

**A Simplified Procedure for Performing Solute Transport Sensitivity
Analyses**

By

Eric Harmsen and David Cercone

© 1996

ABSTRACT

A Simplified Procedure for Performing Solute Transport Sensitivity Analyses

by

Eric Harmsen and David Cercone

Sensitivity analyses are performed in simulation modeling to evaluate the uncertainty of a model result (e.g., constituent cleanup time) based on uncertainty in a model input parameter (e.g., effective porosity). Typically a sensitivity analysis is performed by adjusting the model parameters one at a time and observing the response of the model to changes in each parameter. Another approach adjusts all model parameters simultaneously, each parameter taking on a randomly selected value from its respective probability distribution, as in the case of the Monte Carlo procedure. This approach has the advantage of evaluating the influence of parameter-interaction but the disadvantage of requiring in some cases hundreds of complete runs.

This paper describes a simplified procedure for performing a sensitivity analysis which is applicable to a variety of contaminant transport problems. The procedure is amenable to changing parameters one at a time, or simultaneously as in a Monte Carlo simulation. The theoretical basis for the new method, its development and application to an actual field problem are presented. The new method is validated with data from a formal sensitivity analysis performed using a three-dimensional, numerical, solute transport model. For the test case, the simplified method showed excellent agreement with the numerical model. The cost savings by using the simplified method in this case was estimated at greater than \$10,000. Other benefits of using the new method as well as potential limitations are also discussed.

A SIMPLIFIED PROCEDURE FOR PERFORMING SENSATIVITY ANALYSES

INTRODUCTION

When selecting a groundwater remediation strategy, cleanup time is often a criteria for judging among alternatives; shorter cleanup times being viewed more favorably than longer cleanup times. Most groundwater modelers recognize that certain parameters have a proportional effect on cleanup time. For instance, doubling the retardation factor has the effect of doubling the cleanup time. Unfortunately, use of this heuristic knowledge has not been applied systematically by most modelers. This paper describes a procedure for estimating the cleanup time for a groundwater constituent plume based on linear proportioning, herein referred to as the Proportional Cleanup Time Method (PCTM). Because PCTM requires an initial estimate of cleanup time using a standard procedure (e.g., a numerical solute transport model), its greatest value will be realized when applied to sensitivity or uncertainty analyses. PCTM is quite robust, and can account for relatively complex transport conditions. The procedure is amenable to changing parameters one at a time, or simultaneously as in a Monte Carlo simulation, and can be implemented within a spreadsheet environment. The theoretical basis for PCTM and its development are presented below.

The procedure is validated with a three-dimensional analytical solution and data from two formal sensitivity analyses conducted at a U.S. Government-Owned Facility in Michigan. One of the sites analyzed utilized a one-dimensional numerical solute transport model, the other a three-dimensional numerical solute transport model. For the test cases considered, PCTM showed excellent agreement with the model-calculated cleanup times. The cost savings by using PCTM in lieu of the three-dimensional numerical model was estimated at greater than \$10,000. Other benefits of using PCTM as well as potential limitations are also discussed.

METHOD DEVELOPMENT

In this section the simple PCTM formulae will be derived for estimating the cleanup time of a groundwater contaminant plume. It is assumed that a relatively sophisticated method has been used to obtain the cleanup time under average site conditions, and that this cleanup time is available for use as input into the method. This being the case, PCTM may then be used in lieu of the more expensive sophisticated model to conduct the sensitivity or uncertainty analysis. We shall begin by using a modified form of the advection dispersion equation presented by Freeze and Cherry (1979):

$$R \frac{\partial C}{\partial t} = D_l (\frac{\partial^2 C}{\partial S_l^2}) + D_t (\frac{\partial^2 C}{\partial S_t^2}) + D_v (\frac{\partial^2 C}{\partial S_v^2}) - v_l \frac{\partial C}{\partial S_l} \quad (1)$$

