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A BENCHMARKING ANALYSIS FOR FIVE RADIONUCLIDE VADOSE ZONE MODELS (CHAIN, MULTIMED_DP, FECTUZ, HYDRUS, AND CHAIN 2D) IN SOIL SCREENING LEVEL CALCULATIONS

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ABSTRACT

Five vadose zone models with different degrees of complexity (CHAIN, MULTIMED_DP, FECTUZ, HYDRUS, and CHAIN 2D) were selected for use in radionuclide soil screening level (SSL) calculations. A benchmarking analysis between the models was conducted for a radionuclide (^{99}Tc) release scenario at the Las Cruces Trench Site in New Mexico. Sensitivity of three model outputs to the input parameters were evaluated and compared among the models. The three outputs were peak contaminant concentrations, time to peak concentrations at the water table, and time to exceed the contaminants maximum critical level at a representative receptor well. Model parameters investigated include soil properties such as bulk density, water content, soil water retention parameters and hydraulic conductivity. Chemical properties examined include distribution coefficient, radionuclide half-life, dispersion coefficient, and molecular diffusion. Other soil characteristics, such as recharge rate, also were examined. Model sensitivity was quantified in the form of sensitivity and relative sensitivity coefficients. Relative sensitivities were used to compare the sensitivities of different parameters. The analysis indicates that soil water content, recharge rate, saturated soil water content, and soil retention parameter, β, have a great influence on model outputs. In general, the results of sensitivities and relative sensitivities using five models are similar for a specific scenario. Slight differences were observed in predicted peak contaminant concentrations due to different mathematical treatment among models. The results of benchmarking and sensitivity analysis would facilitate the model selection and application of the model in SSL calculations.

INTRODUCTION

To standardize and accelerate the evaluation and cleanup of soils contaminated with radioactive materials at sites on the National Priorities List (NPL) with anticipated future residential land use scenarios, the U.S. Environmental Protection Agency (EPA) has developed the Soil Screening

Guidance for Radionuclides. The Guidance is aimed to provide a methodology to calculate risk-based, site-specific, soil screening levels (SSLs), for radioactive contaminants in soil. In general, when the radionuclide concentrations equal or exceed SSLs, further study or investigation is needed.

Although SSL equations under certain assumptions and limitations can be used to calculate the site-specific SSLs for surface and subsurface soils, they are simple and are used for preliminary screening purposes. When the site conditions are more complex than the underlined assumptions in the simple SSL equations, a detailed modeling approach is needed. Therefore, selecting a proper model and recognizing the performance of the model are required in the process of SSL calculation. In such an effort to provide background information for SSL calculation, EPA conducted an evaluation of five unsaturated zone fate and transport models for radionucludes. The models evaluated are CHAIN, MULTIMED_DP 1.0, FECTUZ, HYDRUS, and CHAIN 2D models. These five models are a subset of the potential models available to the public, and other models may be applicable for the SSL calculation. This study presents part of the evaluation (benchmarking) results.

In general, different strategies can be used for model evaluation depending on the specific objectives/goals of model evaluation. For example, to calculate the soil cleanup criteria, Sanders (1) compared the predicted leaching of chemicals in the unsaturated soil zone under a hypothetical environmental scenario using four unsaturated zone models -- PRZM, SESOIL, SLMI, and IMPACT. In an evaluation of three multimedia models (MEPAS, MMSOILS, and PRESTO-EPA-CPG) used to support cleanup decision-making at hazardous, mixed, and radioactive waste sites, a review of process modules was conducted based on documentation, on published reviews, and personal interviews by Moskowitz et al. (2). In a series of multimedia benchmarking analyses for three risk assessment models -- RESRAD, MMSOILS, and MEPAS, Laniak et al. (3) and others (4,5,6) examined mathematical constructs and assumptions, similarities, differences of the models, and model performance for a given environmental scenario. In addition to examining the performance of flow and transport processes, Nofziger et al. (7) included sensitivity analysis in their evaluation of Superfund site vadose zone models.

Sensitivity analyses are considered as part of the model evaluation for the SSL calculation because sensitivity analyses serve two purposes: (1) to evaluate the model's response to changes in the input parameters, and (2) to quantify the likely uncertainties of the calibrated model resulting from uncertainties associated with the input parameters, the environmental stresses, and the boundary conditions (8,9). Thus, sensitivity analyses can provide an understanding of the sensitive, important, and non-sensitive nature of model input parameters. Sensitive parameters are those input parameters, which produce significant changes in the model outputs of concern, even though the input changes may be relatively small. Non-sensitive input parameters under certain model scenarios should not be considered as unimportant to the simulation, but merely parameters that contribute little to the model's uncertainty. That is, sensitivity analyses provide the user with an understanding of those input parameters that enhance the robustness of the model and those input parameters that may lead to model uncertainties if care is not sufficiently exercised (10).

