DNAPL spill and plume migration in a naturally heterogeneous aquifer analogue

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Abstract Spills of dense nonaqueous phase liquids (DNAPLs) in highly heterogeneous porous media were simulated using the compositional flow program CompFlow. Detailed realistic data giving the spatial distribution of sedimentary structures was taken from outcrop studies of sand and gravel deposits. For the scenarios studied, pore entry pressure was a major factor controlling the spatial distribution of the DNAPL, and hence its long-term dissolution into the groundwater. Thus the spatial distribution (including connectivity and local contrasts) of low pore entry pressure/high permeability regions is crucial in determining how far the DNAPL migrates the subsurface. The simulations of DNAPL spills based on the outcrop information were compared with similar scenarios simulated using geostatistical realizations of physical parameters. Gaussian realizations showed spreading of the DNAPL at lower saturations due to the inherently smooth parameter contrasts. Indicator geostatistical realizations, through reproducing the structural nature to the parameter heterogeneities and preserving contrasts, appear to lead to a more realistic reproduction of the behaviour of DNAPLs in these sand and gravel deposits. The results highlight the important role of site characterization and representation in the process of predicting the behaviour of NAPLs in heterogeneous porous media.

INTRODUCTION

The migration and fate of non-aqueous phase liquids (NAPLs) can be predicted relatively well for homogeneous porous media. However, natural geological media may exhibit a high degree of heterogeneity in both physical and geochemical parameters, leading to a much greater degree of complexity and uncertainty. Previous studies have often investigated NAPL spills in modelling studies using statistically generated parameter fields. However, it is uncertain how well these fields represent reality. In this study detailed realistic data on the spatial distribution of sedimentary structures is taken from outcrop studies of sand and gravel deposits using an aquifer analogue approach. The features of the distribution of the DNAPL are discussed and a comparison is made with spill scenarios simulated using parameter sets generated by two geostatistical methods based on the statistics of the outcrop data.

CHARACTERIZATION OF HETEROGENEOUS MEDIA: THE AQUIFER ANALOGUE APPROACH

Using outcrops as analogues of aquifer material deposited under similar sedimentary environments is an approach that provides data at a level of detail that can not be obtained by subsurface investigation techniques. In addition to being a source of information on the spatial characteristics of geological deposits, outcrops form accessible areas to obtain samples for the determination of hydraulic and hydrogeochemical parameters. The medium chosen for this study comprised highly heterogeneous sand and gravel deposits typical of alluvial aquifers such as those of the Rhine and Neckar Valleys of Southern Germany. Similar data has been used in modelling studies to investigate the effects of limited sampling on the ability to predict contaminant transport (Whittaker & Teutsch, 1999), the roles of different lithofacies in the nonequilibrium sorption of organic contaminants (Teutsch *et al.*, 1998), and the combined application of geophysical and hydrogeological techniques for subsurface characterization (Dietrich *et al.*, 1998).

SIMULATION OF DNAPL FLOW AND TRANSPORT

The study focuses on the behaviour of DNAPLs, which, as frequently occurring contaminants, pose a great threat due to their high mobililty, low regulatory concentration limits and slow biodegradation rates. The compound trichloroethene (TCE) was taken as representative of the group. Spill scenarios were simulated numerically using the model CompFlow (Unger *et al.*, 1995). A schematic diagram of the model setup is included in Fig. 1. The permeability and porosity values assigned to each sedimentary element were based on values obtained by laboratory and *in situ* determination (Jussel *et al.*, 1994). Since no constitutive relationships were available for these deposits, relationships were scaled according to porosity and permeability from relationships for sands using a modification of the Leverett J-function (Unger *et al.*, 1995). Thus the main effects of the heterogeneity are transmitted to the model through the permeability distribution, which is illustrated in Fig. 2(a). The mapped sedimentary elements represent a two dimensional cross-section through the deposits; it is assumed that the connectivity of the elements is no greater in the third dimension.

