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Non-reactive solute dispersion in Triassic sandstone: laboratory simulation and an application to the field

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Abstract Non-reactive solute dispersion in a Triassic sandstone aquifer in the UK was studied by simulating conservative chemical (chloride and fluoride) plume transport in the subsurface. A new non-invasive imaging technique was developed to investigate plume transport in porous media in the laboratory and a mathematical model was used to simulate the process. Laboratory experiments show that the dispersivity of a two dimensional aquifer made up of glass beads is 0.063 mm. The range of the 50-percentile diameter (median) of particles at the field site is 150–200 μm and the groundwater velocity is approximately 10 m year^{-1}. Field data from two multilevel monitoring boreholes, 130 m and 350 m from the source along the multi-level plume flow path, were simulated. The simulation shows that the vertical dispersivity of the field site is 0.4 mm and this value can successfully predict the transport of other conservative chemicals. The low dispersion coefficient (1.2×10^{-10} m^2 s^{-1}) of the field site may suggest that for low velocity water flow, molecular diffusion is a significant factor which contributes to vertical dispersion.

INTRODUCTION

The Four Ashes plant has manufactured speciality organic chemicals since the site was opened in 1950. The plant overlies the Permo-Triassic Sherwood Sandstone, the second most important aquifer in the UK. Locally it is a fluviatile red-bed sandstone, with a porosity of about 26% and a bulk hydraulic conductivity of about 0.7 m day^{-1}. The water table is about 4 m below ground, and the aquifer is 250 m thick in the vicinity of the site. Flow velocity is about 4–11 m year^{-1} (Fig. 1). The total concentration of organic compounds in the source area is currently 24 800 mg l^{-1}. This includes about 12 500 mg l^{-1} of phenol, substantial concentrations of cresols and xylenols, and low concentrations of monoaromatics and other compounds. Two multilevel observation boreholes, BH59 and BH60, are located down stream of the contaminant source. BH59 is 130 m from the plume source area and samples groundwater to a depth of 30 m b.g.l. BH60 is 350 m from the plume source area and samples groundwater to depth of 45 m b.g.l. The principal oxidants, oxygen and nitrate, are mainly carried by groundwater flow from the back of the plume. At the core of the plume, oxygen and nitrate have been exhausted. The concentration of phenol is over 500–1000 mg l^{-1} (Anon., 1998) and it is toxic to most micro-organisms and acts as an inhibitor to biodegradation. Therefore, in the middle of the plume, biodegradation should be very slow. However, at the fringe of the plume, where the

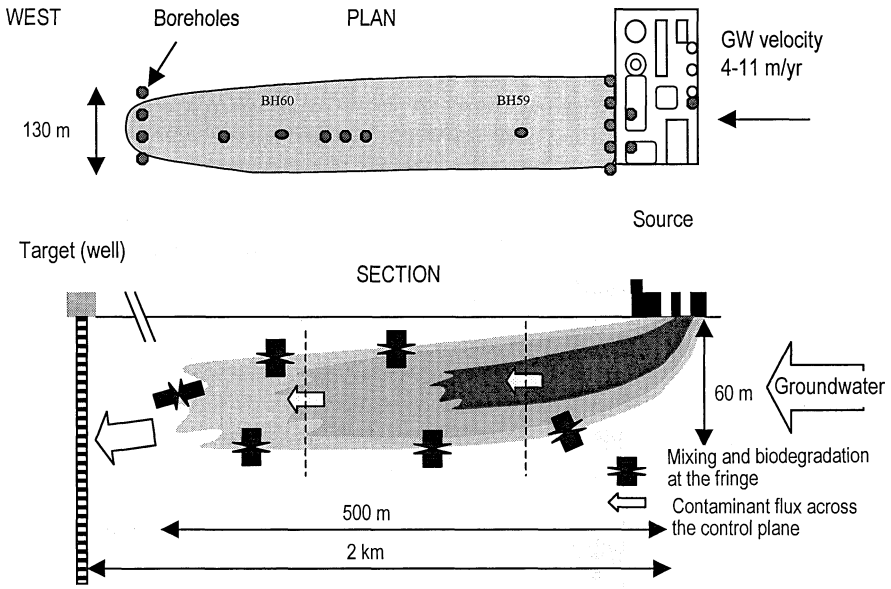


Fig. 1 Concept sketch for attenuation of biodegradables by natural oxidants.

oxidants can mix with the plume and the toxicity is decreased by dilution, faster biodegradation is expected. In this zone, the rate of natural attenuation depends on the rate of dispersive mixing of oxidants into the plume and the nature of the indigenous microbes. Research on transverse dispersion will provide more information to understand natural attenuation at the field site and to make a more valid prediction.