The objectives of this study are to evaluate the technical formulations and performance characteristics of the five unsaturated zone models for radionuclides and to provide the background information for the use of models in the process of the SSL calculation. The flow and transport processes, and inputs/outputs of the five models will be reviewed and evaluated for their capacity for simulating radionuclide migration. Base case simulations and sensitivity analyses will be used to address the model performance. Comparison of the results of the base case simulation and sensitivity analysis will be made for identifying the similarities and difference of model performance.

MODEL DESCRIPTION

The five models selected for this analysis address four essential processes that predominately control the migration of radionuclides in the unsaturated zone: advection (derived from infiltration), dispersion, sorption, and radionuclide decay. Table I provides a summary of model components (processes considered) and the similarities and differences among the models. Table II gives a summary of the use of the model including the model outputs, applicability and limitations. Except for dimensionality, the HYDRUS model is the most comprehensive code for flow and transport in the unsaturated zone. It considers hysteresis of soil water retention. The MULTIMED_DP model was initially developed as a multimedia fate and transport model. The FECTUZ model is the unsaturated module of U.S. EPA's composite model for leachate migration with transformation products (EPACMTP, 11, 12). In general, any of the five models can be used in simulating fate and transport of radionuclides in the unsaturated zone and can provide the time-varying concentrations of radionuclides in the leachate entering ground water. These concentrations are used for the SSL calculation. The detailed procedures for the SSL calculation can be found in the user's guide and the technical background document of the U.S. EPA's Soil Screening Guidance for Radionuclides (13, 14). The reader who is interested in detailed assumptions and mathematical formulations of the models is referred to the specific model theory and user's manuals for CHAIN (15), MULTIMED_DP 1.0 (16, 17, 18), FECTUZ (11, 12), HYDRUS (19), and CHAIN 2D (20).

Table I. Summary Comparisons of the Vadose Zone Models for Radionuclides in the SSL Process

Model component	**HYDRUS**	**MULTIMED-DP**	**FECTUZ**	**CHAIN**	**CHAIN 2D**
Contaminants					
Organics	●	●	●	●	●
Metals	●	●	●	●	●
Radionuclides (parent)	●	●	●	●	●
Radionuclides (progeny)	●	●	●	●	●
Sources types					
Contaminated soil	●	●	●	●	●

Landfill	●	●	●	--	●
Surface impoundment	--	--	●	--	--
Waste piles	--	--	●	--	--
Source term characteristics					
Mass balance	●	●	●	●	●
Multimedia partitioning	●	●	●	--	●
Source decay	--	●	--	--	--
Multiple contaminants per simulations	●	●	●	●	●
Source release mechanisms					
Leaching	●	●	●	●	●
Direct release to:					
Vadose zone	●	●	●	●	●
Groundwater	--	●	●	--	--
Surface water	--	●	--	--	--
Air	--	●	--	--	--
Medium-specific flow					
Surface Hydrology					
Precipitation	--	●	--	--	--
Runoff	--	●	--	--	--
Infiltration	●	●	●	●	●
ET	●	●	--	--	●
Surface Water (Stream discharge)	--	●	--	--	--
Vadose Zone					
Vadose zone (Steady-state infiltration -->soil	●	●	●	●	●
Vadose zone (n-D dynamic)	●	--	--	--	●
Groundwater	--	--	●	--	--
Medium-specific contaminant transport					
Atmosphere (emission through diffusion)	--	●	--	--	--
Surface water (stream interception and mixing)	--	●	--	--	--
Vadose zone (1-D advection and dispersion)	●	●	●	●	●
Vadose zone (2-D advection and dispersion)	--	--	--	--	●
Groundwater					
Homogeneous aquifer (1-D advection and	--	●	●	--	--
Homogeneous aquifer (2-D advection and	--	●	●	--	--
Homogeneous aquifer (3-D advection and	--	●	●	--	--
Medium-specific heat transport	●	--	--	--	●
Contaminant transformations and fate processes					
1st order decay (not decay products)	●	●	●	●	●
1st order decay (with chained daughter and granddaughter decay products) --straight chain	●	●	●	●	●
1st order decay -- branch chain	●	--	●	--	●
Non-1st order decay	●	--	--	--	●
Linear sorption (partitioning between water and soil)	●	●	●	●	●
Nonlinear sorption (partitioning between water and	●	--	●	--	●
Nonequilibrium sorption	●	--	--	--	●

Hydrolysis	--	●	●	--	--
Chemical reactions/speciation	--	●	●	--	--
Intermedia contaminant fluxes					
Surface soil --> Air (volatilization)	●	●	--	●	●
Surface soil --> Vadose zone (leaching)	●	●	●	●	●
Surface soil --> Overland (erosion, runoff)	--	●	--	--	--
Surface water -->Sediment (sedimentation)	--	--	--	--	--
Vadose zone --> groundwater (percolation)	●	●	●	●	●
Vadose zone --> Air (volatilization)	●	●	--	--	●

● denotes component is included in model; -- denotes component is not included in model.