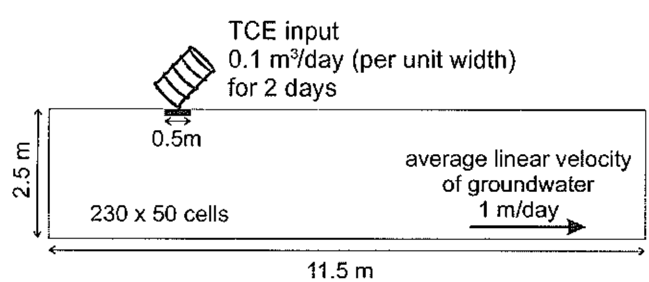

Fig. 1 Schematic diagram of the spill scenario.

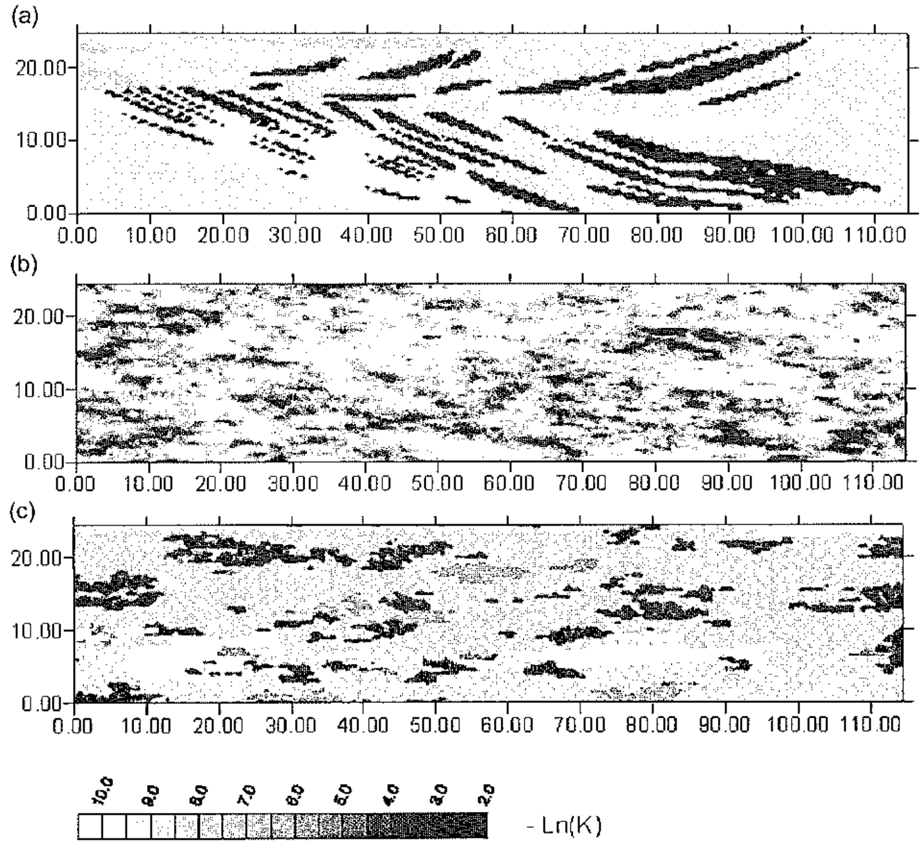

Fig. 2 Log conductivity fields: (a) outcrop data, (b) Gaussian realization, and (c) indicator realization.

FEATURES OF THE DNAPL SPILL

Figure 3(a) shows the DNAPL saturation after percolation into the saturated zone. Since the example data set consists of high permeability gravel lenses embedded in poorly sorted sands and gravels, there are relatively few well-connected regions that would lead to fast pathways for DNAPL migration. Instead, most lenses exhibit low connectivity and are surrounded by material of much lower permeability (and having high pore entry pressures). Thus they act as accumulation areas, where pores can become fully saturated with the NAPL. Thus the major factor controlling the spatial distribution of the DNAPL (and hence its long-term dissolution into the groundwater) in this type of heterogeneous material is found to be the pore entry pressure. A large proportion of the DNAPL is left in high saturation pools, where there is, at most, only very slow water movement. Figure 3(a) shows the development of the plume two days after the end of the spill, highlighting the existence of preferential paths for groundwater flow and solute transport.

