Sensitivity analysis of a contaminant transport model
L'analyse de sensitivité d'un modèle de transport "contaminant"

R.K.Srivastava – *M.N.R. Engineering College, Allahabad, India*

ABSTRACT: Estimation and prediction of transport of pollutants following through porous media (soils/rock mass) reaching ground water and accumulating there, is becoming increasingly important because of its obvious hazard to human health. Various numerical models have been developed for prediction of pollutant transport in porous media based on advection – dispersion equation. The concept of sensitivity plays an important role in parameter estimation. It provides a means to identify the main contributors to uncertainty in the numerical model out put. In the present study sensitivity of a contaminant transport model MT3D with respect to input parameters has been evaluated. Four input parameter viz. Effective porosity, vertical transverse dispersivity horizontal transverse dispersivity and longitudinal dispersivity have been selected to check the sensitivity of this model. For this first a base simulation is carried out. Then subsequent simulations have been taken by varying each parameter by –10% -5% +5% and +10% keeping all other parameters unchanged. The final concentration of pollutants of each subsequent simulation are compared with that of base simulation Results of the analysis indicate that sensitivity coefficient of effective porosity is higher in all cases. It is found to be most sensitive parameter, which may produce more uncertainty in the prediction.

RÉSUMÉ : Le jugement et la prédiction du transport des polluants qui suivent par les media poreux (masse de sols / de rochers), qui descendent jusq' à l'eau soutenaine et qui y accumule, deviennent de plus en plus importants à cause de leur danger évident pour la santé humaine. Plusieurs modèles mumériques ont été développée pour la prédiction du transport des polluants dans les media poreux basés sur l'équation "advection-dispersion". Le concept de sensitivité joue un rôle important dans le judgement des paramètres. Cela aide à identifier les donateurs principaux à l'incertitude dans la production de modèles numériques. Dans l'étude actuelle, on a évalué la sensitivité d'un modèle de transport "contaminant" MT3D pour les paramètres de consommation. On a choisi quatre paramètres de consommation: la porosité effective, la dispersivité verticale transversale, la dispersivité horizontale transversale et la dispersivité horizontale – pour vérifier la sensitivité da ce modèle.Pour faire cela, on effectue d'abord une simulation de base. Après, on effectue les simulations subséquentes en variant tous les paramètres par –10%, –5%, +5% et +10% enretenant inchangés tous les autres paramètres. On compare la dernière concentration de pollutants de chaque simulation de base. Les résultants de l'analyse révèlent que le coefficient de sensitivité de la porosité effective, est supérieur dans tous les cas. C'est le paramètre le plus enesible qui peut produire plu d'incertitude dans la prédiction.

1 INTRODUCTION

Concern over the potential for migration of wastes in the subsurface has generated a great deal of interest in the mechanisms responsible for contaminant transport through ground water systems. Increased attention by both researchers and regulatory agencies to subsurface contamination can be attributed to the growing popularity of waste disposal by means of landfills, sludge lagoons, and deep injection wells and to the concern over subsurface disposal of low to high level, radioactive wastes. Components of the transport process are advection, dispersion (including diffusion) and chemical reactions. Advection refers to movement as a result of differences in head. Dispersion refers to mixing and spreading caused in part by molecular diffusion and microscopic variations in velocities within individual pores. For many filed problems, these effects are negligible in comparison with dispersion caused by large scale heterogeneities with in the aquifer. In the presence of large scale heterogeneities, dispersion occurs as contaminants move selectivity around the less permeable units. However, when advection is weak, mechanical dispersion is negligible relative to molecular diffusion. Molecular diffusion can be important in low velocity systems, especially where high level reductive waste is the contaminant.

To prevent the deterioration of ground water quality, it has become necessary to develop a methodology for monitoring, analyzing, and predicting the movement of contaminants through the subsurface. The hope of formulating such a methodology has motivated the development of predictive tools in the form of mathematical models designed to simulate the transport of contaminants through ground water systems.

