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SOLUTE TRAVEL TIME IN THE VADOSE ZONE UNDER RWMC AT INEL

A Report Prepared By

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SOLUTE TRAVEL TIME IN THE VADOSE ZONE UNDER RWMC AT INEL

1. Introduction

Solute transport in the vadose zone under the Radioactive Waste Management Complex (RWMC) at the Idaho National Engineering Laboratory (INEL) is considered. The objective is to assess the relative importance of variables involved in modeling the travel time of a conservative solute from ground surface to water table.

The vadose zone under RWMC is composed of several layers of basalt flows interceded with sediment layers. The thickness of the layers varies with location. The hydraulic properties also vary. The extents of the variations are large, with standard deviations exceed mean in some instances. The vadose zone is idealized as composed of horizontal layers. Solute transport starts at the ground surface and moves vertically downwards to the water table. The perceived process is one-dimensional.

This study used VS2DT, a computer code developed by the U. S. Geological Survey, for simulating solute transport in variably saturated porous media.

2. Site Characteristics

At RMWC, a layer of surface sediments lies on top of alternating layers of basalt and sedimentary interbeds. The surface sediments layer is made of alluvial sand, loess, and lacustrine deposits and has a thickness varying from 0 to 25 ft (Barracolough, et al., 1976). The overall structure of the basalt and interbed layers can be found in Anderson and Lewis (1989). On the basis of borehole data, the structure of the subsurface was shown with several vertical sections. An example section is reproduced in Fig. 1 to show the general structure and the aerial extent. The shaded layers represent the surface layer and the interbeds at about 110 ft and 240 ft below the surface. The interbeds are made of clay, silt, sand and some gravel. The labels A, B, ... I denote major basalt groups. Significant property variations exist within each interbed as well as within each basalt group. Statistical characterization of the basalt can be found in Knuston, et al. (1990, 1992). Lee (1991) provided statistical data for permeability, porosity, and bulk density for both the surface sediments and the basalt groups.

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Fig. 1 Example ground section at RWMC of INEL (from Anderson and Lewis, 1989)

Layer Thicknesses, Porosities, and Saturated Hydraulic Conductivities

Lee (1991) established a set of layer demarcations by trial and error at 5 foot intervals to find the best statistical fit on permeability data. The resulting layering system reflects the stratigraphy indicated by Anderson and Lewis (1989). The mean and standard deviation of intrinsic permeability k and porosity n for each layer are also provided by Lee (1991). Table 1 summarizes the results. The saturated hydraulic conductivities K_s in Table 1 were converted from Lee's intrinsic permeabilities.

Table 1 Layer Thickness, Saturated Hydraulic Conductivity and Porosity

<u>Layer</u>	<u>Texture</u>	<u>Thickness</u> <u>(m)/(ft)</u>	<u>Porosity n</u> <u>(mean)/(std dev)</u>	<u>Saturated Conductivity K_s</u> <u>(m/day)</u>
1	Sediment	4.6/15	0.429/0.066	0.0657
2	Basalt A	21/70	0.171/no data	0.0552
3	Basalt B	7.6/25	0.152/0.069	0.0055
4	110 Interbed	6/20	0.346/0.086	0.0652
5	Basalt C	19.8/65	0.177/0.076	0.1208
6	Basalt D	14/45	0.165/0.060	0.0059
7	240 Interbed	9/30	0.425/0.060	0.2772
8	Basalt ?	78/255	no data	no data

The standard deviation of K_s , as indicated by Lee (1989) for layers 1 and 7 are 0.0669 and 2.863 m/day, respectively. It is thus anticipated that the standard deviations of K_s exceed the respective mean values. The total thickness of the layers is 160 m or 525 ft. At RWMC, no well was drilled deeper than 240 ft. Consequently, nothing is known about the material other than that it is probably basalt. Beneath the eighth layer is the ground water table.

Because of its substantial thickness, the eighth layer will have significant impact on the travel times. Simulations will be made by assuming the eighth layer to be basalt B, and separately, to be basalt C. These two basalt groups have very different hydraulic properties and thus may bracket the range of properties for the unknown layer.

Moisture Retention Curves and Relative Hydraulic Conductivities

Darcy's law is assumed to be applicable to all layers. The van Genuchten equation (van Genuchten 1980) is used to describe the moisture characteristic curves and the relative hydraulic conductivity curves.

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{[1 + (h/\alpha')^n]^m} \quad (1)$$

and

$$K = K_s \frac{(1 - (h/\alpha')^{n-1} [1 + (h/\alpha')^n]^{-m})^2}{[1 + (h/\alpha')^n]^{m/2}} \quad (2)$$

where θ = moisture content, θ_r = residue moisture content, θ_s = saturated moisture content, h = pressure head, negative when below atmospheric, α' , and n = curve fitting constants, and $m = 1 - 1/n$. Table 2 lists the values used. The data sources are Lee (1991) and Baca et al. (1992).