Table II. Summary of the Use of the Unsaturated Zone Models for Radionuclides in the SSL Process

Model	**Processes, components, outputs**
HYDRUS	- provides leachate radionuclide concentrations entering ground water in order to examine if radionuclide concentrations at a downgradient receptor well exceed acceptable levels - calculates infiltration which can be used as inputs in the SSL calculation - considers soil heterogeneity, nonlinear/nonequilibrium sorption, time-varying infiltration and evapotranspiration - considers hysterisis of soil water retension - outputs radionuclide concentration in soil, cumulative flux across water table - grid discretization for HYDRUS version 6.0 requires extra effort
MULTIMED_DP	- provides leachate radionuclide concentrations entering ground water in order to examine if radionuclide concentrations at a downgradient receptor well exceed acceptable levels - uncertainty of model outputs can be examined - considers runoff, evapotranspiration - linked with a saturated flow and transport model - requires a great amount of input data, expertise because of model complexity
FECTUZ	- provides leachate radionuclide concentrations entering ground water in order to examine if radionuclide concentrations at a downgradient receptor well exceed acceptable levels - uncertainty of model outputs can be examined - linked with a saturated flow and transport model - uses mixed units for the input data
CHAIN	- provides leachate radionuclide concentrations entering ground water in order to examine if radionuclide concentrations at a downgradient receptor well exceed acceptable levels - used for simplified radionuclide-contaminated site scenario - simple-to-use, less input data requirement - as a preliminary assessment tool in SLL estimation

CHAIN 2D	- provides leachate radionuclide concentrations entering ground water in order to examine if radionuclide concentrations at a downgradient receptor well exceed acceptable levels - calculates infiltration which can be used as input in the SSL calculation - considers soil heterogeneity, nonlinear/nonequilibrium sorption, time-varying infiltration and evapotranspiration - outputs radionuclide concentration in soil, cumulative flux across water table - considers two-dimensional soil heterogeneity

METHODOLOGY

Conceptual Site Model for Radionuclide Leaching

To apply the five models evaluated herein in the SSL calculation, a conceptual site model was developed at the Las Cruces Trench Site, New Mexico, and USA. The Site is in the Chihuahuan Desert, on a basin slope of Mount Summerford. Climate in the region is characterized by low relative humidity and an average class a pan evaporation of 239 cm per year. Average annual precipitation is 23 cm. The site has been subject to extensive testing of physical and chemical soil properties and water movement in the unsaturated zone. In addition, results of tracer tests (chloride, bromide, and tritium) are available for the Site (21). For the purpose of this study, it is assumed that the Site had been used as a waste disposal/storage facility where radionuclides from tank leaks or improper waste disposal were released to the soil surface for 1000 days with a total amount for 3×10^{-4} mg /cm ^{99}Tc (^{99}Tc concentration from the waste source is 1.25×10^{-2} mg/L**).** Rainfall infiltration (with a net annual recharge rate of 87 mm/y) is the driving force for the downward migration of radionuclides to the water table. Base values of input parameters are given in Table III. Uniform soil properties and solute transport parameters in Table III are obtained from the layered data of Wierenga et al. (21) and Porro and Wierenga (22), respectively. It is assumed that steady-state uniform water flow occurs at the site. At the time that source release ceases, the soil in the top 150 cm depth contains approximately 1.18×10^{-3} mg/kg of ^{99}Tc. The decay coefficients and the distribution coefficient for ^{99}Tc and its daughter ^{99}Ru are taken from U.S. EPA (14).

The dispersion coefficient D in the unsaturated zone is characterized by a molecular diffusion term and a mechanical dispersion term and is given by Hills et al. (23) as

$$D = \tau_w D_w + D_L \frac{q}{\theta} \qquad \text{(Eq. 1)}$$

where θ is the initial water content of 0.16 cm^3/cm^3, q is the infiltration rate of 8.7 cm/y, D_L is the dispersivity of 4.53 cm, τ_w is the tortuosity factor, and D_w is the diffusion coefficient in free water of 1.73 cm^2/d. The tortuosity factor of 0.19 is calculated from θ (Tomasko et al., 24). Consequently, the dispersion coefficient, D, is 0.33 cm^2/d.