where

R = retardation factor

C = constituent concentration

t = time

S_l = curvilinear coordinate direction directed along the flowline

S_l = coordinate direction directed orthogonal to S_l in the horizontal plane

S_v = coordinate direction directed orthogonal to S_l in the vertical plane

D_l = longitudinal dispersion coefficient = $v_l * \alpha_l$

D_t = transverse lateral dispersion coefficient = $v_l * \alpha_t$

D_v = vertical dispersion coefficient = $v_l * \alpha_v$

α_l = longitudinal dispersivity

α_t = transverse lateral dispersivity

α_v = vertical dispersivity

v_l = average linear velocity = q_l / ϕ along the coordinate direction S_l

q_l = Darcy velocity = $K i$

K = hydraulic conductivity

i = regional hydraulic gradient

ϕ = effective porosity

Equation 1 assumes that solute is being transported along a curvilinear flowline. Solute transport due to advection occurs along the coordinate S_l only, while dispersion occurs in the directions S_t , S_v . The definition of the dispersion coefficients given above assumes that diffusion is small compared to dispersion and therefore can be ignored. The retardation factor can be defined in two ways:

$$R = 1 + (\rho_b f_{OC} K_{OC}) / \phi, \text{ and} \quad (2)$$

$$R = v_l / v_c \quad (3)$$

where

K_{OC} = equilibrium partition coefficient

f_{OC} = organic carbon fraction

ρ_b = bulk density

v_c = average solute velocity

Combining equation 3 with equation 1 and rearranging yields

$$\partial t = \partial C / v_c [\alpha_l (\partial^2 C / \partial S_l^2) + \alpha_t (\partial^2 C / \partial S_t^2) + \alpha_v (\partial^2 C / \partial S_v^2) - \partial C / \partial S_l] \quad (4)$$

Equation 4 indicates that ∂t is proportional to $1 / v_c$, or in terms of the fundamental transport parameters K , i , ϕ , ρ_b , f_{OC} and K_{OC} :

$$1/v_c = R/v_l = [\phi + \rho_b f_{oc} K_{oc}] / K_i \quad (5)$$

For convenience we shall make the following definitions:

$$A = \partial C / [\alpha_l (\partial^2 C / \partial S_l^2) + \alpha_f (\partial^2 C / \partial S_f^2) + \alpha_v (\partial^2 C / \partial S_v^2) - \partial C / \partial S_l] \quad (6)$$

$$\partial t_1 = 1/v_{c1} A \quad (7)$$

$$\partial t_2 = 1/v_{c2} A \quad (8)$$

In the equations listed above, the subscripts 1 and 2 simply represent two different solutions, one for $v_c = v_{c1}$ and the other for $v_c = v_{c2}$. Dividing equation 8 by equation 7 yields:

$$dt_2 = (v_{c1} / v_{c2}) dt_1 \quad (9)$$

By eliminating A, equation 9 is greatly simplified, and is reduced from a partial to an ordinary differential equation. Integrating the left hand side of equation 9 from 0 to T_2 and the right hand side from 0 to T_1 yields:

$$T_2 = v_{c1} T_1 / v_{c2} \quad (10a)$$

$$= (T_1 v_l R_2) / v_l R_1 \quad (10b)$$

$$= T_1 K_1 i_1 (\phi_2 + \rho_{b2} K_{oc2} f_{oc2}) / K_2 i_2 (\phi_1 + \rho_{b1} K_{oc1} f_{oc1}) \quad (10c)$$

Equations 10a, 10b and 10c are different forms of the PCTM equations. Equation 10a indicates that if we know the cleanup time for condition 1, and the values of the average solute velocity for the two conditions, we can estimate the cleanup time for condition 2. This result is potentially useful for aiding in the performance of a solute transport model sensitivity or uncertainty analysis. Note that having T_2 expressed as Equations 10b and 10c is useful since the sensitivity or uncertainty analysis may consider variations in R and v_l directly, or may wish to consider the more fundamental parameters K, i, ϕ , ρ_b , f_{oc} and K_{oc} . It should be noted that the product $f_{oc} K_{oc}$ should be replaced by the distribution coefficient, K_d , in the case of an inorganic solute.