Table 2 Parameters used in the van Genuchten equations

Layer	Layer Texture	θ_s	θ_r	$\alpha'(-m)$	n
1	Surficial Sediment	0.429	0.1	0.822	1.360
2	Basalt A	0.171	0.015	0.260	1.474
3	Basalt B	0.152	0.015	0.260	1.474
4	110 Interbed	0.346	0.1	0.822	1.360
5	Basalt C	0.177	0.015	0.260	1.474
6	Basalt D	0.165	0.015	0.260	1.474
7	240 Interbed	0.425	0.1	0.822	1.360

The saturated moisture contents is assumed to be equal to the porosities shown in Table 1. The remaining data are adopted from Baca et al. (1992).

Fig. 2 shows the moisture contents (top) and the hydraulic conductivities (bottom) as functions of pressure head using the tabulated parameter values. Since θ_r and θ_s are physical (as

Fig. 2 Estimated moisture contents (top) and Hydraulic conductivities (bottom) of the layers

opposed to curve fitting) parameters, and since Lee (1991) has shown considerable variations in porosity (and hence θ_r), the sensitivity of the moisture retention and the hydraulic conductivity curves with θ_r and θ_s were explored. The curves in Fig. 3 were obtained by increasing θ_r 's by 10 percent. The curves in Fig. 4 were obtained by increasing θ_s 's by 10 percent. Comparing Figs. 3 and 4 with Fig. 2 shows that the moisture retention and the conductivity curves are sensitive to θ_r , but not to θ_s . The effect of porosity on solute travel time will be discussed later.

Net Infiltration Rate

In water travel-time predictions, Baca et al. (1992) assumed the infiltration rate as a random variable with a uniform distribution from 1.0 to 10.0 cm per year. This assumption is adopted. The corresponding mean infiltration rate is 0.00015 m/day, and the standard deviation of infiltration rate is 0.00007 m/day.

Hydrodynamic Dispersion of Solute

No data on dispersivity for the layers at RWMC were found. Domenico and Schwartz (1990) indicate that dispersivity increases with scale, and show some dispersivities and the corresponding migration distance for fractured rocks. For a migration distance of 160 m, the dispersivity is on the order of 10 m. Healy (1990) shows an example of solute transport in a 160 m column of saturated soil with a dispersivity of 10 m. A longitudinal dispersivity of 10 m is used. VS2DT treats the dispersivity as a constant. No estimation of transverse dispersivity is made as the solute transport process is one-dimensional.

Molecular diffusion is ignored in this study.

3. The Need for a Probabilistic Approach

In addressing nonuniform homogeneous ground water flows, Freeze (1975) demonstrated the importance of the standard deviation of the model parameters. Changing the standard deviations leads to different means of the output even when the mean values of the model parameters remain fixed. Because of the nonuniformity in model parameters, Freeze contented the validity of deterministic modeling using a single value for each of the model parameters.

At RWMC, significant variations in model parameters exist within each main group of

Fig. 3 Moisture contents and hydraulic conductivities when θ_r is increased by 10 percent

Fig. 4 Moisture contents and hydraulic conductivities when θ_s is increased by 10 percent

the basalt flows and interbeds. Deterministic modeling using representative or "conservative" model parameters may not be meaningful. Baca et al. (1992) used Monte Carlo simulations to predict the water travel time beneath RWMC. A probabilistic approach, such as the Monte Carlo method, provides information on the uncertainty of the model output.

In Monte Carlo simulations, multiple runs of the model are made. For each run, the model parameters are chosen from pertinent probability density functions. A distribution of the model output emerges as the number of runs increases. The process continues until the mean of the outputs converges. When the number of random model parameters is large, a very large number of runs are needed. The method becomes too CPU intensive to be practical.

4. Approximate Probabilistic Methods by Rosenblueth and Harr

Rosenblueth (1981) presented a point estimation method that avoids the shortcoming of the Monte Carlo method. Consider a function Y of a single random variable X . The probability density function of X is represented by two point estimates. Using the point estimates, the function Y is evaluated twice. Using the evaluated Y values and the point estimates of X , the mean and the standard deviation of Y can be estimated. The efficiency of the point estimation method is due to that fact that only two properly chosen evaluations of Y are needed while the Monte Carlo method requires numerous evaluations of Y .

The point estimates can be visualized by using an analogy between a probability density function and a similarly distributed vertical load on a rigid horizontal beam with two supports. Suppose that the mean x_m and the standard deviation σ_x of X are known. The two reactions p_+ acting at x_+ and p_- acting at x_- can be computed from

$$p_+ = p_- = 0.5 \quad (3)$$

$$x_+ = x_m + \sigma_x \quad (4)$$

$$x_- = x_m - \sigma_x \quad (5)$$

Let y_+ and y_- be the value of Y evaluated at x_+ and x_- respectively. Then the mean and the standard deviation of Y can be estimated from

$$y_m = p y_- + P y_+ \quad (6)$$

$$\sigma_y = \sqrt{p y_-^2 + P y_+^2} \quad (7)$$

Thus it is seen that by simply evaluating two properly chosen Y , the central tendency and the scatter of Y can be estimated. Details of this example with one random variable, including non-zero skew of X can be found in Harr (1987).