LABORATORY EXPERIMENT

A physical model was developed to simulate non-reactive solute transport in porous media. The schematic of the experimental setup is shown in Fig. 2. The experimental procedures were as follows. A relationship between image brightness and tracer concentration was established by measuring the brightness of different tracer concentrations under uniform conditions. A water pump created a uniform velocity of 2.17×10^{-6} m s^{-1}. A continuous input of tracer (sodium fluorescein) was started. The tracer was excited by UV light and emitted green light, and images were captured with a CCD camera every 180 s.

LABORATORY EXPERIMENT RESULTS

Imaging pictures at time 24 h, 24.5 h and 25 h totally overlap, which suggests that tracer transport has reached a steady state. The plume from a continuous line source in uniform porous media is described by (Domenico & Robbins, 1985):

$$C(x,y) = (C_0/2)\{\mathrm{erf}[(y+Y/2)/(2(\alpha_y x)^{1/2})] - \mathrm{erf}[(y-Y/2)/(2(\alpha_y x)1/2)]\} \quad (1)$$

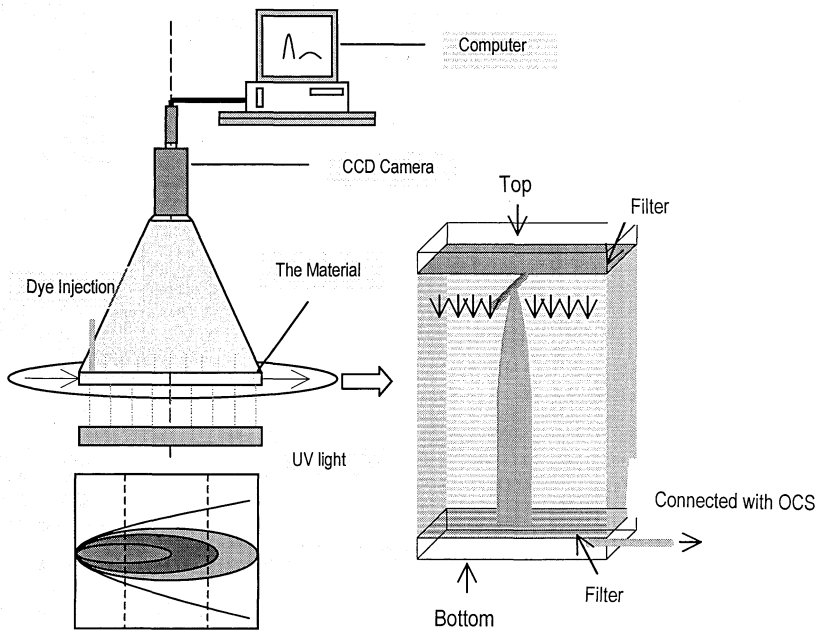


Fig. 2 Schematic of CCD-camera measurement system.

where C is concentration, C_0 is the source concentration, x is the direction of the water flow, y is the transverse direction, Y is the size of the source. To estimate how the model fits to the experimental results, we have adopted model efficiency (Vonsperling, 1993):

$$\text{Model efficiency} = 100 \times \left(1 - \frac{\sum_{i=1}^{n} (X_{Ei} - X_{Si})^2}{\sum_{i=1}^{n} (X_{Ei} - \overline{X_{Ei}})^2} \right) \tag{2}$$

were X_{Ei} is experimental data, X_{Si} is simulation data, n is the number of experimental data. Table 1 shows that model efficiencies are greater than 95% in all simulations.

Table 1 Analysis of simulation reliability.

Section X (mm)	24	80	96	135	157	174	185	202
n	136	136	136	136	136	136	136	136
Model efficiency (%)	97.4	95.9	97.3	98.0	96.7	96.6	96.2	96.7

Randomly selected sections at $X = 96$ mm (Fig. 3), 135 mm, 157 mm, 174 mm and 202 mm are simulated by equation (1). These simulations all support one value of transverse dispersivity, 0.063 mm. These simulations confirm that the equation is suitable for simulating non-reactive conservative chemical transport in the homogeneous aquifer.

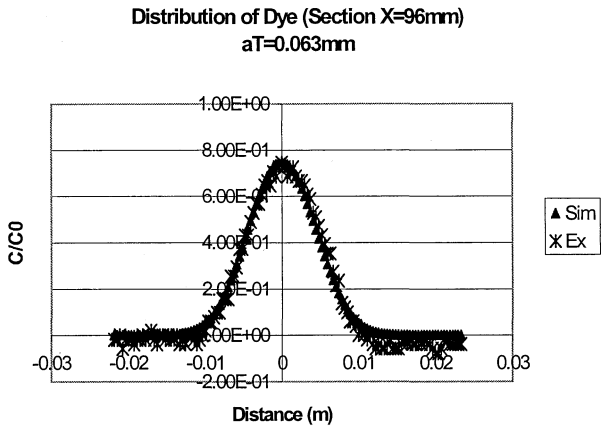


Fig. 3 Distribution of tracer at section $X = 96$ mm.

