Study of Modeling and Numerical Sensitivity Analysis at a Contaminated Site

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1. Introduction

Recently, soil and groundwater contamination caused by hazardous waste materials has become a serious social problem. In general, it is difficult to evaluate the degree of contamination over the whole site with only field investigations, because soil and groundwater contamination progress in the underground. To carry out proper countermeasures, it is very important to predict accurately the contaminant distribution at the site using results from field investigations. Numerical simulation enables prediction and visualization of the contaminant distribution, and therefore is a very effective tool for supporting planning of the countermeasures.

At the illegal dumping site described in this paper, some countermeasures are urgently needed because contaminants have already penetrated into the deep aquifer. The object of this study is to examine the countermeasure by applying numerical simulation to this site. In a previous study[1], as the first analysis for the modeling of this site, a three-dimensional geographical and geological model was developed, and contaminant distribution in the first aquifer was predicted. However, there were still differences between the calculated and observed values. To predict the future distribution accurately, it is necessary to re-examine the parameters through sensitivity analysis. In addition, although the contaminants have already penetrated into the deep aquifer, analysis in the second aquifer has not yet been carried out. To complete the modeling of contamination over the site, the distribution of contaminants in the second aquifer should be also predicted.

In this study, the effect of each parameter on future contaminant distribution in the first aquifer was confirmed by sensitivity analysis, and the contaminant distribution in the second aquifer was predicted. Based on these results, items requiring re-investigation were proposed.

2. Site Description

The illegal dumping site described in this paper is a least controlled landfill site. Ash, sludge and waste oil, including some hazardous materials, were illegally dumped into the landfill site about three years ago. These hazardous materials, which include chlorinated organic compounds and aromatics, have contaminated the groundwater around the site.

The site is located on a terrace near a river, as shown in Fig. 1. The area of the landfill

site is 2,800 m² and the maximum depth is 14.7 m. Alternating gravel layers and clay layers occur above bedrock. The bedrock presents about 22 m below the ground level at the landfill site. It was found from field investigation that the aquifer is divided into two (the first and second aquifer) by an impermeable layer about 10 m below the

Fig.1 The plan of the contaminated site

ground level. The water table in the waste layer is about 5 m below ground level. It was expected that because the waste layer penetrated into the second aquifer, both the first aquifer and the second aquifer might be contaminated. In addition, it was also expected from the regional geographic and geological features around the site that there might be difference in the direction of groundwater flow between the first and second aquifer.
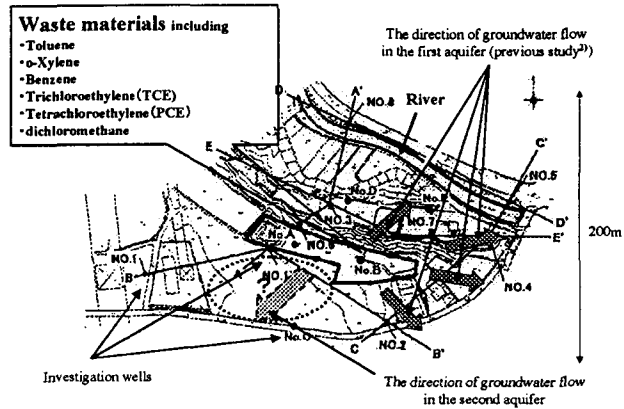
3. Prediction of contaminant distribution in the first aquifer

As the first analysis of this site, the groundwater flow and contaminant transport in the first aquifer were simulated numerically in the previous study[1]. The procedure was:

(1) A three-dimensional geological structure model was developed from the nine bore logs. The geological structure estimation software GEORAMA (CRC Research Institute, Inc.) was used for this modeling.

(2) A calculation area and boundary conditions were set.

(3) A grid was set over the calculation area, and the necessary data (geological structure, initial hydraulic conductivity, and initial groundwater level) were set at each node.