MT3D is a modular three dimensional transport model for simulation of advection, dispersion and chemical reactions of dissolved constituents in ground-water systems. The MT3D transport model uses a mixed Eulerian - Lagrangian approach to the solution of the three-dimensional advective – dispersive – reactive equation in three basic options : the method of characteristics (MOC) the modified method of characteristics (MMOC) and a hybrid of these two methods (HMOC). The availability of both MOC and MMOC options and their selective use based on an automatic adaptive procedure under the HMOC option make MT3D uniquely suitable for a wide range of field problems. The MT3D transport model is intended to be used in conjunction with any block – centered finite difference flow model such as MODFLOW and is based on the assumption that changes in the concentration filed will not affect the flow field measurably. MT3D accommodates the following spatial discretization capabilities and transport boundary conditions:

1. Confined, unconfined variably confined / unconfined aquifer layers.
2. Inclined model layers and variable cell thickness within the same layer.
3. Specified concentration or mass flux boundaries, and
4. The solute transport effects of external sources and sinks such as wells, drain, river, areal recharge evapotranspiration.

MODFLOW is a three-dimensional finite difference ground water flow model. It simulates steady and non-steady flow in an irregularly shaped flow system in which aquifer layers can be confined, unconfmed, or a combination of confined and unconfined. Flow from external stresses, such as a flow to wells, areal recharge, evaportranspiration, flow to drains, and flow through river beds, can be simulated. Hydraulic conductivities or transmissivities for any layer may differ spatially and be anisotrapic and the storage coefficient may be heterogeneous. The model requires input of the ratio of vertical hydraulic conductivity to distance between vertically adjacent block centres MODFLOW is currently the most used numerical model in the US Geological survey for ground water flow problems.

Due to these reasons, in the present study, sensitivity of contaminant transport model, MT3D, developed by Zheng (1990) for U.S.E.AP.A. with respect to input parameters, has been checked. Four input parameters have been selected to check sensitivity. These parameters are effective porosity, vertical transverse dispersivity, horizontal transverse dispersivity, and longitudinal dispersivity. Firstly, a base simulation is carried out. Then subsequent simulation has been taken by varying each parameter by −10% −5%, 5% and 10%, keeping all other parameters unchanged. The final concentrations of pollutants of each subsequent simulation are compared with that of base simulation. For comparison purpose, eight observation cells in one layer of the aquifer have been chosen. By comparison, sensitivity coefficient of each parameter for each percentage variation is calculated.

2 PROBLEM FORMULATION

A four layered hypothetical aquifer is assumed. Each layer is divided in 61 rows and 40 column. All layers are of equal thickness. It is assumed that each layers are homogenous in nature.

2.1 Details of hypothetical aquifer.

Cell thickness, effective porosity and dispersion coefficient for the four layers of the assumed aquifer are presented in Table 1 and location of observation points are presented in Table 2.

Table 1. Layer details

Layer No.	Cell thickness (m)	Effective porosity	Dispersion parameters (m)
1	0.25	0.30	0.10
2	0.25	0.30	0.10
3	0.25	0.30	0.10
4	0.25	0.30	0.10

Initial concentration for 1st layer = 0.0
Initial concentration for 4th layer = 0.0
Horizontal transverse dispersivity / longitudinal dispersivity = 0.20
Vertical transverse dispersivity / longitudenal dispersivity = 0.20
Diffusion coefficient = 0.0
Longitudenal dispersivity = 10
Sorption constant no. 1 = 1.0 cm^3/G
Sorption constant no. 2 = 1.0 cm^3/G
No. of observation points = 8

Table 2. Location of observation points

Layer No.	Cell thickness (m)	Effective porosity	Dispersion parameters (m)
1	3	11	29
2	3	19	26
3	3	26	23
4	3	33	20
5	3	40	17
6	3	48	14
7	3	48	9
8	3	52	17

3 RESULTS

To check the sensitivity of the model a base simulation is carried out varying layer parameters between − 10% to + 10%. The value of parameters for subsequent different variation is given is Table 3. Eight observation points are chosen. The final concentration of pollutants after 500 days and 1000 days for each subsequent simulation and base simulation are compared and sensitivity coefficient in the normalised form are calculated by adjoint technique. Few typical results are presented in Tables 4, 5, 6 and 7. Finally, these sensitivity coefficients are compared to check the sensitivity of the parameters (Table 8).

