Calibration and Reliability in Groundwater Modelling (Proceedings of the ModelCARE 99 Conference held at Zürich, Switzerland, September 1999). IAHS Publ. no. 265, 2000.

Calibration and sensitivity analysis of the 3-D Cape Cod tracer test

S. WAGNER, F. HÄFNER, S. BOY & A. BEHR

Institute of Drilling Technology and Fluid Mining, Freiberg University of Mining and Technology, Akademiestrasse 6, D-09596 Freiberg, Germany

e-mail: wagner@bohr1.tbt.tu-freiberg.de

Abstract The three-dimensional (3-D) simulation of the Cape Cod tracer test with the density-dependent simulation software MODCALIF, shows that the results of the test evaluation which have been published up to now do not lead to any satisfactory correspondence with the observed bromide plumes. Neither the maximum concentration of the plume, nor the movement of the centre of mass, nor the vertical drift, correspond to the observed data. In particular, the simulated vertical drift of the plume is only about 2.5 m (observed: 4 to 5 m), and the simulated maximum concentrations are too low. A sensitivity analysis shows that the previous assumption of a homogeneous hydraulic conductivity is not valid. By integrating the calibration method into MODCALIF, the anisotropy and spatial distribution of the hydraulic conductivity was determined which leads to a small vertical discharge (Darcy-velocity) component. Furthermore, it can be shown that the transport of the bromide plume can be simulated very well assuming inhomogeneous conductivity and very small dispersivities.

INTRODUCTION

The Cape Cod natural-gradient experiment was planned and carried out by the US Geological Survey. The first evaluations (LeBlanc *et al.*, 1991; Garabedian *et al.*, 1991; Hess *et al.*, 1992) ignored the density effect and assumed a homogeneous hydraulic conductivity of ~1.27×10^{-3} m s^{-1} with a vertical anisotropy factor of 0.2 to 0.5. The dispersivity was determined from the movement of the respective centre of mass of the bromide plume, and the change with respect to the travel time of the second moment (longitudinal dispersivity: 96 cm, transversal dispersivities: 0.15 to 1.8 cm) (Fitts, 1996; Zhang *et al.*, 1998; Dagan, 1998; Fiori & Dagan, 1999).

CRITICAL ASSESSMENT OF THE PREVIOUS RESULTS

The large number of measured concentrations (28 130) show a diffuse image of the plume. Therefore we have tried to simplify the problem by graphical analysis of the maximum concentration and the mass percentage 1 mg l^{-1} (mass of the plume with concentrations higher than 1 mg l^{-1} divided by the total mass), and the centre of mass of the plume versus time. The time variability of the observed data is shown in Figs 1, 2 and 3. These variabilities are a hint of the non-symmetrical concentration distributions which are caused by macroscale and nonstochastic (deterministic) heterogeneities of the hydraulic conductivity. The three-dimensional (3-D) graph of the plume's trail