(4) The hydraulic conductivity was estimated by inverse analysis, and was used to simulate the groundwater flow, using PC UNISSIF (CRC Research Institute, Inc.) which provides semi-three-dimensional groundwater flow analysis.

(5) Transflow (CRC Research Institute, Inc.) was used for the contaminant transport analysis. The concentration at each node was calculated, and was compared with the observed value.

In this previous study, four cases (two options for the hydraulic conductivity, and two options for the dispersivity) were simulated. The best agreement between calculated and observed values of the contaminant distribution was obtained with the parameters presented in Table 1

Table1. Parameters used in the analysis of the first aquifer

distribution coefficient	0.023mL/g
octanol-water distribution coefficient	18.2L/kg
fraction organic corborn	0.00125mg/L
soil density	0.2g/cm³
dispersivity	10m/1m
molecular diffusion coefficient.	0
curvature rate	0
effective porosity	0.2
specific storage coefficient	0.0003

and 2. Fig.2 shows the trichloroetylene (TCE) distribution 3 years after the illegal dumping. The distributions of tetrachloro-ethylene (PCE) and toluene were also predicted but are not illustrated. For these three contaminants, the difference in the concentration between calculated and observed values was within one order of magnitude. Fig. 3 shows the predicted future TCE distribution after 13 years. At the beginning of the analysis, it was expected that the contaminants might be transported in the first aquifer from the landfill site to the river. However, it was found from Fig.3 that the contaminants would be transported not only to the north but also in northeasterly, easterly and southeasterly directions.

Table2. Hydraulic conductivity used in the analysis of the first aquifer

symbol	hydraulic conductivity (m/day)	note
W	7.00	waste layer
B	4.32×10^{-7}	banking
F	4.32×10^{-7}	surface soil
Ac	4.32×10^{-21}	
Ag	50.0	
tDg	3.08	first aquifer
tDc	4.32×10^{-21}	
Dc	4.32×10^{-21}	
Ds	4.32×10^{-21}	
Dg	3.88×10^{-2}	second aquifer
TCTS	4.32×10^{-21}	base

* The symbol shows the stratum in the field.
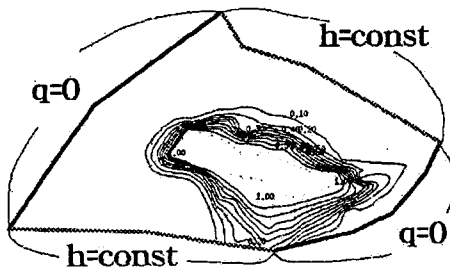* The end character of symbol: c is clay g is gravel and s is sand.

Fig.2 TCE distribution in the first aquifer
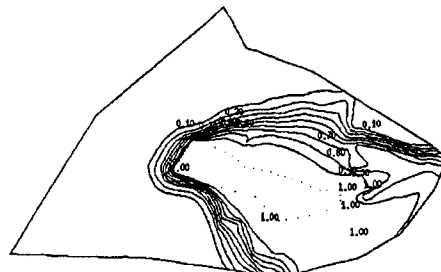(3 years after the illegal dumping)

Fig.3 TCE distribution in the first aquifer
(after 13 years)

4. Sensitivity analysis for the first aquifer

4.1 Objectives of sensitivity analysis

The current distribution of contaminants in the first aquifer could be predicted approximately, as described above. However there were still problems with the prediction of the future contaminant distribution. To confirm the effect of each parameter on the future distribution, a sensitivity analysis for the first aquifer was carried out. Using this sensitivity analysis, the accuracy necessary in the measurement of each parameter could be confirmed, and items to be re-investigated could be proposed.

The parameters examined in this study were hydraulic conductivity, dispersivity, effective porosity, and fraction organic carbon.

4.2 Calculation conditions and evaluation method

Changing one parameter at a time, the sensitivity analysis was carried out considering those parameters listed in Table 1 and 2 as a standard. The range of values considered for each parameter was determined by considering maximum ranges in the literature values[2, 3]. In this analysis, 32 cases were calculated. A part of the calculation conditions is shown in Table 3.