The point estimation method enables the mean and the standard deviation of the dependent variable be approximated from the mean, the standard deviation, and the skewness of the independent variables. If the independent variables are correlated, then correlation coefficients between the independent variables are needed in estimating the mean and the standard deviation of the dependent variable. An example of the Rosenblueth point estimation method to a problem with three independent random variables can be found in Harr (1989).

In the point estimation method, the probability distributions of the independent random variables do not have to be known as long as their first few moments are known. In addition, Rosenblueth (1981) shows, at least for simple functions, that the mean and the standard deviation of the dependent variable are not sensitive to the skewness of the independent variables. Thus, if there is no reason to suspect the variable to be skewed, the skewness coefficient can be assumed to be zero. Knowing the mean and the standard deviation of the random variables alone enables reasonable estimations for the central tendency and the scatter of the function or the dependent variable.

In vadose zone modeling, the means and the standard deviations of model parameters are often known but their distributions are not. In addition, some of the independent variables may be correlated. Thus, besides computational efficiency, the point estimation method offers some theoretical advantages over the Monte Carlo method. The latter requires the distributions of the random variables to be known and the independent variables not correlated.

For a function with m independent random variables, the mean and the standard deviation for each variable, and a set of $m(m - 1)/2$ correlation coefficients among the random variables

can be established. Based on the means, the standard deviations, and the correlation coefficients of the m random variables, 2^m estimates (reactions) of the m independent random variables and 2^m properly chosen evaluations of the function can be made. The estimates scale the evaluations according to the correlation coefficients. For large m , the Rosenblueth method can still be very CPU intensive as 2^m increases rapidly as m increases. In this study, ten independent random variables are used and $2^m = 1024$. Since, for some cases, one VS2DT run sometimes requires almost 20 hours on a 486/33 PC. The CPU requirement is still too intensive for the method to be practical for problems with a large m .

Yen and Guymon (1990) and Guymon and Yen (1990) used the point estimation method to model regional ground water flow. They suggested that, when m exceeds 9, the Monte Carlo method may be more efficient than the point estimation method since 2^9 becomes quite large.

Harr (1989) proposed an alternative point estimation method that reduces the number of function evaluations from 2^m , required by the Rosenblueth method, to $2m$. For this study and with ten independent random variables, only 20 VS2DT runs are needed. This is a very significant reduction in efforts and in CPU time, and makes approximate probabilistic estimation of solute arrival time feasible. The Harr's method is briefly reviewed next.

When there are m independent random variables, an m by m symmetrical correlation matrix can be established from data. The eigenvalues and eigenvectors of the correlation matrix can be readily computed. The correlation matrix can be rotated in the direction of the eigenvectors so that the standardized independent variables are not correlated. Harr (1989) demonstrated that the correlation matrix can be represented by a hypersphere (for $m > 3$) with a radius $m^{0.5}$. The hypersphere is centered at the mean point of the Cartesian coordinate system of the random variables. Each eigenvector emanates from the center and intersects the sphere at two points. Thus there are $2m$ intersections on the sphere. The coordinates of these $2m$ points replace those of the 2^m points in the Rosenblueth method. Because the standardized independent random variables are not correlated, the magnitude of the reactions in the Harr's method is simply $1/m$. The mean of the dependent variable is simply the arithmetic mean of the m evaluations. The variance of the dependent variable is the weighted sum of the variances of respective eigenvectors. For each eigenvector, the weighing factor equals the respective eigenvalue divided by m .

5. Applying the Harr's Method to Solute Travel Time at RWMC

Ten random variables were selected for estimating the solute travel time probabilistically. They are the hydraulic conductivities $K_1, K_2, K_3, K_4, K_5, K_6, K_7, K_8$ of the eight layers, the infiltration rate f , and the longitudinal dispersivity D_l . These random variables are assumed to be uncorrelated. It is further assumed that the sample sizes of the ten random variables are so large that the correlation coefficients are zero. Let $dK_1, dK_2, dK_3, dK_4, dK_5, dK_6, dK_7, dK_8, df$ and dD_l be the standard deviations of the perspective variables. In applying the Harr's method to estimating the solute travel time, twenty VS2DT runs were made at the points in the domain of the independent variables. These points are shown in Table 3.