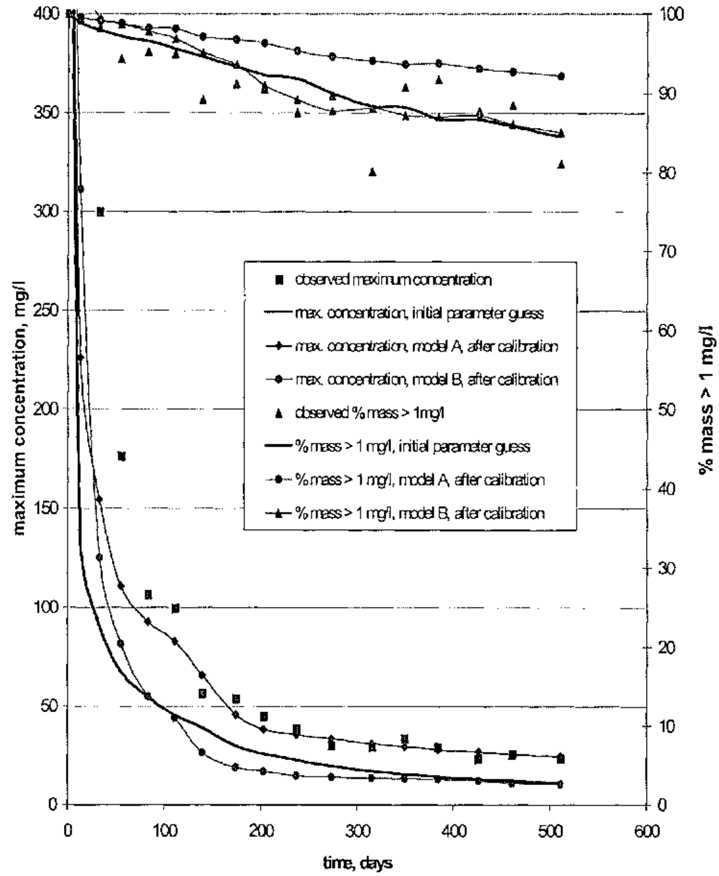

Fig. 1 Maximum concentration of the bromide plume and mass percentage (C > 1 mg l^{-1}) *vs* time.(“maximum observed concentration” is the mean of the largest 1% of observations).

(3D-TECPLOT) showsdeviations from the groundwater path line which confirms this statement (Fig. 4). In particular, the trail of the plume shows a typical “meandering” which is caused by well known conductivity channels in aquifers.

The determinations of parameters: hydraulic conductivity, longitudinal dispersivity, transverse-horizontal, and transverse-vertical dispersivities, are based upon models which neglect inhomogeneity and anisotropy of the hydraulic conductivity as well as the density effects and groundwater recharge. Thus, all these influences necessarily reappear in the values of dispersivities as only the dispersion—and the molecular diffusion to a minimal extent—can lead to the observed spreading of the plume. Thus, the effects of the usual model simplifications (constant density), but also serious model errors (macroscale heterogeneities, anisotropy, groundwater recharge), are replaced by the stochastic macrodispersion. But 3-D calculations show that the maximum concentration of the plume is much too low (Fig. 1). Furthermore, density-dependent simulations considering groundwater recharge show that the vertical drift of the plume is too small (Fig. 2).

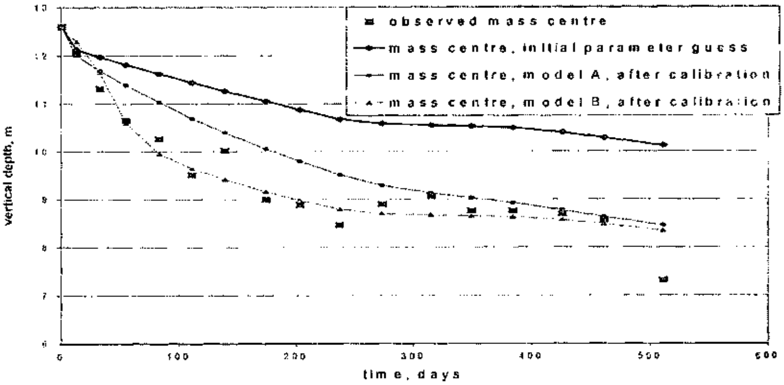

Fig. 2 Depth of the centre of mass *vs* time.

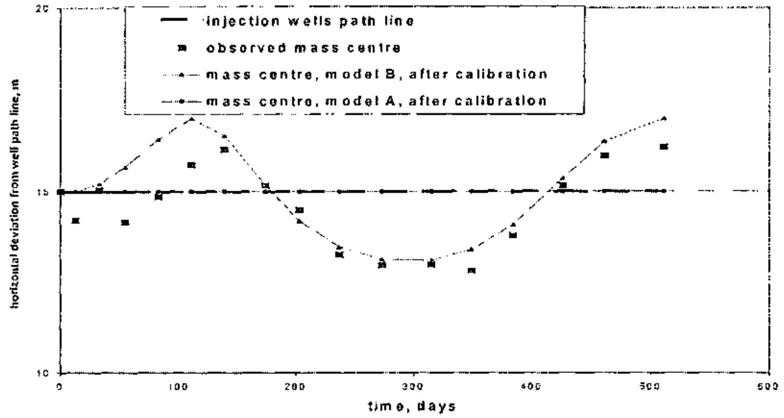

Fig. 3 Horizontal deviation of the centre of mass from the well path line.