METHOD VALIDATION

In this section we shall evaluate the accuracy of PCTM for estimating cleanup time by comparing it with several other more sophisticated methods. In Test No. 1, PCTM (equation 10a) is compared to a three-dimensional analytical solute transport solution. The purpose of the test is to compare PCTM to an exact solution. Test No. 2 involves data from two numerical modeling sensitivity analysis studies. The purpose of this test is not only to verify the accuracy of the

method but to illustrate that the method can be used to solve relatively complex practical problems.

Test No. 1

An expanded form of the three-dimensional analytical solution to the advection-dispersion equation presented by Freeze and Cherry (1979) will be used:

$$C = \frac{M_0}{8 \cdot (\pi \cdot t)^{\frac{3}{2}} \cdot \sqrt{\alpha_L \cdot \alpha_T \cdot \alpha_V \cdot v_c^3}} \cdot \exp \left[-\frac{(x - v_c \cdot t)^2}{4 \cdot \alpha_L \cdot v_c \cdot t} - \frac{y^2}{4 \cdot \alpha_T \cdot v_c \cdot t} - \frac{z^2}{4 \cdot \alpha_V \cdot v_c \cdot t} \right] \quad (11)$$

In equation 11, x , y and z are spatial coordinates, M_0 is the initial mass of solute, α_x , α_y and α_z are the dispersivities in the x , y and z directions, respectively, and all other symbols have been previously defined. Diffusion is assumed to be small relative to dispersion and therefore can be ignored. Equation 11 assumes that a mass of solute M_0 is instantaneously released into the aquifer at $x = y = z = 0$ at $t = 0$. Groundwater flow is one-dimensional in the x direction and is steady-state. It is assumed that the solute exits the aquifer as it encounters a stream at the right hand boundary located at $x = 244$ m. The assumed dispersivities are: $\alpha_x = 9.14$ m, $\alpha_y = 0.91$ m and $\alpha_z = 0.09$ m.

The objective of this test is to calculate the cleanup times (T_1 and T_2) using the exact solution (equation 11) for two different conditions (i.e., for v_{c1} and v_{c2}). Using T_1 from the exact solution and the values of v_{c1} and v_{c2} , T_2 will be calculated using equation 10a and compared with the T_2 value calculated using equation 11. Table 1 lists the input used in the test problem, and the cleanup times (T_1 and T_2) as estimated by equations 11 and 10a. In Case 1, the cleanup criteria (CUC) is $2 \mu\text{g/L}$ and according to equation 11 the peak of the concentration curve drops below the CUC before reaching the stream (Figure 1). In Case 2, the CUC is $1 \mu\text{g/L}$ and the cleanup criteria is met at the stream some time after the peak of the concentration distribution reached the stream (Figure 1). Table 1 indicates exact agreement in the T_2 estimates calculated with equations 11 and 10a.

Table 1. Input Data and Results of Example Problem.

Case 1

$CUC = 2 \mu\text{g/L}$

$M_o = 0.1 \text{ kg}$

$v_{c1} = 0.15 \text{ m/day}$

$T_1 = 772 \text{ days}$ (Equation 11)

$v_{c2} = 0.52 \text{ m/day}$

$T_2 = 227 \text{ days}$ (Equation 11)

$T_2 = v_{c1} T_1 / v_{c2} = (0.15 \text{ m/day} * 772 \text{ days}) / 0.52 \text{ m/day} = 227 \text{ days}$ (Equation 10a)

Case 2

$CUC = 1 \mu\text{g/L}$

$M_o = 1 \text{ kg}$

$v_{c1} = 0.15 \text{ m/day}$

$T_1 = 2465 \text{ days}$

(Equation 11)

$v_{c2} = 0.52 \text{ m/day}$

$T_2 = 725 \text{ days}$ (Equation 11)

$T_2 = v_{c1} T_1 / v_{c2} = (0.15 \text{ m/day} * 2465 \text{ days}) / 0.52 \text{ /day} = 725 \text{ days}$ (Equation 10a)

Test No. 2

Obviously the proposed method would have little value if only one or two cleanup time estimates were desired as in the case of Test No. 1. In Test 2, the method is used to perform two sensitivity analyses involving a large number of cleanup time estimates. The sensitivity analyses were previously performed using two numerical models and these results will be compared to the PCTM results. The models were developed for the purpose of comparing remedial alternatives. The numerical studies were conducted at a U.S. Government-Owned Facility in Michigan.