Table III. Values of Model Input Parameters

Parameters	**Values**
Source-Specific Parameters	
Area of disposal facility (m^2)	400
Width of disposal facility (m)	20
Length of disposal facility (m)	20
Mass release of Radionuclide ^{99}TC (mg/cm^2)	3×10^{-4}
Concentration of ^{99}Tc in recharge water from waste source (mg/L)	1.25×10^{-2}
Duration of waste source being completely released (days)	1000
Potential recharge rate (cm/d)	0.024
Initial water content (cm^3/cm^3)	0.16
Soil Properties in Unsaturated Zone	
Saturated hydraulic conductivity, K_s, (cm/d)	270.1
Porosity (--)	0.358
Saturated water content (cm^3/cm^3)	0.321
Residual water content (cm^3/cm^3)	0.083
Bulk density (g/cm^3)	1.70
van Genuchten alpha coefficient, α, (cm^{-1})	0.055
van Genuchten beta coefficient, β (--)	1.509
Depth to water table (m)	6
Solute Transport Parameters	
Decay coefficient for parent product ^{99}Tc (1/d)	9×10^{-9}
Decay coefficient for daughter product ^{99}Ru (1/d)	stable
Distribution coefficient for parent product ^{99}Tc (cm^3/g)	0.007
Distribution coefficient for daughter product ^{99}Ru (cm^3/g)	5
Dispersion coefficient (cm^2/d)	1.01
Dispersivity (cm)	4.53
Diffusion coefficient in free water (cm^2/d)	1.73
Apparent molecular dispersion coefficient (cm^2/d)	0.33

Model Outputs of Interest

Using the base values of the input parameters (Table III), the time evolution of the radionuclide ^{99}Tc concentration in the leachate at the bottom of the unsaturated zone (i.e., at the entry point to the water table, 6 m below the ground surface) is obtained (Figure 1). The solid line in Figure 1 represents the typical breakthrough curve (BTC) for the base scenario of the conceptual model using the CHAIN model.

In the SSL process, the concentration at a receptor well is assumed to exceed the Maximum Contaminant Level (MCL) whenever the concentration at the ground water entry point exceeds the MCL times a dilution attenuation factor (DAF). A value of 20 for DAF is proposed in U.S. EPA (14). When this occurs, the radionuclide concentrations in soil (mass units of mg/Kg) exceed SSLs. The MCL for ^{99}Tc is 5.3×10^{-5} mg/L (14). Three characteristics of the BTCs are of interest in this study:

1. The peak concentration of the radionuclide, C_{peak},
2. The time to reach peak concentration, T_{peak}, and
3. The time when the concentration of radionuclide is high enough for the resulting concentration at a receptor well to exceed the MCL. The time to reach MCL is denoted by T_{MCL}.

In Figure 1, the arrow indicates a time point where ^{99}Tc concentration / DAF exceeds the MCL, i.e. T_{MCL}. Similarly, the peak concentration of ^{99}Tc, C_{peak}, and the time to reach peak concentration can be read from the y-axis (concentration axis) and x-axis (time axis) respectively.

Sensitivity Analysis

The sensitivity of a model is a measure of the change in a selected model output resulting from a specified change in an input parameter. Mathematically, the sensitivity coefficient S_{ij} of a model's output y_i to a model's input parameter x_j is the partial derivative of y_i with respect to x_j, while holding other pertinent input parameters fixed, and it is expressed as:

$$S_{i,j} = \frac{\partial y_i}{\partial x_j} \qquad \text{(Eq. 2)}$$

Here, the model's output, y_i, could be one of the three output quantities: C_{peak}, T_{peak} and T_{MCL} The model's input parameter, x_j, could be any one of the model input parameters given in Table III. In the current analyses, only 12 parameters are included in the sensitivity analysis. They are the distribution coefficient for parent product ^{99}Tc, recharge rate, initial water content, bulk density, dispersion coefficient, dispersivity, diffusion coefficient in free water, saturated hydraulic conductivity, saturated water content, residual water content, van Genuchten alpha coefficient, α, and van Genuchten beta coefficient, β.

The dimensions of S_{ij} are those of y_i divided by those of x_j. Since S_{ij}, in general, is dimensional, it may be difficult and confusing to compare sensitivities for different input parameters. These problems are overcome by introducing a normalized form of S_{ij}, called the relative sensitivity coefficient, defined by:

$$S^r_{i,j} = \frac{\partial y_i}{\partial x_j} \frac{x_j}{y_i} \qquad \text{(Eq. 3)}$$

By definition, S^r_{ij} is dimensionless, and comparison of the sensitivity coefficients between two input parameters can be made. For example, S^r for T_{peak} to recharge rate is -1.0, and S^r for T_{peak} to initial water content is 0.80. Then T_{peak} is more sensitive to the recharge rate than to initial water content. Note that the comparison is made on the absolute values of two relative sensitivity coefficients. The negative S^r value for recharge rate indicates that T_{peak} decreases with an increase in recharge rate.