Table 3 Locations of Point Estimates

Run	K_1	K_2	K_3	K_4	K_5	K_6	K_7	K_8	f	D_l
1	<i>max</i>	mean	mean	mean	mean	mean	mean	mean	mean	mean
2	<i>min</i>	mean	mean	mean	mean	mean	mean	mean	mean	mean
3	mean	<i>max</i>	mean	mean	mean	mean	mean	mean	mean	mean
4	mean	<i>min</i>	mean	mean	mean	mean	mean	mean	mean	mean
5	mean	mean	<i>max</i>	mean	mean	mean	mean	mean	mean	mean
6	mean	mean	<i>min</i>	mean	mean	mean	mean	mean	mean	mean
7	mean	mean	mean	<i>max</i>	mean	mean	mean	mean	mean	mean
8	mean	mean	mean	<i>min</i>	mean	mean	mean	mean	mean	mean
9	mean	mean	mean	mean	<i>max</i>	mean	mean	mean	mean	mean
10	mean	mean	mean	mean	<i>min</i>	mean	mean	mean	mean	mean
11	mean	mean	mean	mean	mean	<i>max</i>	mean	mean	mean	mean
12	mean	mean	mean	mean	mean	<i>min</i>	mean	mean	mean	mean
13	mean	mean	mean	mean	mean	mean	<i>max</i>	mean	mean	mean
14	mean	mean	mean	mean	mean	mean	<i>min</i>	mean	mean	mean
15	mean	mean	mean	mean	mean	mean	mean	<i>max</i>	mean	mean
16	mean	mean	mean	mean	mean	mean	mean	<i>min</i>	mean	mean
17	mean	mean	mean	mean	mean	mean	mean	mean	<i>max</i>	mean
18	mean	mean	mean	mean	mean	mean	mean	mean	<i>min</i>	mean
19	mean	mean	mean	mean	mean	mean	mean	mean	mean	<i>max</i>
20	mean	mean	mean	mean	mean	mean	mean	mean	mean	<i>min</i>

In Table 3 and for each variable, the max and min values are computed from

$$\text{max} = \text{mean} + \sqrt{10} \text{ standard deviation} \quad (8)$$

$$\text{min} = \text{mean} - \sqrt{10} \text{ standard deviation} \quad (9)$$

Eqs. 8 and 9 are simplified from the Harr's presentation that allows non-zero correlation coefficients (Harr, 1989).

In applying Eq. 9, the min values of the independent variables become negative because of large standard deviations. Consequently, the min values are nonphysical and VS2DT simulations become impossible. To overcome this difficulty, it is assumed that except for the infiltration rate, the standard deviations equal to 30 percent of their respective mean values. Because long term weather data can be constructed for the site (Baca et al. 1992), the uncertainty on infiltration rate may be less than those of other variables. Consequently, the standard deviation for the infiltration is assumed to be 15 percent of its mean value.

Obviously, the above assumptions on the standard deviations artificially reduce the scatter of the data on the independent variables. As a result, the mean and the standard deviation of the simulated solute travel times are affected. However, the assumptions serve the purpose of evaluating the sensitivity of solute travel time with respect to the independent variables.

Let y_i be the travel time for the i -th VS2DT run. The mean travel y_m time is simply

$$y_m = \frac{1}{20} \sum_{i=1}^{20} y_i \quad (10)$$

The standard deviation of the estimated travel time σ_y is the square root of the weighted sum of variances for the respective eigenvectors

$$\sigma_y = \sqrt{\frac{1}{10} \sum_{i=1}^{10} \sigma_i^2} \quad (11)$$

where

$$\sigma_i^2 = \left[\frac{y_{\max}^2 + y_{\min}^2}{2} - \left(\frac{y_{\max} + y_{\min}}{2} \right)^2 \right]_i \text{ for } i = 1, 2, \dots, 10 \quad (12)$$

In Eq. 12, $y_{\max}$ and $y_{\min}$ are the travel time evaluated from VS2DT using the max and min independent variables as indicated in Table 3.

Two sets of probabilistic simulations were made. In the first set, the eighth layer (with unknown properties) is assumed to have hydraulic properties identical to basalt B. In the second set, the eighth layer is assumed to have hydraulic properties identical to basalt C.

6. Modeling Considerations

Considerable effort was spent on determining the spatial grid spacing and the time-step size in using VS2DT. A variable spatial grid was used. The grid spacing was as small as 0.1 m at layer interfaces and as large as 15 m in the interior of the eighth layer where changes are expected to be more gradual. A total of 100 grid space was used, which is the maximum provided for by VS2DT.

For hydraulic computations, a maximum time-step of 0.25 year and a minimum time-step of 0.001 year are specified. VS2DT attempts to use the maximum step. When convergence is not achieved, the time step is reduced by half. If convergence is still not obtained after three reductions, the simulation is terminated. In solving the equation of solute mass conservation, the central differencing scheme for the advective component and the fully implicit temporal differencing options are used. The specified time-step was determined by comparing the simulated results using progressively smaller time-step size.

The input file using the mean values for all the properties and with the eighth layer treated as basalt C is included in the Appendix.