Site Background

During the early 1960s organic solvents and petroleum products were released to the subsurface at two locations at the facility. At Location 1, a three-dimensional, numerical groundwater flow and solute transport analysis was performed for trichloroethylene (TCE) and tetrachloroethylene (PCE). At Location 2, TCE, benzene and m-xylene were modeled using a one-dimensional, numerical solute transport model.

At the facility, the shallow unconfined aquifer consists of medium to coarse grained sand, with some gravel and silt stringers. Saturated thickness varies between 12.2 and 15.2 meters. The shallow aquifer is underlain by a thick layer of clay averaging 30 m in thickness. Groundwater discharges to a lake located east of the site and a river located south of the site. Seepage velocities across the site ranged from 0.27 to 0.73 m/day. Typical hydraulic gradients vary from 0.001 to 0.005 m/m. Vertical flow was generally downward, however, upward gradients were observed within a few hundred feet of the lake. Differences in groundwater elevations in well

pairs ranged from zero to 0.1 m. Vertical gradients were observed near pumping wells and near discharge areas. From aquifer pumping tests, transmissivity of the shallow aquifer ranged from 465 to 1,860 m²/day; horizontal hydraulic conductivity ranged from 23 to 94.5 m/day, and specific yield was estimated to be 0.20. Estimated horizontal hydraulic conductivity of shallow wells tended to be greater than those estimated from deeper wells.

Location 1 Model Information

- Three-dimensional groundwater flow model, MODFLOW (McDonald and Harbaugh, 1984)
- Three-dimensional solute transport model, MT3D (Zheng, 1992)
- Constituents: TCE and PCE
- Four remedial alternatives: no action, groundwater extraction (one pumping well), groundwater extraction (two pumping wells), and air sparging (sparge curtain located along facility boundary). (Note, air sparging was simulated by setting the solute transport model cells along the sparge curtain to constant zero concentration cells. Consequently, constituents located upgradient of the curtain were prevented from passing through the curtain into the downgradient area)
- TCE cleanup time was calculated for three cleanup levels: 7.7 µg/L, 5.0 µg/L and 2.2 µg/L
- PCE cleanup time was calculated for two cleanup levels: 5.0 µg/L and 1 µg/L
- Condition 1 parameter values: $\alpha_{l1} = 3$ m, $\alpha_{t1} = \alpha_{l1} / 10$, $\alpha_{v1} = \alpha_{l1} / 200$, $K_1 = 36.6$ m/day, $i_1 = 0.0033$, $\phi_1 = 0.30$, $\rho_{b1} = 1.55$ g/cm³, $f_{oc1} = 0.001$, $K_{oc1} = 165$ cm³/gm (TCE), and $K_{oc1} = 364$ cm³/gm (PCE).
- Conditions 2 parameter variations: retardation factor (doubled and halved), effective porosity (0.18 and 0.43) and hydraulic gradient (+0.33 m and -0.33 m lake elevation).

Location 2 Model Information

- One-dimensional groundwater flow and solute transport
- Model: one-dimensional finite-difference method
- Constituents: benzene, TCE and m-xylene
- Five remedial alternatives: no action, limited action (current pumping), enhanced groundwater extraction, hot air sparging within upgradient portion of plumes, hot-spot removal (Note, hot air sparging and hot-spot removal were not actually simulated, initial concentrations were simply set to zero in these area.)
- Cleanup time was based on the following cleanup criteria: benzene and TCE, 5.0 µg/L; m-xylene, 280 µg/L.
- Condition 1 parameter values: $\alpha_{l1} = 30.5$ m, $\phi_1 = 0.25$, $\rho_{b1} = 1.55$ g/cm³, $f_{oc1} = 0.001$, $K_{oc1} = 100$ cm³/gm (benzene), $K_{oc1} = 140$ cm³/gm (TCE), and $K_{oc1} = 1580$ cm³/gm (m-xylene).
- Condition 2 parameter variations: retardation factor (doubled and halved) and average linear groundwater velocity (doubled and halved).