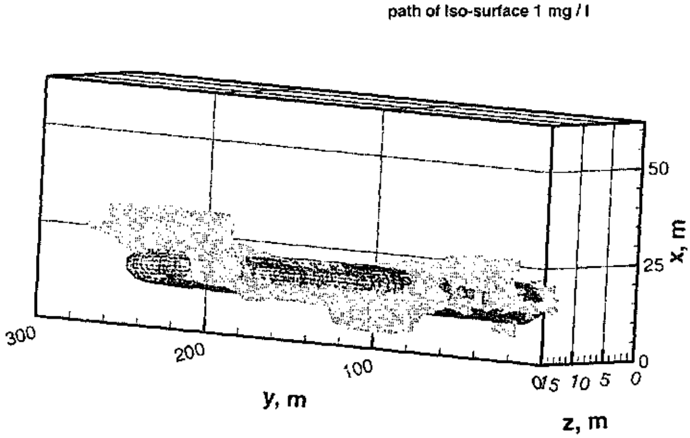

Fig. 4 3-D trail of the bromide plume (iso-surface C = 1 mg l^{-1}), at all observation times. (Flooded volume: observed concentration, mesh volume: concentration simulated with the initial parameter set).

THEORY

The non-reactive mass transport equation and the variable density flow equation are solved numerically according to the control volume method. The program system MODCALIF solves the flow equation completely implicitly and the transport equation semi-implicitly according to the FRONT LIMITATION algorithm (Haefner *et al.*, 1997). The program system considers all hydrological characteristics which are also considered by MODFLOW/MT3D and runs under VISUAL MODFLOW (Waterloo Hydrogeologic) and CADSHELL (IHU Nordhausen). MODCALIF is not bound to the usual Peclet condition (grid Peclet number <2 to 10), and therefore, a coarse grid net can also be used without causing essential errors due to numerical dispersion. MODCALIF includes a tool for automatic parameter calibration (sensitivity method) which enables the evaluation of an optimum parameter set (Haefner *et al.*, 1998).

A comparison with the exact analytical solution for the 3D-DIRAC volume source gives evidence of the error of MODCALIF due to numerical dispersion that can be neglected even in the case of a coarse grid. The injection of the bromide solution is considered to be a DIRAC impulse within the source volume; density influences and groundwater recharge are neglected. The comparing MODCALIF simulation applies a grid net of 21 × 45 × 30 cells with a horizontal increment of 2–10 m and a vertical increment of 0.5 m. The deviations of the MODCALIF isolines are always smaller than one cell increment as far as the plume extent is concerned. All MODCALIF simulations are carried out on PC Pentium II (233 MHz). One complete calculation (511 days) lasts 20–60 min.

CAPE COD EVALUATION NEGLECTING GROUNDWATER RECHARGE AND DENSITY EFFECTS

In this case, the results on the subject of dispersion that have been published so far can be verified by the analytical solution (3D-DIRAC volume source). The analytical solution with the dispersivities $\delta_L = 0.96$ m and $\delta_T = 0.018$ m, leads to plumes whose volumes are too big and whose maximum concentrations are too low compared with the measured values. A much better correspondence can be obtained with the parameters $\delta_L = 0.27$ m and $\delta_T = 0.005$ m. As there are no numerical errors in the exact solution and MODCALIF provides nearly the same results, one has to conclude that the stochastic interpretation of the dispersion according to Fitts (1996), Dagan (1998) and Fiori & Dagan (1999), results in exaggerated dispersivities being obtained and, therefore, too small a maximum concentration.