7. Hydraulic Considerations

A fixed flow is imposed at the surface to represent the infiltration. A fixed head of zero is imposed at the bottom of the eighth layer to represent the ground water table. An initial head of -5 m is imposed everywhere as the initial boundary condition. Simulation is then carried out for sufficiently long period until the flow leaving the bottom of the eighth layer (and discharging into the ground water) equation the infiltration. Thereafter, the water retained in the vadose zone is constant. This process is shown in Fig. 5. This figure also indicates that a good water mass balance was maintained by the code.

Fig. 7 shows the pressure head and the water content traces at selected locations in the vadose zone shown in Fig. 6. These results were obtained using the average value for all properties and assuming the eighth layer as basalt C. Initially, because the initial head of -5 m is not an equilibrium condition, the pressure heads and the water contents vary rapidly to seek an equilibrium. The oscillation at location H is believed to be numerical as the spatial grid size is the largest. Despite this oscillation, an equilibrium is reached. Since solute transport takes place in the period of steady state flow, the oscillation should not affect the results. Step changes occur later as the water, infiltrated from the surface, arrive at the various depths. Thereafter, a steady state flow of water prevails.

After the water content reaches an equilibrium, a conservative solute with a concentration of unity is added to the infiltration. The time of introducing the solute into the vadose zone is at 250 years. VS2DT simulates the solute movement towards the water table. The simulation stops when the solute concentration in the exiting flow becomes substantial. Fig. 8 shows the concentration variation at the bottom of each layer over time. Because of numerical dispersion associated with the solution procedure, the trace amount of solute that first appears at the water table, see Fig. 9, may not be physical, and thus should not be used to mark the arrival of the solute at the water table. Instead, arrival times using a criterion of 1 percent, ten percent, and at the instant of maximum rate of rise (RAR) of solute concentration at the water table are used.

The rationale for adding a solute to the infiltration only after a steady state flow is reached is explained next. Exploratory VS2DT simulations show that the change in the water content in the vadose zone significantly affects the travel time. Change of water content occurs when the initial water content in VS2DT simulation can not be sustained by the infiltration over

Fig. 5 Volumes of inflow, out flow, and storage indicating good water mass balance

Fig. 6 Layer schematic and locations of output sections

Fig. 7 Pressure and water content traces using mean properties - the eighth layer is basalt C

Fig. 8 Traces of solute concentration levels at the water table - the eighth layer is basalt C

Fig. 9 Logarithmic plot of Fig. 8 showing details at lower concentrations

the long run. Since the initial water content is not known a priori, a -5 m of pressure head (and the corresponding water content) is used to start the computation toward an equilibrium hydraulic condition. The water content of this equilibrium condition is then viewed at the "initial" water content for solute transport modeling.

8. Results

Approximate probabilistic estimates for the solute travel time are summarized in Tables 4 and 5 for the case where the eighth layer is basalt B. The mean solute travel time varies depending on the solute concentration at the exit flow. It varies from 392 years for the 1 percent solute concentration to first appear at the water table level, 564 years for the 10 percent solute concentration, and 980 years for the solute concentration to rise at a maximum rate. The former two can be viewed as the prelude due to hydrodynamic dispersion, while the latter signifies the arrival of the solute by advection to the water table.

The standard deviations for the three travel times are 88, 144, and 298 years. Recall that we have assumed a standard deviation of 30% of mean for all independent variables except the infiltration. For the latter, we assumed a standard deviation of 15%. The actual scatters in the data for the independent variables are greater than those assumed.

The sensitivity of solute travel time with respect to each of the independent variables are indicated by the percentage distribution of the variance associated with the respective variables. It is seen that the infiltration rate and the longitudinal dispersivity account for most of the variance. The hydraulic conductivities of the layers, combined as a whole, contribute about 3 percent or less to the overall variance.

Similar results were obtained for the case where the eighth layer is basalt C. The results are shown in Tables 6 and 7. Since basalt C has a much greater hydraulic conductivity than that of basalt B (0.2772 m/day versus 0.0055m/day), the travel times are shorter. They are 344, 476, and 879 years compared with 392, 564, and 980 years for the previous case. Fig. 10 shows the time traces of the solute concentration for the two cases.

The infiltration and longitudinal dispersivity again contributed most of the variance. The hydraulic conductivities, combined as a whole, contributed about seven percent or less of the overall variance. Of this meager contribution, most of it comes from the unknown eighth layer.

