrocarbon Benzene Spill with Vapor Loss GWSCREEN Ver 2.5  (
------------------------------------------------------------------------------
Model Run Options
------------------------------------------------------------------------------
IMODE Contaminant Type and Impacts:                              5
ITYPE (1) Vert Avg (2) 3D Point (3) 3d Avg:                      1
IDISP (0) Fixed Dispersivity (1-3) Spatially Varying:            0
KFLAG (1) Max Conc (2) Conc vs Time (3) Grid Output:             1
IDIL (1) No dilution factor (2) Include Dilution Factor:         1
IMOIST Source Moisture Content Option:                           1
IMOISTU Unsaturated Moisture Content Option:                     1
IMODEL (1) Surface/Burried Src (2) Pond (3) Usr Def:             1
ISOLVE (1) Gaussian Quarature (2) Simpsons Rule: (Aquifer)       1
ISOLVEU (1) Gaussian Quarature (2) Simpsons Rule: (Unsat Zone)  1
Health Effects: Carcinogenic incidence risk for non-radiological contaminants
Output mass/activity units:   mg
Output concentration units:   mg/m**3
Dose/Risk Conversion Units:   kg-d/mg
Output health effects units:  carcinogenic risk
------------------------------------------------------------------------------
Exposure Parameters
------------------------------------------------------------------------------
Body Mass (kg):              70.       Averaging Time (days):       25550.
Water Ingestion (L/d):       2.000E+00 Exposure Freq (day/year):    3.500E+02
Exposure Duration (y):       3.000E+01 Limiting Dose:               1.000E-06
------------------------------------------------------------------------------
Site Parameters
------------------------------------------------------------------------------
X Coordinate:                0.000E+00  Y Coordinate:                0.000E+00
Source Length (m):           1.500E+01  Source Width (m):            2.500E+01
Percolation Rate (m/y):      1.000E-01
Source Thickness (m):        2.000E+00  Src Bulk Density (g/cc):     1.500E+00
Source Moisture Content:     3.000E-01
------------------------------------------------------------------------------
Unsaturated Zone Parameters
------------------------------------------------------------------------------
Unsat Zone Thickness (m):    1.000E-01  Unsat Bulk Density:          1.900E+00
Unsat Dispersivity (m):      0.000E+00  Unsat Moisture Content:      9.000E-02
------------------------------------------------------------------------------
Aquifer Zone Parameters
------------------------------------------------------------------------------
Longitudinal Disp (m):       9.000E+00  Transverse Disp (m):         4.000E+00
Aquifer Thickness (m):       7.600E+01  Well Screen Thickness (m):   1.500E+01
Darcy Velocity (m/y):        5.700E+01  Aquifer Porosity:            1.000E-01
Bulk Density (g/cc):         1.900E+00
------------------------------------------------------------------------------
Calculated Flow Parameters
------------------------------------------------------------------------------
Percolation Water Flux (m3/y):  3.7500E+01
Unsat Pore Velocity (m/y):      1.1111E+00
Aquifer Pore Velocity (m/y):    5.7000E+02
Longitudinal Disp (m**2/y):     5.1300E+03
Transverse Disp (m**2/y):       2.2800E+03
------------------------------------------------------------------------------
Contaminant Data
------------------------------------------------------------------------------
Contaminant Name:              Benzene
Half Life (y):                   9.500E-01
Other Source Loss Rate (1/y):   1.130E-02
Kd Source (ml/g):               2.500E-01
Solubility Limit (mg/L):        1.780E+03
Molecular Weight (mg/L):        7.810E+01
Initial mass/activity:          5.620E+08
Kd Unsat (ml/g):                2.500E-01
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Kd Aquifer (ml/g):              2.500E-01
Risk/Dose Conversion Factor     5.200E-02
-----------------------------------------------------------------------------
Calculated Contaminant Values
-----------------------------------------------------------------------------
Decay Constants (1/y):          7.2963E-01
Leach Rate Constant (1/y):      7.4074E-02
Solubility Limited Mass (mg):   9.0113E+08
Unsat Retardation Factor:       6.2778E+00
Mean Unsat Transit Time (y):    5.6500E-01
Aquifer Retardation Factor:     5.750E+00
Minimum Peak Window Time (y):   6.0031E-01
Maximum Peak Window Time (y):   3.1644E+01
-----------------------------------------------------------------------------
Results for Receptor X =  2.50000E+01 Y = 0.00000E+00
-----------------------------------------------------------------------------
Peak Concentration (mg/m**3):          3.947E+02
Time of Peak (y):                      1.1105E+00
Concentrations Averaged Between:       5.6500E-01 and  3.0565E+01 years
Average Concentration (mg/m**3):       2.330E+01
Maximum Dose:                          1.422E-05
Maximum Allowable Inventory (mg):      3.951E+07
Execution Time (Seconds):    0
```