The evaluation of sensitivity (ES) on each parameter was given by equation 1), being the sum of squares of the difference in concentration at each node. C1 and C2 are relative concentrations (the concentration of contamination source being taken as unity) after 13 years, calculated using standard values and changed values, respectively. ES was also normalized (NES) to compare the sensitivity of one parameter with other parameters.

$$ES = \sum_{i}^{nodes} \left(C1_i - C2_i \right)^2 \qquad \text{1)}$$

$$NES = ES \Big/ \left[\frac{range\ of\ value\ for\ parameter}{\max imum\ range\ of\ value\ for\ parameter} \right] \qquad \text{2)}$$

4.3 Result and discussion

The calculated ES and NES are shown in Table 3, and the contaminant distribution in each case is shown in Fig.4, 5, 6 and 7. The NES of the hydraulic conductivity was found to be larger than other parameters. In particular, the NES in cases 1 and 2 were much larger than that in case 3. In cases 1 and 2, the hydraulic conductivity of only the waste layer and the first aquifer, respectively, was changed. On the other hand, in case 3, the hydraulic conductivities of all the layers were changed. It was confirmed that the effect of the hydraulic conductivity ratio change was especially large. In addition, the change in concentration in the north and south area was found to be so large, when the distributions of Fig.4 and 5 were compared with that of Fig. 3. That is responsible for the hydraulic conductivity ratio. Because the hydraulic conductivity of the first aquifer was measured, the hydraulic conductivity of the waste layer should be also measured.

Table3. Result of sensitivity analysis

| case	changed parameter	maximum range of value	changed value	ES	NES	note
1	hydraulic conductivity (waste layer) [m/day]	100	7→0.7	25.48	254.80	Fig.4
2	hydraulic conductivity (first aquifer) [m/day]	100	3.075→30.75	28.00	280.00	Fig.5
3	hydraulic conductivity (all layer) [m/day]	100	10→100	1.33	13.30	
4	dispersivity [m] (length : width)	3	10:1→5:0.5	3.70	7.40	Fig.6
5	effective porosity [-]	1.5	0.2→0.25	0.04	0.05	
6	fraction organic carbon [-]	10	0.00125→0.00625	0.08	0.16	Fig.7
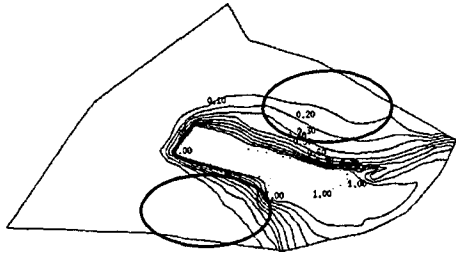
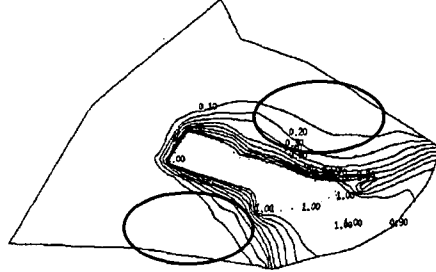Fig. 4 Contaminant distribution in the first aquifer
(TCE,case1,after 13 years)

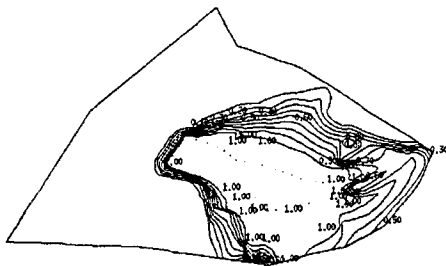Fig. 5 Contaminant distribution in the first aquifer
(TCE,case2,after 13 years)