CAPE COD EVALUATION WITH GROUNDWATER RECHARGE AND DENSITY EFFECT

Groundwater recharge and density effect

Garabedian *et al.* (1991) pointed out that the recharge was very high in the first 270 days (974 mm year^{-1}). In the spring/summer of 1986 (270–384 days), however, recharge was nearly nil, but later on it approached the mean value. Constant recharge and time dependent recharge were simulated but there were no significant differences in the vertical drift. They have already assessed the influence of bromide density on the vertical drift at about 1 m. The MODCALIF simulations with variable density prove that the influence of the increased density of the bromide plume is low and smaller than 1 m in the vertical drift after 511 days (Fig. 2). The recharge causes a vertical drift of about 1.8 m.

Inhomogeneity and anisotropy of hydraulic conductivity (permeability)

Inhomogeneity and anisotropy remain the only possible causes of a vertical movement. Guided by the geological situation (LeBlanc *et al.*, 1991), the calibration of hydraulic conductivity and vertical anisotropy was attempted on the basis of the observed hydraulic heads. The result of this calibration is unsatisfactory in so far as the observed heads give too little information concerning the vertical gradient. Calibration led to a mean value of conductivity of 1.273×10^{-3} m s^{-1}. The quantity of concentration measurements (28 130 observations, sensitivity = 0.01 mg l^{-1}) is much better than the quantity of the hydraulic head measurements (~300 observations, sensitivity ~0.01 m). Thus, the weighted concentration measurements (weighted with the maximum concentration of the corresponding plume) were used as a matching criterion for horizontal and vertical conductivities. The calibration of conductivity led to a reduction of the A-model error of 0.122 to 0.105 (model A neglects the channelling of the aquifer; model B includes a calibrated channelling of the hydraulic conductivity). Figures 1, 2 and 3 show the effect of changes in conductivity, especially the good calibration of the vertical movement of the plume.

Dispersion

A surprising result of the calibration of the hydraulic conductivity is the fact that the following determination of dispersivities always leads to very small values. Figure 5 shows that the values used here (model B) reflect the spreading of the plume well. A subsequent calibration of the dispersivities did not lead to essentially different results. Corresponding to its description as a compensation process, the dispersion may often tend to replace other physical processes (dilution by groundwater recharge etc.). In order to ensure the uniqueness of this result the calibration of anisotropy and dispersivities was carried out simultaneously. The sensitivities showed that the observed concentrations are decisively influenced by inhomogeneous conductivity but only insignificantly by dispersion. After calibration of the hydraulic conductivity in subdomains (model B) the macroscale meandering of the plume (Fig. 3, Fig. 5) can be simulated. In this case the dispersivity is very small, of the order of magnitude of the pore-scale values.

CONCLUSIONS

- The stochastic analysis of Cape Cod dispersion is based on homogeneous and isotropic hydraulic parameters and tries to explain the full spreading of the plume by macro-dispersion.