Fig. 10 Traces of solute concentration at the water table - comparing basalt B and basalt C as the eighth layer

Table 4 Solute travel times in years - Bottom layer is basalt B

<u>run</u>	<u>1%</u>	<u>10%</u>	<u>RAR</u>
1	371	517	889
2	374	520	896
3	367	512	877
4	397	549	906
5	369	514	881
6	380	527	901
7	370	515	894
8	381	528	905
9	367	513	874
10	388	533	895
11	369	514	886
12	380	529	893
13	366	516	890
14	385	536	896
15	348	500	874
16	438	593	957
17	231	333	616
18	754	1020	2076
19	316	456	707
20	487	1048	1891
mean	392	564	980

Table 5 Variances and their distributions - Bottom layer is basalt B

<u>variable</u>	<u>1%</u>	<u>distrib</u>	<u>10%</u>	<u>distrib</u>	<u>RAR</u>	<u>distrib</u>
K_1	2	0.01	2	0.00	12	0.00
K_2	225	0.29	342	0.16	210	0.02
K_3	30	0.04	42	0.02	100	0.01
K_4	30	0.04	42	0.02	30	0.00
K_5	110	0.14	100	0.05	110	0.01
K_6	30	0.04	56	0.03	12	0.00
K_7	90	0.12	100	0.05	9	0.00
K_8	2025	2.59	2162	1.03	1722	0.19
f	68382	87.41	117992	56.60	532900	60.17
D_1	7310	9.34	87616	42.03	350464	39.57
std dev	88		144		298	

Table 6 Solute travel times in years - Bottom layer is basalt C

<u>run</u>	<u>1%</u>	<u>10%</u>	<u>RAR</u>
1	331	463	845
2	334	467	855
3	327	460	846
4	350	485	872
5	332	464	850
6	340	473	858
7	332	464	838
8	357	493	876
9	328	459	841
10	365	503	873
11	328	459	841
12	354	488	883
13	332	463	844
14	340	474	847
15	321	447	833
16	409	541	917
17	203	296	501
18	563	796	1311
19	242	368	684
20	395	465	1372
<i>mean</i>	344	476	879

Table 7 Variances and their distributions - Bottom layer is basalt C

<u>variable</u>	<u>1%</u>	<u>distrib</u>	<u>10%</u>	<u>distrib</u>	<u>RAR</u>	<u>distrib</u>
K_1	2	0.01	4	0.006	25	0.01
K_2	132	0.32	156	0.229	169	0.06
K_3	16	0.04	20	0.030	16	0.01
K_4	156	0.38	210	0.308	361	0.13
K_5	342	0.83	484	0.710	256	0.09
K_6	169	0.41	210	0.308	441	0.16
K_7	16	0.04	30	0.044	2	0.00
K_8	1936	4.72	2209	3.240	1764	0.62
f	32400	78.98	62500	91.67	164025	57.47
D_1	5852	14.27	2352	3.45	118336	41.46
<i>std dev</i>	64		83		169	

These results indicate that, for solute travel time estimations, the infiltration rate and the longitudinal dispersivities of the vadose zone are, by far, the most important parameters. Efforts to reduce their scatter will significantly improve the travel time estimations.

The next most significant unknown is the eighth layer. The tables show that the difference in the travel times between the two cases (basalt B or basalt C as the eighth layer) exceeds the differences in the travel time caused by the scatter in each of the hydraulic conductivities of the top seven layers. This is because of the thickness of the eighth layer is about 49 percent of the total thickness of the vadose zone (see Table 1). Thus, for solute travel time estimations, further refinement of the hydraulic conductivity data for the top 7 layers will yield little improvement before gaining a better understanding of the properties of the eighth layer.

The effect of porosity on the solute travel time is estimated next. Instead of varying the porosity for individual layers, two simulations were made where the porosities, as a group, were increased and then decreased by 30 percent of the mean values. The computed solute concentration traces at the water table are shown in Figs. 11 and 12. To see how significant the differences are, Figs. 11 and 12 are compared with Figs. 13 and 14 where the solute concentration traces are shown for the point estimates with variations in the longitudinal dispersivity. It can be seen that the porosities significantly affect the solute travel time.

Consequently, another probabilistic estimation for the mean and the standard deviation of solute travel time are made. In this estimation, the infiltration rate f , the longitudinal dispersivity D_L , and the porosity n for all the layers as a group are treated as the three independent random variables. Consistent with the previous assumptions, the assumed standard deviations are 30 percent of the mean values for the longitudinal dispersivity and porosity, and 15 percent of mean for infiltration. The eighth layer is assumed to be basalt C. The mean hydraulic conductivities are used. The locations of the point estimates are shown in Table 8. The *max* and *min* values are computed according to Eqs. 8 and 9. The results are summarized in Tables 9 and 10. It is seen that the mean travel times are comparable to those shown in Table 6 while the standard deviations are about twice as those shown in Table 7. The contributions to the total variance are approximately 75 percent for porosity, 20 percent for infiltration rate, and 5 percent for longitudinal dispersivity.