Figure 2 compares PCTM and model-calculated cleanup times. The figure indicates excellent agreement between the methods. The calculated regression coefficient (r^2) for the data presented in Figure 2 was 0.9992 (sample size = 180). The results presented in Figure 2 suggest that PCTM is quite robust and will potentially work well under a variety of realistic conditions. For example, Location 1 included multiple pumping wells, highly nonuniform, three-dimensional, initial concentration distributions, and stagnation points.

It is important to keep in mind that each of the data points in Figure 2 corresponding with the horizontal axis were obtained by using a numerical model. In addition to running the model, the analysis involved post processing the data in order to extract the cleanup times from the output. In the case of the Location 1 numerical model, the post-processing presented a significant quality control challenge. The Location 1 sensitivity analysis was accomplished in approximately one week using four individuals. Use of PCTM to obtain essentially identical results required one person less than four hours. The cost savings to the client in this case would have been greater than \$10,000.

METHOD LIMITATIONS

Equation 10a, 10b and 10c are not functions of dispersivity. Unlike R and v_l , dispersivity has a complex relationship with the cleanup time. Figure 3 shows the results of cleanup time as calculated by a one-dimensional transport model (Fischer, et al., 1979, Equ. 2.30). Cleanup time is shown for two distances (L) between the origin and the point of compliance, and for six values of the ratio C_0/CUC . A $C_0/CUC = 1000$ means that the initial solute concentration is 1000 times higher than the cleanup criteria (e.g, $C_0 = 1000 \mu\text{g/L}$ and $CUC = 1 \mu\text{g/L}$). The conditions modeled include $v_l = 0.34 \text{ m/day}$, $R = 1$, and a slug source of concentration C_0 extending from $x = 0$ to $x = 91 \text{ m}$.

Figure 3 shows that cleanup time is highly dependent on L and the ratio C_0/CUC . For the conditions modeled, increases in dispersivity caused the cleanup time to increase in some cases and decrease in others. The complex relationship shown in the figure can be explained partly in terms of where along the travel path the concentration drops below the CUC. For the $L = 3,000 \text{ m}$ case, for example, all cleanup times below 40 years resulted from the peak concentration dropping below the CUC value prior to reaching the point of compliance, whereas, for cleanup times greater than 40 years, the CUC was achieved at the point of compliance within the tail of the plume.

It is recommended that if PCTM is used, that the solute transport model be used to estimate cleanup time for several values of dispersivity (e.g, low, baseline and high values). Then using PCTM, a sensitivity or uncertainty analysis be performed on the parameters K , i , ϕ , ρ_b , f_{OC} and K_{OC} using the T_1 associated with each different value of dispersivity evaluated.

Other potential limitations of PCTM are listed below:

- The validation of PCTM presented above should not be interpreted to mean that PCTM will work under all conditions. The method will not provide reliable results for conditions which violate the assumptions upon which the method is based. Conditions under which PCTM may not provide reliable results include: highly heterogeneous or anisotropic aquifers conditions, sites where residual free product is present, problems involving large temporal and/or spatial variations in the groundwater velocity, or problems involving biodegradation, radioactive decay and/or coupled multi-species transport.
- PCTM is limited to linear equilibrium partitioning between the liquid and solid phases.
- PCTM will not provide reliable estimates of cleanup time for diffusion dominated problems.
- PCTM is based on the assumption that the critical pathline does not change under the altered condition. The critical pathline is the pathline which controls the cleanup time (i.e., the solute concentration along this pathline requires more time to drop below the CUC than any other pathline). As an example of a situation in which PCTM would not be expected to provide a reliable cleanup time, suppose that the critical pathline terminates at a groundwater recovery well under the baseline condition. Under the altered condition, however, the capture zone becomes greatly reduced in size and the critical pathline no longer terminates at the recovery well. This condition could potentially exist if a large value were used for the groundwater hydraulic gradient.