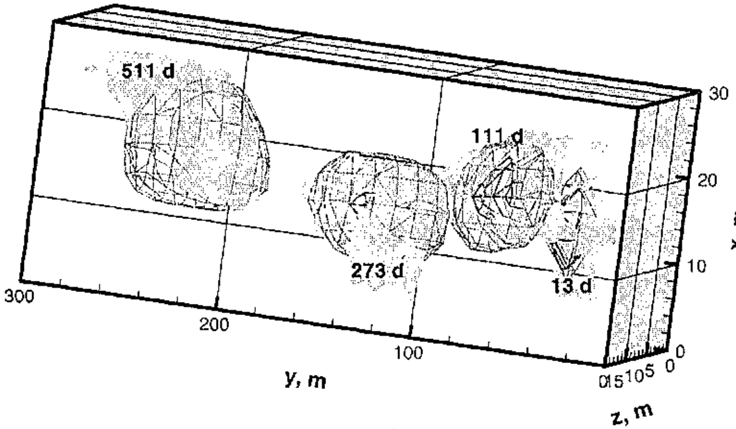

Fig. 5 3-D iso-surfaces (1, 10, 100 mg l^{-1}) of the Cape Cod bromide plume at 13, 111, 273 and 511 days, with the calibrated parameter set (model B). The *y*-axis is the principal direction. (Flooded volume: observed concentration, mesh volume: concentration simulated with the calibrated parameter set).

- The parameters for hydraulic conductivity, anisotropy and the dispersivities determined in this paper can reproduce the Cape Cod field experiment well.
- The 3-D evaluation of the Cape Cod data has proven that the 1-D or 2-D vertical section simulation cannot describe the plume movement.
- The results of a field test parameter evaluation—independent of the evaluation method—should always be verified by a full-scale simulation to avoid what we have described as only one process (like macro-dispersion) and have "offered violence to" a lot of other decisive processes (like advective transport).

REFERENCES

Dagan, G. (1998) Solute concentration fluctuations in aquifer transport: theory, simulations and field experiments. In: *Groundwater Quality: Remediation and Protection* (ed. by M. Herbert & K. Kovar) (Proc. GQ'98 Conf., Tübingen, Germany, September 1998), 575–578. IAHS Publ. no. 250.

Fiori, A. & Dagan, G. (1999) Concentration fluctuations in transport by groundwater: comparison between theory and field experiments. *Wat. Resour. Res.* **35**(1), 105–112.

Fitts, C. R. (1996) Uncertainty in deterministic groundwater transport models due to the assumption of macrodispersive mixing: evidence from the Cape Cod (Massachusetts, USA) and Borden (Ontario, Canada) tracer tests. *J. Contam. Hydrol.* **23**, 69–84.

Garabedian, S. P., LeBlanc, D. R., Gelhar, L. W. & Celia, M. A. (1991) Large-scale natural gradient tracer test in sand and gravel, Cape Cod, Massachusetts. 2. Analysis of spatial moments for a nonreactive tracer. *Wat. Resour. Res.* **27**(5), 911–924.

Haefner, F., Boy, S., Wagner, S., Behr, A., Piskarev, V. & Palatnik, B. M. (1997) The "Front Limitation" algorithm: a new and fast finite-difference method for groundwater pollution problems. *J. Contam. Hydrol.* **27**, 43–61.

Haefner, F., Boy, S., Behr, A., Kelbe, B. & Germeshuyse, T. (1998) Parameter calibration using CALIF for density-dependent groundwater flow and transport In: *Groundwater Quality: Remediation and Protection* (ed. by M. Herbert & K. Kovar) (Proc. GQ'98 Conf., Tübingen, Germany, September 1998), 521–528. IAHS Publ. no. 250.

Hess, K. M., Wolf, S. H. & Celia, M. A. (1992) Large-scale natural gradient test in sand and gravel, Cape Cod, Massachusetts. 3. Hydraulic conductivity variability and calculated macrodispersivities *Wat. Resour. Res.* **28**(8), 2011–2027.

LeBlanc, D. R., Garabedian, S. P., Hess, K. M., Gelhar, L. W., Quadri, R. D., Stollenwerk, K. G. & Wood, W. W. (1991) Large-scale natural gradient tracer test in sand and gravel, Cape Cod, Massachusetts. 1. Experimental design and observed tracer movement. *Wat. Resour. Res.* **27**(5), 895–910.

Zhang, H., Schwartz, F. W., Wood, W. W., Garabedian, S. P. & LeBlanc, D. R. (1998) Simulation of variable-density flow and transport of reactive and nonreactive solutes during a tracer test at Cape Cod, Massachusetts. *Wat. Resour. Res.* **34**(1), 67–82.