Fig. 11 Traces of solute concentration at the water table - Comparing results with 30 percent increase and 30 percent decrease in group porosity - The eighth layer is basalt B

Fig. 12 Traces of solute concentration at the water table - Comparing results with 30 percent increase and 30 percent decrease in group porosity - The eighth layer is basalt C

Fig. 13 Traces of solute concentration at the water table - Comparing results with 30 percent increase and 30 percent decrease in dispersivity - The eighth layer is basalt B

Fig. 14 Traces of solute concentration at the water table - Comparing results with 30 percent increase and 30 percent decrease in dispersivity - The eighth layer is basalt C

Table 8 Location of point estimates - 3 random variable case

<u>run</u>	<u>f</u>	<u>D_i</u>	<u>n</u>
1	<i>max</i>	mean	mean
2	<i>min</i>	mean	mean
3	mean	<i>max</i>	mean
4	mean	<i>min</i>	mean
5	mean	mean	<i>max</i>
6	mean	mean	<i>min</i>

Table 9 Solute travel time (years) using 3 random Variables - Bottom layer is basalt C

<u>run</u>	<u>1%</u>	<u>10%</u>	<u>RAR</u>
1	249	356	635
2	456	627	1152
3	272	401	747
4	412	537	855
5	544	738	1286
6	122	190	317
<i>mean</i>	343	475	832

Table 10 Variances and their distributions using 3 random variables-Bottom layer is basalt C

<u>variable</u>	<u>1%</u>	<u>distrib</u>	<u>10%</u>	<u>distrib</u>	<u>RAR</u>	<u>distrib</u>
<i>f</i>	10712	18	18496	19	66822	22
<i>D_i</i>	4900	8	4624	5	2916	1
<i>n</i>	44521	74	75076	76	234740	77
<i>std dev</i>	142		181		319	

Approximate probabilistic estimates of the solute travel time with parameter standard variations other than those used can be easily made using Figs. 15, 16, and 17. These figures are discussed in the next section.

9. Validity of the Harr's Method

One way to check the validity the Harr's approximate probabilistic estimates is to repeat the problem using the Monte Carlo simulations. This was not attempted because computer resources needed to carry out a large number of VS2DT simulations were not available. The validity of the Harr's estimates for solute travel time can be only inferred indirectly.

Yen and Guymon (1990) compared the Rosenbuleth's point estimation method with the Monte Carlo method in determining water table levels of a regional aquifer. They concluded that the point estimation method is only generally valid for linear problems where the coefficient of variation of uncertain parameters is small. Further, the method may be applied to slightly nonlinear problems with good results if coefficients of variation are small. Since the Harr's method is an extension of the Rosenblueth's method, Yen and Guymon's conclusion may be applicable to the Harr's method. Therefore, the degree of linearity of the function is an issue.

Shown in Figs. 15, 16, and 17 are the travel time estimates when the infiltration rate, the longitudinal dispersivity, and the group porosity are varied separately. Each figure shows three lines that correspond to the 1 percent, 10 percent, and the maximum rate of rise criteria of solute arrival. The travel time appears to be an approximately linear function of the infiltration rate for all the three criteria. The travel time also appears to be an approximately linear function of longitudinal dispersivity and group porosity for the 1 and 10 percent arrival criteria. For the criterion of maximum rate of rise, linearity of travel time with dispersivity and group porosity becomes questionable.

On the basis of the linearity demonstrated, it is concluded that the Harr's method yields acceptable approximations for the travel time provided the solute concentration arrived at the water table is less than 10 percent.

10. Summary and Conclusions

The relative importance of variables in estimating travel times of a conservative solute from ground surface to water table in the vadose zone below RWMC at INEL are investigated. The vadose zone is viewed as an eight-layer system with one-dimensional vertical flow. The independent random variables considered are the infiltration rate, the hydraulic conductivities of the layers, the longitudinal dispersivity, and the porosity of the layers as a group. The 255 ft

Fig. 15 Variation of solute travel time with infiltration rate

Fig. 16 Variation of solute travel time with longitudinal dispersivity

Fig. 17 Variation of solute travel time with group porosity

unknown layer directly above the water table is treated as basalt B and separately, as basalt C. It is hoped that the different properties of basalt B and basalt C bracket the properties of the unknown layer.

Because of lacking of some data, and because of large standard deviations in the available data, there are significant uncertainties in the variables themselves. Consequently, probabilistic estimates are needed. The approximate probabilistic method by Harr in conjunction with the VS2DT code by the US Geological Survey are used in this study. In using the VS2DT code, it is implicitly assumed that fractured basalt layers can be equivalenced to a homogeneous porous medium.

The Harr's method requires some solute travel times be evaluated at points where the values of independent variables are at predetermined amounts below their mean values. Because of the large standard deviations, the required variable values become negative and thus are not physically possible in VS2DT simulations. Consequently, all standard deviations except that for the infiltration rate are assumed to be 30 percent of the respective mean values. The standard deviation of the infiltration rate is assumed at 15 percent of its mean. Separately, inadequate data prevents the correlation coefficients, if non zero, from being established. Out of necessity, this study assumes that the independent random variables are uncorrelated.