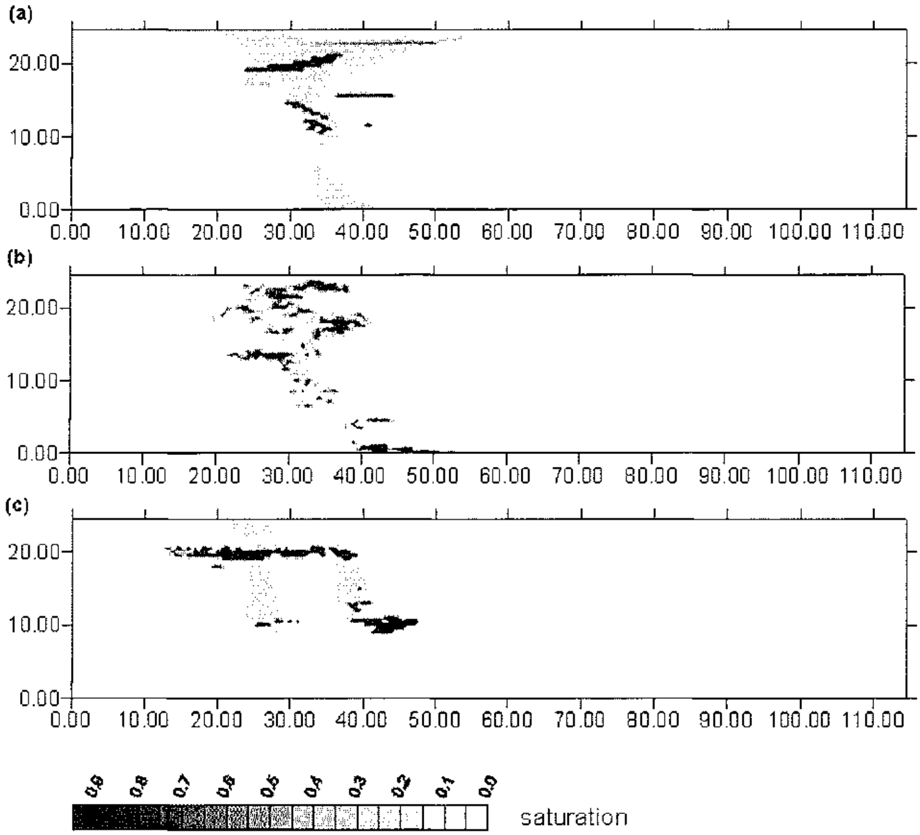

Fig. 3 TCE phase saturation: (a) outcrop data, (b) Gaussian realization and (c) indicator realization.

REPRESENTATION OF THE HETEROGENEOUS POROUS MEDIUM BY GEOSTATISTICAL REALIZATIONS

For many purposes there is a need to predict groundwater flow and contaminant transport over larger scales than are feasibly characterized through aquifer analogue studies; there is thus a requirement to be able to generate synthetic, but realistic data for input into such models. The simulations of DNAPL spills based on the outcrop information were compared with similar scenarios simulated using two geostatistical simulation techniques. The statistical parameters required by each of the techniques were based on the exhaustive data; the added complexity of parameter uncertainty through limited sampling of the geological medium was not considered.

Although Gaussian realizations are frequently applied to represent heterogeneous porous media, they have inherent characteristics that appear to differ from natural heterogeneous material (Fig. 2). Firstly, Gaussian realizations show low contrasts in parameter values, i.e. there are always smooth transitions from low to high values.

This is obviously in contrast to the sand and gravel deposits examined in this study, where depositional and erosional events may lead to sharp contrasts in material properties. Secondly, there is low correlation of extreme values, so that both low and high permeability areas have little structure and connectivity. These features of the statistical realizations lead to the DNAPL being distributed at lower saturations (Fig. 3(b)), meaning that the groundwater is able to flow through the contaminant source area at higher velocities, transporting the DNAPL solute away from the source at a faster rate, as illustrated by the progression of the plume (Fig. 4(b)).