FIELD SITE DATA SIMULATION

At the field site, the subsurface geology is mainly sandstone with uniform properties. Two monitoring boreholes, BH59 and BH60, are located along the groundwater flow and contaminant plume. This allows us to simulate the transport using two-dimensional (2-D) models. The situation at the field site is very complicated. The conservative chemicals and contaminants were released at different times, concentrations and depths. The field site investigation shows that one chemical has usually formed several plumes. After the chemicals are released, they first move vertically downward to the subsurface and then are transported down gradient by advection and dispersion. The different plumes may mix at their borders. However, the upper fringe of the top plume and lower fringe of the bottom plume will not mix with other plumes and will remain unchanged. Before simulating the conservative chemicals, we assumed that the top and bottom fringes of the plumes are not disturbed by other plumes; conservative chemicals are transported without retardation and reaction, and the plumes are at steady state. Chloride, bromide and fluoride were selected as conservative chemicals to investigate transverse dispersivity at the field site. Several observations at different times showed that the distribution of these chemicals changed little in the last two years. The vertical section of the two monitoring boreholes, BH59 and BH60, is considered a 2-D transport process with line sources. Applying equation (1) to the field situation, we can simulate the conservative chemicals mentioned above.

CHLORIDE SIMULATION

Chloride simulations are shown in Figs 4 and 5. The results show that the vertical transverse dispersivity α_T is 0.4 mm. Table 2 gives an analysis of the model's efficiency at simulating the field situation; model efficiencies are greater than 95%.

The results of other studies (Gelhar *et al.*, 1992; Aldo, 1998) are shown in Table 3. There are mainly two factors responsible for transverse dispersion: molecular thermal

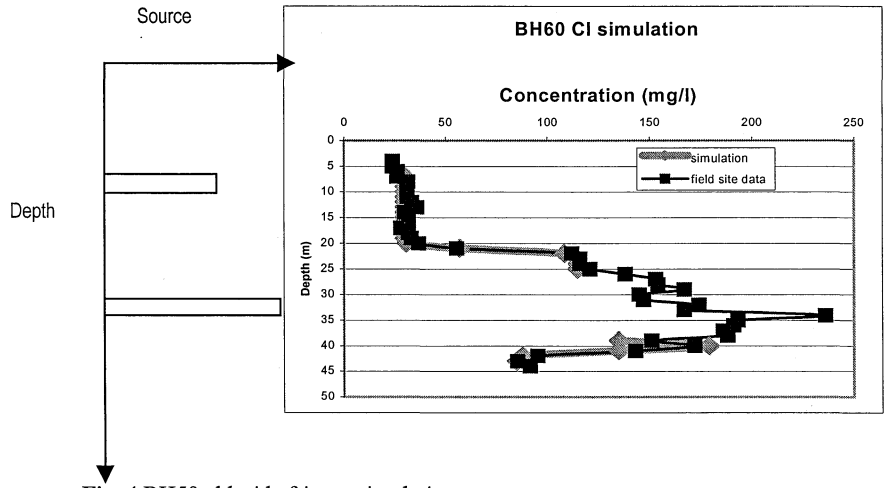


Fig. 4 BH59 chloride fringes simulation.

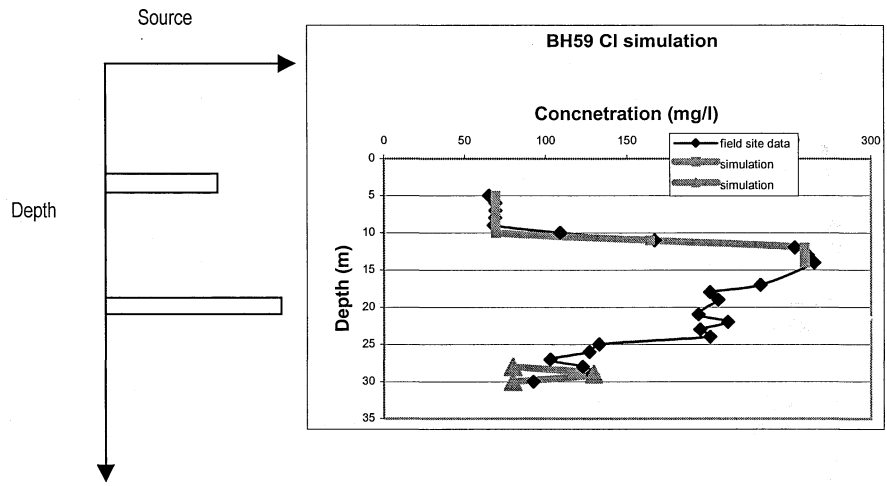


Fig. 5 BH60 chloride fringes simulation.