Procedures Followed in the Sensitivity Analyses

The procedures for conducting a sensitivity analysis are as follows:

1. Select a model for analysis;
2. Select the model outputs of interest, namely C_{peak}, T_{peak}, and T_{MCL};
3. Select a particular variable input parameter and select a range for this parameter;
4. Run model simulations using the base parameter values except for the input parameter being evaluated;
5. Calculate the sensitivity (S) and relative sensitivity (S^r) of a model output to the various input parameters following the approach (Equations 3 and 4) described above.

The procedures given above are repeated for each input parameter considered in each model.

RESULTS AND DISCUSSION

Impact of Input Parameters on BTC

Figure 1 gives the breakthrough curves of ^{99}Tc at the hypothetical water table located at 6 m below the ground surface. The solid curve represents the breakthrough curve of ^{99}Tc using the base value of 0.024 cm/d for recharge rate using the CHAIN model. In the sensitivity analysis for recharge rate, a range of recharge rates around the base values (0.024 cm/d) were used to obtain the BTCs. For example, the dotted curve in Figure 1 represents the breakthrough curve of ^{99}Tc using the base values in Table III except using a lower bound of 0.014 cm/d for recharge rate. In this manner, the impacts of changing recharge rate on the BTCs can be evaluated. As shown in Figure 1, a decrease of recharge rate results in an increase of travel time for ^{99}Tc to first reach the entering point (water table) and an increase of the residence time of ^{99}Tc in the unsaturated zone.

The residence time is the time lag between the time where the source was released and the time where ^{99}Tc is completely leached out of the unsaturated zone. For the three outputs of interest, C_{peak} increases with an increase in recharge rate; T_{peak} and T_{MCL} decrease with an increase in recharge rate.

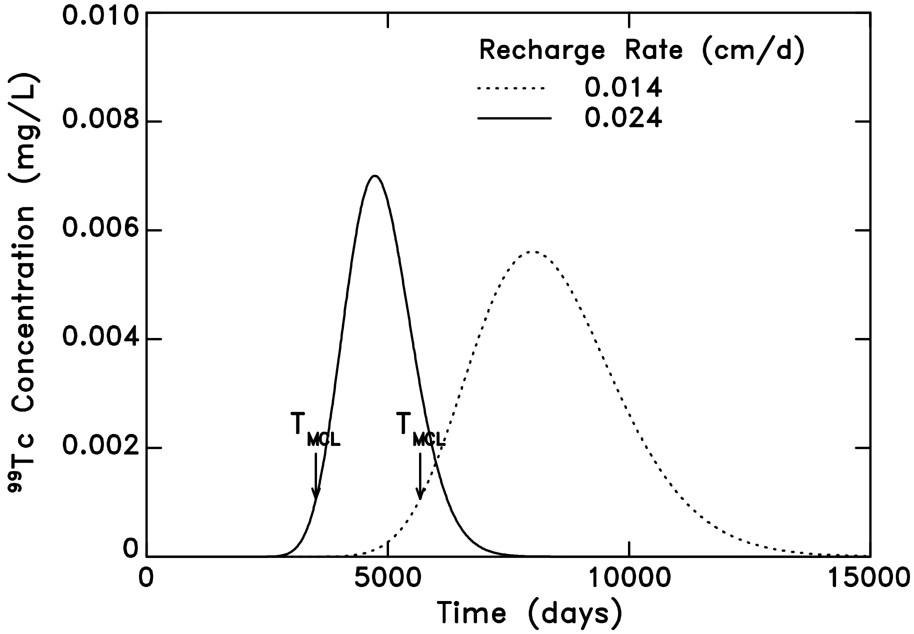

Fig. 1. Sensitivity of ^{99}TC breakthrough curve (through the unsaturated zone) to the recharge rate using the CHAIN model.

When C_{peak} was plotted in correspondence to recharge rate, a curve as given in Figure 2(a) was obtained. Figure 2(a) indicates an increase of C_{peak} with an increase in recharge rate. The sensitivity of C_{peak} to recharge rate, as shown in Figure 2(b), can be obtained using equation 2. Similarly, the relative sensitivity of C_{peak} to recharge rate as shown in Figure 2(c) can be obtained using equation 3. Central finite difference approximation was used for the calculations of sensitivity and relative sensitivity. According to equations 2 and 3, relative sensitivity has the same sign as sensitivity. In this manner, the sensitivities and relative sensitivities of C_{peak}, T_{peak} and T_{MCL} to twelve input parameters using the five models were obtained.