Simulations of DNAPL migration on parameter fields generated by indicator geostatistics (Deutsch & Journel, 1992) lead to accumulation of DNAPL in high saturation pools similar to those observed for the outcrop data. Indicator techniques, however, represent a higher demand for site data interpretation than does the Gaussian method. Frequencies and correlation structures are required for each different indicator bandwidth. Thus, given enough information, it is possible to define the structural characteristics of each category of sedimentary element.

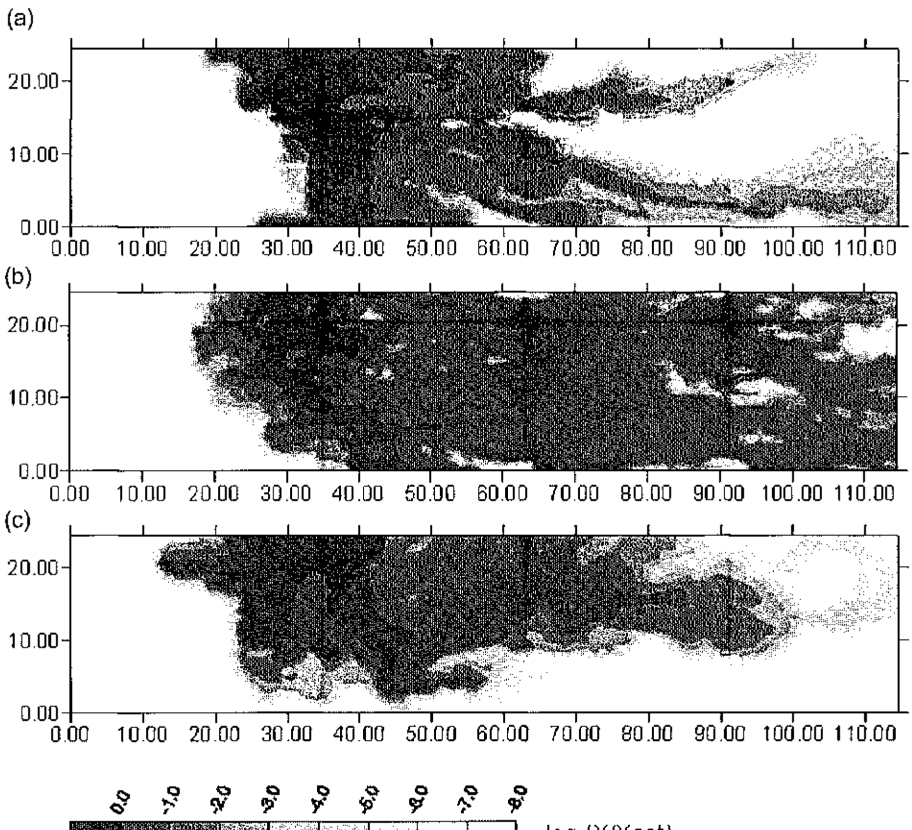

Fig. 4 TCE solute concentration (as molar fraction X); (a) outcrop data, (b) Gaussian realization and (c) Indicator realization.

CONCLUSIONS

The aquifer analogue approach was used in a numerical investigation of the characteristics of a DNAPL spill in a highly heterogeneous porous medium. The degree of connectivity of the geological structures, and the contrasts in hydraulic values, have a large influence on the extent of DNAPL penetration and the spatial saturation distribution. Comparisons were made with spills simulated for parameter fields generated by geostatistical methods. Indicator realizations were able to reproduce areas of accumulation of DNAPL at high saturations similar to those observed using the outcrop data. However, Gaussian realizations resulted in more even spreading of the DNAPL and consequently higher groundwater velocities flowing through the contaminant source area. The simulations highlight the important role of site characterization and representation in the process of predicting the behaviour of a NAPL in a heterogeneous porous medium.

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