Table 3. Value of different parameters for variation used in sensitivity analysis

S. No.	Parameter	% variation	Value
1	Effecting Porosity	−10	0.270
		−5	0.285
		+5	0.317
		+10	0.330
2	Vertical transverse dispersivity / logitudenal dispersivity	−10	0.180
		−5	0.190
		+5	0.210
		+10	0.220
3	Horizontal transverse dispersivity / longitudinal dispersivity	−10	0.180
		−5	0.190
		+5	0.210
		+10	0.220

Table 4. Sensitivity coefficients simulation of −10% variation in effective porosity.

Location of observation point	Final concentration		IΔC_nI	IΔC_{n2}I	ΔC_n^2	ΔC_{n2}^2
	C_n	C_{n2}				
1	04.3	01.1	0.6	0.0	0.36	0
2	23.3	05.1	1.8	1.7	3.24	2.89
3	40.7	11.6	2.0	1.4	4.00	1.96
4	38.6	20.2	1.8	0.9	3.24	0.81
5	32.0	21.1	0.3	2.1	0.09	4.41
6	16.7	14.7	0.6	0.2	0.36	0.04
7	04.8	06.4	1.3	0.1	1.69	0.01
8	02.5	01.7	0.1	0.0	0.01	0
					$\sum = 12.99$	$\sum = 10.12$

ΔC_n – Change in concentration from base simulation after 500 days.
ΔC_{n2} – Change in final concentration from base simulation after 1000 days.

Table 5. Coefficients in simulation of −5% variation in vertical transverse dispersitivity.

Location of observation point	Final concentration		IΔC_nI	IΔC_{n2}I	ΔC_n^2	ΔC_{n2}^2
	C_n	C_{n2}				
1	4.9	1.1	0	0	0	0
2	24.4	6.0	0.7	0.8	0.49	0.64
3	42.4	12.7	0.3	0.3	0.09	0.09
4	37.8	21.5	1.0	0.4	1.0	0.16
5	33.7	21.9	2.0	1.3	4.0	1.69
6	16.1	15.6	0	1.7	0	0.49
7	5.1	6.6	0.5	0.3	0.25	0.09
8	2.6	1.8	0.2	0.1	0.04	0.01
					$\sum = 5.87$	$\sum = 3.17$

4 DISCUSSION AND CONCLUSION

Comparison of the sensitivity coefficients of selected parameters for their respective simulations shows that effective porosity is most sensitive parameter. It is observed that the sensitivity coefficients of parameters vary in same pattern for − 10% and + 5% variation-simulation in both cases (after 500 days and 1000 days). For + 10% variation, the ranking pattern is different in both cases. In transport calculation, porosity enters not only to calculate seepage velocity, but also to calculate the solute mass in a given volume of aquifer and the rate at which mass changes with time. If advection is assumed to be the only transport process, the storage of solute mass can occur only with in the mobile fraction of water. As a result, the effective porosity used in calculating the seepage velocity also governs solute mass accumulation. When dispersion transport is considered, two different values of porosity might be required because pore scale diffusion can cause solute to spiral into portions of interstitial water in which there is little or no fluid movement. One porosity is required for seepage velocity calculation and other for evaluating the rate of mass accumulation. If the mixing of solutes caused by diffusion from mobile to immobile portions of the pore water is assumed to be instantaneous, these two porosities are both equivalent to the total porosity. If mixing is assumed to be negligible, the two porosities are both equivalent to the effective porosity.

It is convention in advection, dispersion analysis to use a single value of porosity in place of two porosities. So a single effective porosity is defined for calculating both seepage velocity and rate of solute mass accumulation. In this way, one may conclude, that the porosity is difficult to determine in partice. In some cases, where two very different porosities (e.g. fractured and unfractured media) occur in close association, if may be nearly impossible to define a single effective porosity which fills both roles.

It is generally assumed that the porous medium is isotropic with respect to dispersion. Under this assumption dispersion coefficient is based on two dispersivties, longitudinal dispersivties and transverse dispersivity. For anisotropy's medium, it is assumed that dispersion coefficient requires three dispersivities, longitudinal dispersivity, horizontal transverse dispersivity and vertical transverse dispersivity.

To define dispersivity value for use in field scale transport simulation is difficult and has been subject of some controversy. Values of dispersivity generally appear to be dependent on the scale of observation. Dispersivity values derived from tracer test, which are usually performed on relatively local or small scale, tend to be smaller than those developed from field observations which involve larger scales. In case of longitudinal dispersivity, data reliability is necessary because of the wide range of heterogeneity in the aquifers in which tests are conducted and in the method of interpretation by which results are obtained. But it is observed that reliable data falls in the small scale range. As scale increases, data reliability decreases.