Fig. 6 Contaminant distribution in the first aquifer
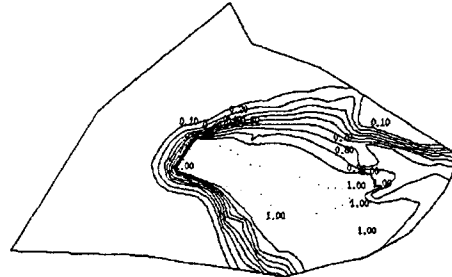(TCE,case4,after 13 years)

Fig. 7 Contaminant distribution in the first aquifer
(TCE,case6,after 13 years)

5. Prediction of contaminant distribution in the second aquifer

As described above, the waste layer penetrates into the second aquifer. Therefore it was expected that the second aquifer would be also contaminated. In addition, it was expected that the groundwater in the second aquifer would flow in an opposite direction to the first aquifer. Therefore, the distribution of contaminants in the second aquifer was also modeled.

Because it was found from the sensitivity analysis that the value used for the hydraulic conductivity had a large effect on the distribution, the hydraulic conductivities of the second aquifer, waste layer and base were determined by inverse analysis. For this analysis, a groundwater level estimation program, which also provides inverse analysis, was developed. As a result of inverse analysis, three patterns of hydraulic conductivity valued (A, B and C) were obtained. They are shown in Table 4. Fig.8 shows the TCE distribution in the second aquifer in the case of pattern C, which is the calculated distribution that is most consistent with the observed values. It was

Table4. Estimated hydraulic conductivity

	pattern A		pattern B		pattern C ◎	
	initial value	estimated value	initial value	estimated value	initial value	estimated value
waste layer	8.10E-03	6.11E+02	5.00E-03	4.95E+01	2.70E-03	1.92E+01
second aquifer	8.84E-03	6.98E-01	3.00E-03	4.05E-01	2.40E-03	2.83E-01
TCTS(base)	8.84E-06	3.58E+00	8.84E-06	1.85E+00	4.00E-02	5.74E-02
sum of squares	9.318		9.386		9.456	

suggested from Fig.8 that the contaminants might be transported toward the south-southwest of the site through the second aquifer. In field investigations, toluene and xylene were detected at low level in this area. Therefore, further investigation in the south-southwest area is needed to evaluate the contamination in the second aquifer.
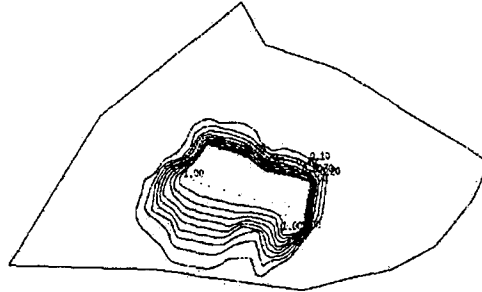

Fig. 8 TCE distribution in the second aquifer
(after 3 years)

6. Conclusion

(1) Sensitivity analysis in the first aquifer showed that the effect of hydraulic conductivity on the future contaminant distribution was larger than other parameters.

(2) In particular, the effect of the change of the hydraulic conductivity ratio was very large. Because the hydraulic conductivity of the first aquifer had already been measured, it is necessary to measure the hydraulic conductivity of the waste layer to predict the future contaminant distribution more accurately.

(3) As a result of the prediction of contaminant distribution in the second aquifer, it was suggested that the contaminants might be transported toward the south-southwest area of the site through the second aquifer. It is necessary to investigate the south-southwest area to evaluate the contamination in the second aquifer.

References

1) T. Kobayashi, T. Furuichi, K. Ishii and T. Imai (2000), The Selection of Remedial Countermeasures in Soil and Groundwater Pollution by Numerical Simulation Considering Contaminant Characteristics, Proceedings of the 11th Annual Conference of the Japan Society of Waste Management Experts, pp. 1234-1236

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3) T. H. Wiedmeier, H. S. Rifai, C. J. Newell and F. T. Wilson (1999), Natural Attenuation of Fuels and Chlorinated Solvents in the Subsurface, John Wiley & Sons, Inc., p147