With the assumptions stated above, the ranking of variables, accordance to their contribution to the variance in the solute travel times, is: (1) group porosity (75 percent), (2) infiltration rate (20 percent), (3) longitudinal dispersivity (5 percent), and (4) hydraulic conductivities (5 percent). The percentages indicated are approximate and only indicate the relative importance of the variables.

The Harr's method is demonstrated in detail for uncorrelated independent random variables. This method only requires $2m$ evaluations of the function or the dependent variable for a problem with m independent random variables. Due to the large number of independent variables required in modeling the transport process in the vadose zone, the Harr's method offers a decidedly important advantage in efficiency over the Monte Carlo method and the Rosenblueth's point estimation method. The validity of Harr's method in estimating solute travel time under steady hydraulic conditions has been discussed in terms of the linearity of the travel time regarding porosity, longitudinal dispersivity, and infiltration rate.

11. Recommendations

Further works to improve solute travel time estimations are suggested in three areas.

Data

The scatter in the porosity data needs to be reduced. This may be achieved by re-establishing the layering structure using Lee's method of layer demarcation (Lee 1991) but using porosity instead of permeability as the criterion for best fit.

Statistical estimations on the porosity for the 255 ft unknown layer directly above the water table need to be made.

Correlation coefficients or lack of correlation among independent variables need be investigated.

Long term net infiltration rate needs to be established.

Data on decay and adsorption for the various solutes at the site should, if not already, be established.

Data on longitudinal dispersivity as a function of solute travel distance is needed

Hydraulic and Solute Transport Model

The single and constant value allowed for longitudinal dispersivity in VS2DT may not be realistic. Code modifications to allow for dispersivity increase with scale are needed.

The solute travel time estimations should be repeated where the porosities for the eight layers should be treated as separate random variables.

VS2DT is developed for porous media. When VS2DT is applied to the RWMC at INEL, it is implicitly assumed that the fractured basalt mass is hydraulically equivalent to a porous medium. In the future, if data describing the interconnecting fractures in the basalt flows emerge, other models that handle fractured rocks should be considered

Probabilistic Methods

The Harr's method offers a practical way to obtain probabilistic estimates. This method needs to be verified against the Monte Carlo method directly for problems with uncorrelated independent variables. A method to quantify the error of the Harr's method, such as using the linearity of the function as an index, needs to be established.

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13. Appendix - Sample data file for VS2DT (2 pages)

Input file for VS2DT Program:

One-Dimensional Infiltration (8 layers)

1750 0 0	A2
M YEAR KG	A3
4 100	A4
2 50000	A5
FTT	A6
TTF	A6A
TFTTF	A7
TFTFF	A8
0 .1	A9
1. 1. 1. 1.	A10
0 .1	A11
1. 2. 8. 12. 12. 8. 2. 1.	
1. 2. 4. 8. 12. 30. 48. 48. 30. 12. 8. 4. 2. 1.	
1. 2. 4. 8. 23. 23. 8. 4. 2. 1.	
1. 2. 4. 8. 15. 15. 8. 4. 2. 1.	
1. 2. 4. 8. 12. 30. 42. 42. 30. 12. 8. 4. 2. 1.	
1. 2. 4. 8. 12. 20. 23. 23. 20. 12. 8. 4. 2. 1.	
1. 2. 4. 8. 12. 18. 18. 12. 8. 4. 2. 1.	
1. 2. 4. 8. 20. 40. 60. 100. 155. 155. 100. 60. 40. 20.	
8. 4. 2. 1.	A12
7	A13
50 100 150 180 300 400 500	A14
6	A15
22 2 42 2 82 2 90 2 97 2 99 2	A16
2	A17
13 16	A18
.001 0.4 0.0 0.001	B1
5 200	B3
T	B4
8 6 6	B5
1	B6
1 23.9805 .0 .429 -.8224 .1 1.36	B7
10. 0. 0. 0. 0. 0.	B7A
2	B6
1 20.148 .0 .171 -.2604 .015 1.474	B7
10. 0. 0. 0. 0. 0.	B7A
3	B6
1 2.0075 .0 .152 -.2604 .015 1.474	B7
10. 0. 0. 0. 0. 0.	B7A
4	B6
1 23.798 .0 .346 -.8224 .1 1.36	B7
10. 0. 0. 0. 0. 0.	B7A
5	B6
1 44.092 .0 .177 -.2604 .015 1.474	B7
10. 0. 0. 0. 0. 0.	B7A
6	B6
1 2.1535 .0 .165 -.2604 .015 1.474	B7
10. 0. 0. 0. 0. 0.	B7A
7	B6
1 101.178 .0 .425 -.8224 .1 1.36	B7
10. 0. 0. 0. 0. 0.	B7A

8
 1 44.092 0 .177 -.2604 .015 1.474
 10. 0. 0. 0. 0. 0.
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 1 4 22 2
 1 4 32 3
 1 4 42 4
 1 4 56 5
 1 4 70 6
 1 4 82 7
 1 4 100 8
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