In any case, it is recommended that several (e.g., three or four) runs be made with the numerical model, varying parameter values, for the purpose of comparing and testing the validity of PCTM before deciding to use it. If the PCTM-estimated cleanup times are in reasonable agreement with the model estimated cleanup times then PCTM can be used as a substitute for the numerical model when performing the sensitivity analysis.

SUMMARY

This paper described the Proportional Cleanup Time Method (PCTM). PCTM is a simple and inexpensive method for estimating groundwater solute plume cleanup times. The method requires as input a baseline cleanup time estimate from a standard method (e.g., numerical model), along with parameters for the baseline and new conditions. The method is potentially valuable for performing sensitivity and uncertainty analyses. Parameters that can be evaluated include v_L , R , v_C , K , i , ϕ , ρ_b , f_{OC} and K_{OC} (K_d in the case of an inorganic solute). The method showed excellent agreement with a three-dimensional analytical solute transport solution, and two numerical models. An example was provided in which the use of PCTM would have resulted in a savings to the client of greater than \$10,000. Potential limitations of the method were also discussed.

REFERENCES

- Fischer, H. B., E. J. List, R. C. Y. Koh, J. Imberger and N. H. Brooks, 1979. *Mixing in Inland and Coastal Waters*. Academic Press.
- Freeze, A. R. and J. A. Cherry. 1979. *Groundwater*. Prentice Hall Publisher
- McDonald, M. G. and A. W. Harbaugh. 1984. *A Modular Three-Dimensional Finite Difference Ground-Water Flow Model*. U.S. Geological Survey.
- Zheng, C. 1992. *MT3D A Modular Three Dimensional Transport Model for Simulation of Advection, Dispersion and Chemical Reactions in Groundwater Systems*. U.S. EPA.