Table IV summarizes the relative sensitivities of C_{peak}, T_{peak} and T_{MCL} at the base scenario (i.e., using the base values as given in Table III). For all of the models, the sensitivities with respect to distribution coefficient for parent product ^{99}Tc, recharge rate, initial water content, bulk density, dispersion coefficient, dispersivity, and diffusion coefficient in free water were obtained under the constant, uniform water content (recharge rate) conditions. The sensitivities with respect to saturated hydraulic conductivity, saturated water content, residual water content, van Genuchten alpha coefficient, α, and van Genuchten beta coefficient, β, were obtained under the nonuniform

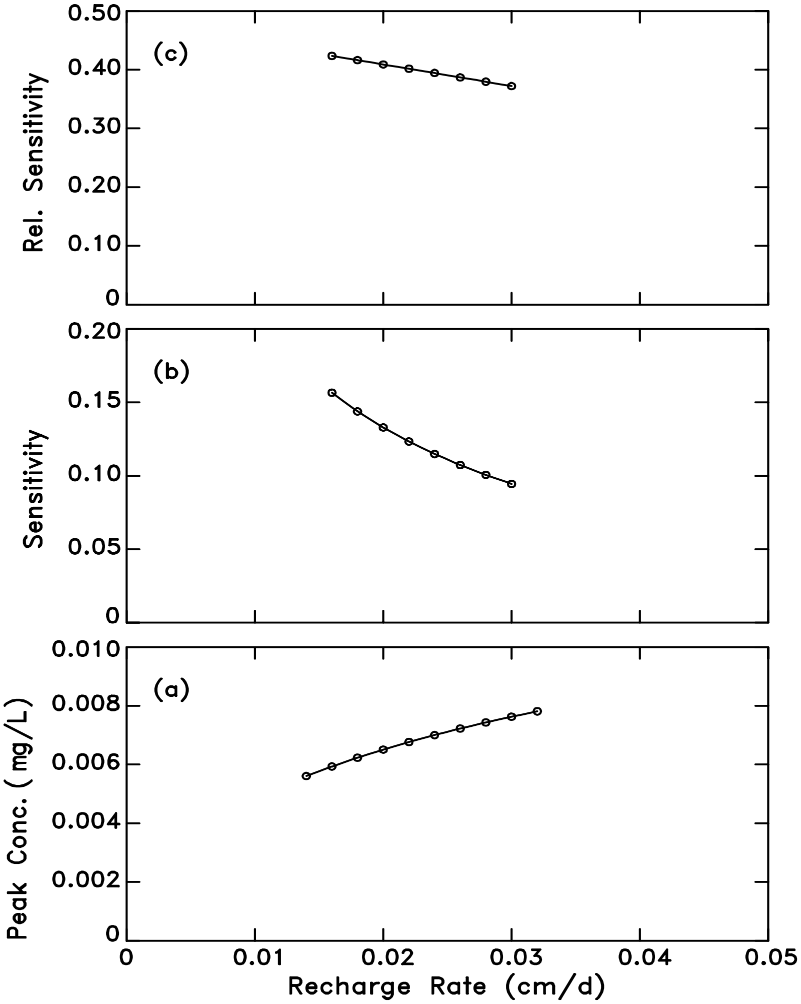

Fig. 2. Sensitivity and relative sensitivity of peak concentrations at the depth of 6 m to the CHAIN model.

moisture content condition. The main reason is because uniform water content and recharge rate are assumptions in the CHAIN model. In doing so, model comparison on sensitivity results can be made. In the latter case, such restriction does not exist.

The results given in Table IV indicate that

1. Similar magnitudes of relative sensitivity were observed using five models;
2. Initial water content, van Genuchten beta coefficient, β, and saturated water content are the most sensitive input parameters to predicted C_{peak};
3. Recharge rate, initial water content, van Genuchten beta coefficient, β, and saturated water content are the most sensitive input parameters to predicted T_{peak} and T_{MCL};

In other words, the advection process is the predominant process for the radionuclide ^{99}Tc transport in the hypothesized scenario. Note that the input parameters -- recharge rate, initial water content, van Genuchten beta coefficient, β, and saturated water content are the controlling parameters in water flow. As a result, they significantly influence the transport of ^{99}Tc. Conversely, sorption (^{99}Tc having a relatively small distribution coefficient, 0.007 cm^3/g) and dispersion are less dominant processes.

Table IV. Summary of Realtive Sensitivities for All Models, Outputs, and Input Parameters