Transverse dispersivites are observed to be smaller than longitudinal dispersivity and also influenced by scale of observations. It also shows the same pattern as discussed in longitudinal dispersivity.

There are two limitations in sensitivity analysis carried out in this study.

1. In sensitivity analysis, parameters are assumed to be uncorelated and each parameter is varied independently. In reality, parameters are often correlated to certain degree.

Table 6. Sensitivity coefficients in simulation of 5% variation in horizontal transverse dispersivity.

Location of observation point	Final concentration		$I\Delta C_n I$	$I\Delta C_{n2} I$	ΔC_n^2	ΔC_{n2}^2
	C_n	C_{n2}				
1	4.8	1.1	0.1	0	0.01	0
2	25.1	5.8	0	1.0	0	1.00
3	42.1	13.2	0.6	0.2	0.36	0.04
4	36.8	21.4	0	0.3	0	0.09
5	31.7	23.0	0	0.2	0	0.04
6	16.1	14.9	0	0	0	0
7	5.7	6.3	0.4	0	0.16	0
8	2.5	1.8	0.1	0.1	0.01	0.01
					$\sum = 0.23$	$\sum = 2.56$

Table 7. Sensitivity coefficients in simulation of 10% variation in longitudinal dispersivity.

Location of observation point	Final concentration		$I\Delta C_n I$	$I\Delta C_{n2} I$	ΔC_n^2	ΔC_{n2}^2
	C_n	C_{n2}				
1	5.0	1.0	0.1	0.1	0.01	0.01
2	25.1	6.2	0.0	0.0	0	0.36
3	41.6	13.3	1.1	1.21	1.21	0.09
4	36.9	21.4	0.1	0.01	0.01	0.09
5	32.0	23.0	0.3	0.09	0.09	0.04
6	15.9	15.4	0.2	0.04	0.04	0.25
7	5.7	6.4	0.4	0.16	0.16	0.01
8	2.3	1.9	0.1	0.1	0.01	0.04
					$\sum = 1.53$	$\sum = 0.89$

Table 8. Sensitivity coefficients of parameter for 500 and 1000 days.

S.No.	% Variation	Parameter	500 days		1000 days	
			Rank	Sensitivity Coefficient	Rank	Sensitivity Coefficient
1	-10	Effective porosity	1	129.9	1	101.2
		Vertical Transverse dispersivity	2	65.6	2	73.0
		Horizontal transverse dispersivity	4	9.1	4	25.6
		Longitudinal	3	38.7	3	36.0
2	-5	Effective porosity	1	188.8	1	80.0
		Vertical Transverse dispersivity	2	117.4	2	63.4
		Horizontal transverse dispersivity	4	4.6	4	51.2
		Longitudinal	3	69.0	3	62.4
3	+5	Effective porosity	1	115.6	1	118.4
		Vertical Transverse dispersivity	2	23.4	2	62.4
		Horizontal transverse dispersivity	3	10.8	3	23.4
		Longitudinal	4	0	4	0
4	+10	Effective porosity	1	186.7	1	193.5
		Vertical Transverse dispersivity	3	10.1	2	33.1
		Horizontal transverse dispersivity	4	6.3	3	12.3
		Longitudinal	2	15.3	4	8.4

2. The use of sensitivity coefficient implies a linear relationship whereas model prediction is a non-linear function of the input parameters.

From this study of sensitivity analysis of a contaminant transport model. MT3D, following conclusions may be drawn.

1. It is very difficult to measure the values of effective porosity, longitudinal dispersivity, vertical transverse dispersivity, horizontal transverse dispersivity in field.

In comparison of sensitivity coefficient, effective porosity is found most sensitive parameters. So, it may produce more uncertainty in the model output.

In dispersivities, vertical transverse dispersivity is more sensitive than other two.

REFERENCES

Zheng, C. 1990. MT3D: A Modular Three dimensional transport model for simulation of Advection dispersion and chemical reaction, of contaminates in ground water systme. *Report to the U.S. Environmental Protection Agency, Ada.*