Table 2 Model efficiency analysis of field site simulation.

	BH59 Cl (upper fringe)	BH60 Cl (upper fringe)	BH60 (lower fringe)
Model efficiency (%)	97.6	99.2	96.4

movement and and the tortuous nature of the flow path. At much smaller velocities, mechanical dispersion and molecular diffusion will be of comparable importance and possibly of similar magnitude. Several recent investigations suggest low values of transverse dispersivity. Table 4 compares the molecular diffusion coefficient and hydrodynamic dispersion coefficient. Conversely, when the velocity of water flow is high, mechanical dispersion will be the dominant factor for transverse dispersion. So in some cases transverse dispersivity may have a higher value.

Table 3 Values of transverse dispersivity obtained in other studies (Gelhar *et al.*, 1992; Aldo, 1998).

Reference and site name	Aquifer material	Tracer	Monitoring	Velocity (m day^{-1})	Scale of test (m)	Transverse dispersivity (m)
Bredehoeft & Pinder (1973), Brunswick, Georgia	Limestone	Cl^-	2-D	–	2000	52
Freyberg (1986), Borden	Glaciofluvial sand	Cl^- Br^-	3-D	0.09	90	0.039
Fried (1975), Rhine aquifer southern Alsace, France	Alluvial	Cl^-	3-D	–	800	1
Grove (1977), NRTS, Idaho	Basaltic lava and sediment	Cl^-	2-D	–	20 000	91
Gupta *et al.* (1975), Sutter basin, California	Sandstone, shale, sand and alluvial sediment	Cl^-	2-D	3.5	50 000	8-20
New Zealand Min. of Work and Development (1977), Heretaunga aquifer	Gravel with cobbles	Cl^-	3-D	120–200	54–59	0.04–0.10
Hastings city rubbish dump	Alluvium (gravels)	Cl^-	3-D	20	290	0.07
Rabinowitz & Gross (1972), Roswell basin, New Mexico	Glaciofluvial	Cl^- Br^-	3-D	11–21	90	0.0022
Segol & Pinder (1976), Cutler area, Biscayne Bay aquifer, Florida	Fractured limestone	Cl^-	3-D	20	490	0.67
Sykes *et al.* (1982, 1983) Borden	Glaciofluvial sand	Cl^-	2-D	–	700	0.31
Aldo & Gedeon (Aldo, 1998), Borden Site	Sandstone and sediment	–	2-D	–	–	0.0005
Garabedian *et al.* (1988) Cape Cod, Massachusetts	Coarse sand	Br^-	3-D	0.43	250	0.0015
New Zealand Min. of Work and Development (1977) Roys Hill Site	Alluvium (gravels)	Br^-	3-D	20–25	25	0.06
GPRG (1999), Four Ashes, UK aquifer	Sandstone and sediment	Cl^- Br^- F^- SO_4^{2-}	2-D	0.027	350	0.0004

Table 4 Comparison of diffusion coefficient and transverse hydrodynamic coefficient.

Compounds	Materials	Diffusion coefficient ($m^2 s^{-1}$)	Transverse hydrodynamic coefficient ($m^2 s^{-1}$)
Chloride	Clay	5×10^{-10}	–
Tritium	Culebra dolomite	4×10^{-11}	–
TCE	Triassic sandstone	7.5×10^{-11}	–
Chloride	Triassic sandstone	–	1.26×10^{-10}
Fluorescein	Glass beads	–	1.09×10^{-10}

SIMULATIONS OF OTHER CONSERVATIVE CHEMICALS

Using a value of vertical transverse dispersivity α_T of 0.4 mm, we also simulated other conservative chemicals (bromide and fluoride). The results show that all simulations support this value of $\alpha_T = 0.4$ mm.

CONCLUSION

A newly developed non-invasive technique can successfully simulate 2-D solute transport in the laboratory. The advantages of this technique are that it allows non-destructive and non-invasive measurement, enables visualization of the transport process and it can effectively record information about the 2-D transport process fully. In the future, this technique will be used to investigate reactive transport in porous media in the laboratory. Equation (1) can accurately simulate the 2-D continuous line source transport and give reliable results. Using a value of vertical transverse dispersivity of 0.4 mm it can successfully simulate all the conservative plumes at the field site. Laboratory and field investigations show that the transverse hydrodynamic coefficient is approximately 10^{-10} m^2 s^{-1}, which is close to the magnitude of the pure molecular diffusion coefficient ($10^{-10} \sim 10^{-11}$ m^2 s^{-1}). The lower values suggest that in conditions of low velocity water flow, molecular diffusion may play an important role in transverse dispersion.

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