Model Input Parameter	**C_{peak}**					**T_{peak}**					**T_{MCL}**				
	CHAIN	MULTIMED-DP 1.0	FECTUZ	CHAIN 2D	HYDRUS	CHAIN	MULTIMED-DP 1.0	FECTUZ	CHAIN 2D	HYDRUS	CHAIN	MULTIMED-DP 1.0	FECTUZ	CHAIN 2D	HYDRUS
Distribution coefficient	-0.06	-0.06	-0.05	-0.06	-0.06	+0.06	+0.06	+0.07	+0.06	+0.06	+0.07	+0.07	+0.08	+0.07	+0.07
Recharge rate	+0.40	+0.00	+0.00	+0.11	+0.12	-1.00	-1.00	-0.98	-1.00	-1.00	-0.89	-1.00	-1.00	-0.98	-0.98
Initial water content	-1.16	-0.80	-0.68	-1.03	-1.10	+0.80	+0.80	+0.81	+0.78	+0.88	+0.83	+0.88	+0.92	+0.84	+0.95
Bulk density	-0.17	-0.06	-0.05	-0.05	-0.05	+0.06	+0.06	+0.08	+0.07	+0.05	+0.08	+0.06	+0.07	+0.07	+0.07
Dispersion coefficient	-0.38	—	—	—	—	-0.02	—	—	—	—	-0.10	—	—	—	—
Dispersivity	—	-0.17	-0.36	-0.28	-0.28	—	-0.01	-0.02	-0.02	-0.02	—	-0.05	-0.09	-0.08	-0.07
Diffusion coef. in water	—	—	—	-0.10	-0.10	—	—	—	-0.01	-0.01	—	—	—	-0.03	-0.03
Saturated conductivity	—	+0.04	+0.00	+0.05	+0.05	—	-0.05	-0.00	-0.04	-0.04	—	-0.05	-0.00	-0.04	-0.04
Saturated water content	—	-0.60	-0.51	-0.66	-0.66	—	+0.58	+0.58	+0.57	+0.57	—	+0.64	+0.68	+0.64	+0.64
Resisual water content	—	-0.23	-0.20	-0.31	-0.27	—	+0.23	+0.22	+0.24	+0.23	—	+0.24	+0.26	+0.25	+0.24
van Genuchten alpha	—	+0.05	+0.06	+0.11	+0.14	—	-0.05	-0.09	-0.05	-0.05	—	-0.05	-0.09	-0.06	-0.05
van Genuchten beta	—	+0.98	+0.86	+1.30	+1.38	—	-0.96	-1.04	-1.00	-1.00	—	-1.06	-1.13	-1.04	-1.03

Comparison of Flow and Transport in the Base Scenario

The models, except the CHAIN model, have a module for water flow in the unsaturated zone and use the same van Genuchten model for soil water retention. For the base scenario, a uniform soil layer is assumed with a constant flux boundary at the top and a water table at a depth of 6 m. The soil moisture distributions using the HYDRUS, CHAIN 2D, FECTUZ and MULTIMED_DP models are shown in Figure 3. An error in the originally distributed MULTIMED_DP 1.0 code was detected (solid square points). The error arose from the incorrect use of the residual water content in the van Genuchten model for the soil water retention. When this error was corrected, the new water content results (solid triangle) give reasonably consistent results with the other three models.

Parallel to the comparison of simulating water flow in the unsaturated zone, the predicted BTCs were obtained using the base values for the CHAIN, HYDRUS, CHAIN 2D, FECTUZ, and MULTIMED_DP models. A constant and uniform soil moisture profile was assumed. The results are presented in Figure 4. It was found that

1. All five models give very similar BTCs except that the MULTIMED_DP and FECTUZ models predict higher peak concentrations of ^{99}Tc than the CHAIN, HYDRUS and CHAIN 2D models.
2. The differences in the predicted BTCs are mainly attributed to neglecting the molecular diffusion in the MULTIMED_DP and FECTUZ model. Both models assume molecular diffusion (the first right-hand term of equation 1) is not significant compared to mechanical dispersion (the second right-hand term of equation 2). Using the base values in Table III, a resulting dispersion coefficient of 1.01 cm^2/d is obtained for the CHAIN, HYDRUS and CHAIN 2D models and 0.68 cm^2/d for the MULTIMED_DP and FECTUZ models. When the dispersivity, D_L, of 4.53 cm (base value) was replaced by 6.53 cm, a value for the dispersion coefficient was obtained for the FECTUZ model (the first right-hand term is zero in equation 1). The resulting BTC using the FECTUZ model is reasonably close to those BTCs given by the CHAIN, HYDRUS and CHAIN 2D models. The same is true for the MULTIMED_DP model (not shown).
3. The selection of the proper inverse Laplace Transform algorithm for solving the transport equation is important in using MULTIMED_DP model. Both the Stehfest and DeHoog algorithm are available in the MULTIMED_DP model. A stable solution can be obtained using the DeHoog algorithm but not the Stehfest. The DeHoog algorithm is also used in the FECTUZ model.

The model comparison results also depict that similar predicted BTCs are expected to be obtained when the models were constructed for the same essential flow and transport processes. Minor differences may come from different numerical techniques or grid sizes.