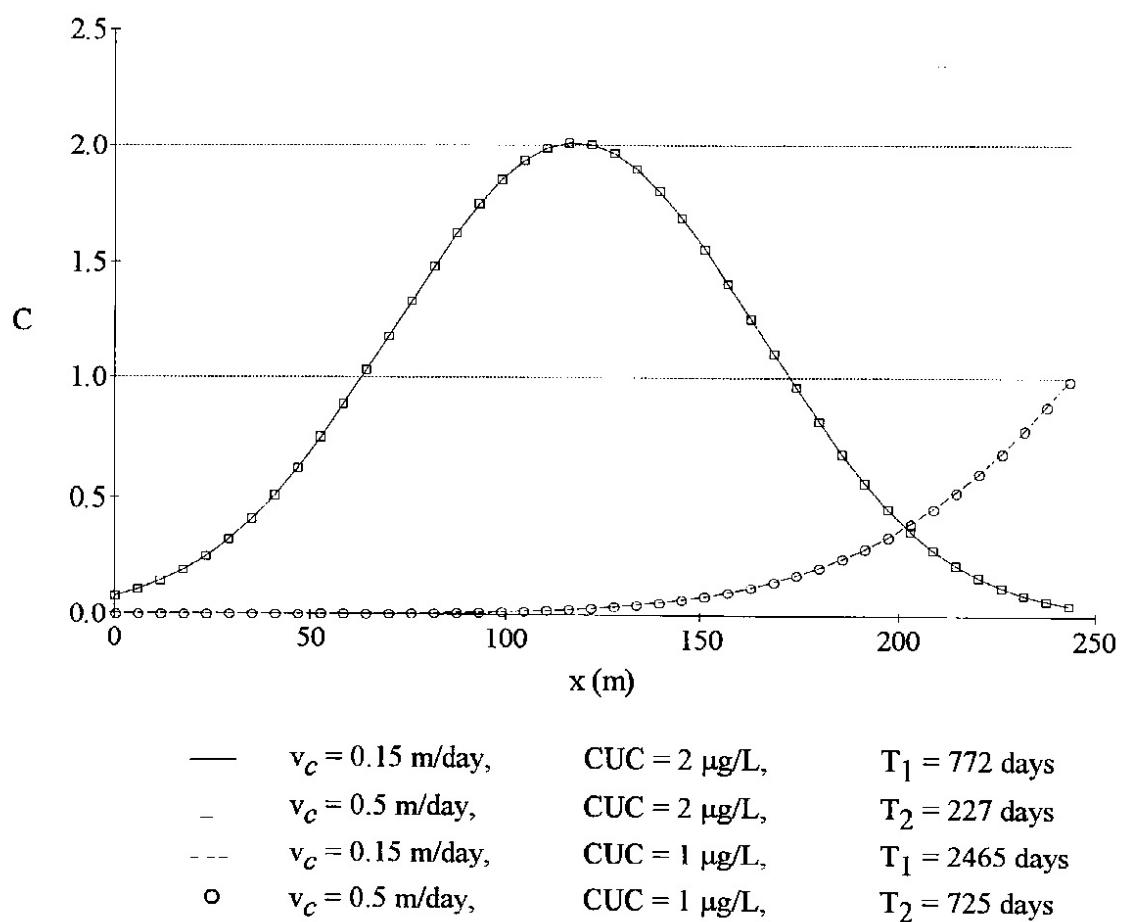


Figure 1. Estimated solute concentration distributions plotted at times associated with achievement of cleanup criteria (CUCs).

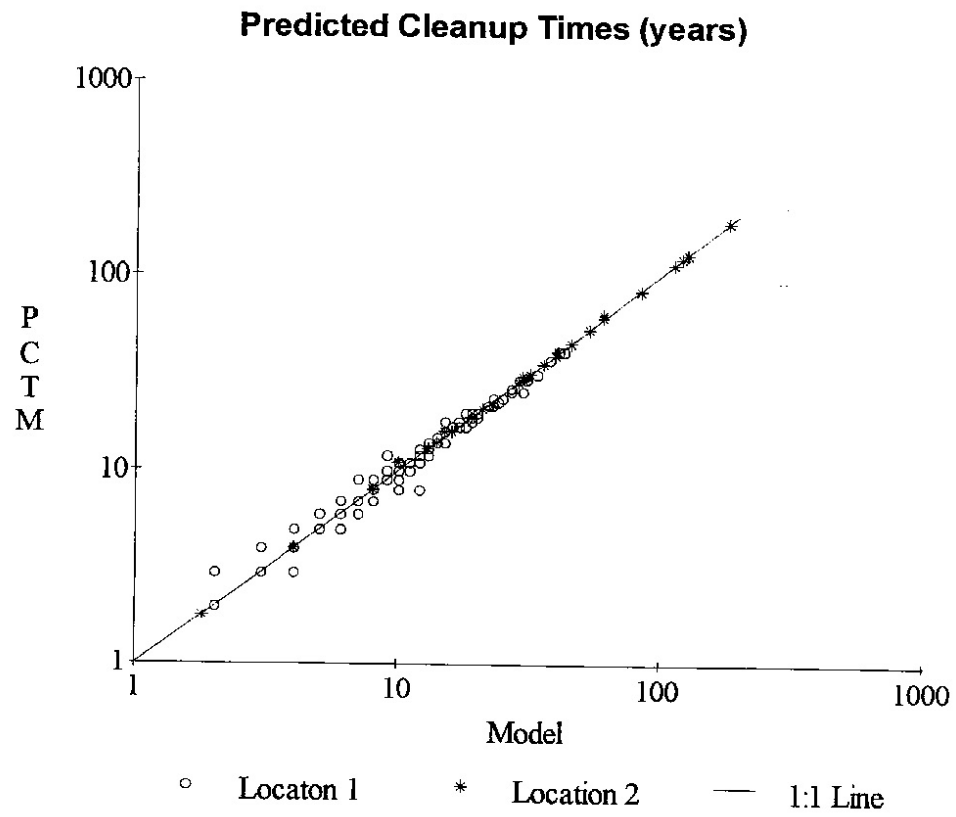


Figure 2. Comparison of cleanup time (years) between PCTM and Location 1 and 2 numerical solute transport models.