The above analyses are conducted to compare the performance of the five models used for the SSL calculation at a hypothetical scenario. Each model has additional functions/capacities that are not addressed in this study. A detailed evaluation of these five models can be seen in U.S. EPA (14) and Chen et al. (25)

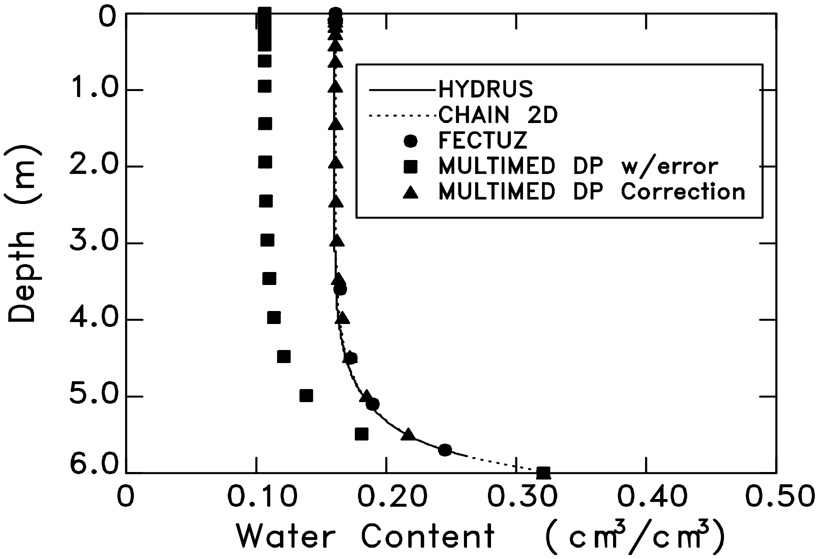

Fig. 3. Water content distributions predicted by the HYDRUS, CHAIN 2D, FECTUZ, and MULTIMED DP 1.0 models. Note that the water contents (ϑ) obtained from the originally distributed MULTIMED DP 1.0 code are in an error. The corrected code gives a consistent water content distribution (ϑ) with the other three models.

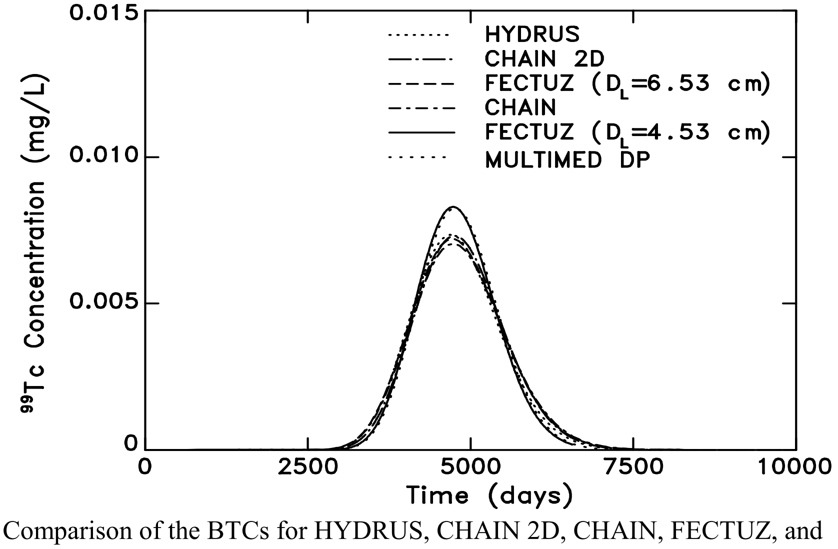

Fig. 4. Comparison of the BTCs for HYDRUS, CHAIN 2D, CHAIN, FECTUZ, and MULTIMED_DP models for the base values of the input parameters with the BTC for the FECTUZ model with the base value of D_L = 4.53 cm replaced by the value D_L = 6.53 cm.

CONCLUSION

The results of the model evaluation based on model capacity, sensitivity analysis and inter-model comparison for a hypothetical scenario at the Las Cruces Trench Site in New Mexico, indicate that:

1. Any of the five models is capable of simulating fate and transport of radionuclides in the unsaturated zone and can provide the time-varying concentrations of radionuclide in the leachate for the purpose of the SSL calculation;
2. Recharge rate, initial water content, van Genuchten beta coefficient, β, and saturated water content are the most sensitive input parameters to predicted C_{peak}, T_{peak} and T_{MCL};
3. The HYDRUS, CHAIN 2D, FECTUZ and MULTIMED_DP models, in general, provide consistent results in water flow simulation assuming the detected error in the MULTIPED_DP was corrected;
4. The CHAIN, HYDRUS, CHAIN 2D, FECTUZ and MULTIMED_DP models predicted very similar BTCs; The differences in the predicted peak concentrations of ^{99}Tc using different models are due to the differences in the implementation of the dispersion term. Neglecting a molecular diffusion in the FECTUZ and MULTIMED_DP model results in a lower dispersion coefficient and higher C_{peak}. When adjustment for dispersion coefficient is made, all five models predict similar BTCs for the SSL calculation.

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