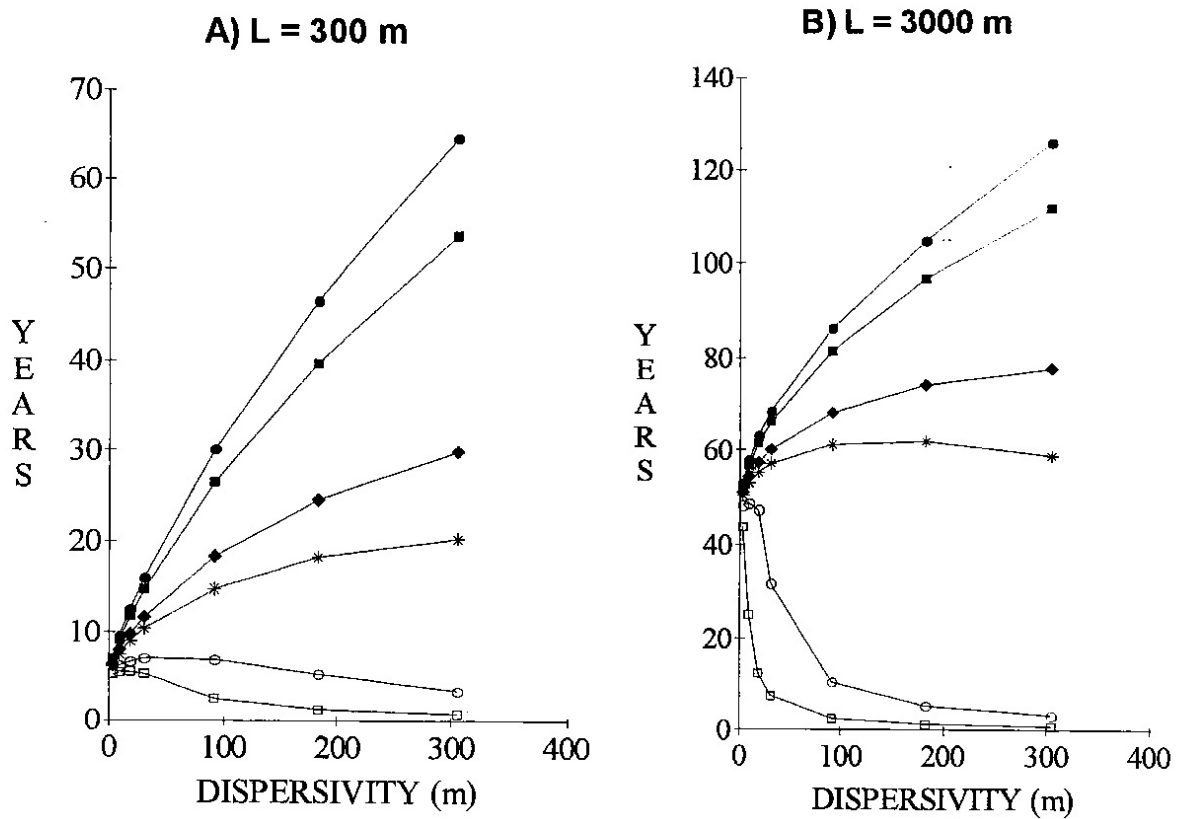


Figure 3. Cleanup time as a function of longitudinal dispersivity. A) L = 300 m; B) L = 3000 m. (solid circle $C_0/CUC = 1000$, solid square $C_0/CUC = 500$, solid diamond $C_0/CUC = 100$, asterisk $C_0/CUC = 50$, open circle $C_0/CUC = 10$, open square $C_0/CUC = 5$)