INTRODUCTION

Dense non-aqueous phase liquids (DNAPLs) are notoriously difficult to locate in the subsurface. This single factor has serious implications when assessing the risk to groundwater from dissolution of DNAPLs, or to targeting a DNAPL source zone with a specific remediation technology. Characterising DNAPL source zones requires reliable estimates of the mass distribution of the DNAPL in the subsurface, based on the nature of the DNAPL release, the geological structure, and the physicochemical properties of the DNAPL.

The subsurface migration of a DNAPL is largely determined by the geological structure, in particular by heterogeneities in the rock – where rock fractures represent an extreme end-member. Where rock fractures are present they will, at least in the early stages of migration, provide the primary pathway for DNAPL movement (Whittaker et al., 1998). However, it is exceedingly difficult, and probably not possible, to fully characterise the spatial distribution and physical properties of all fractures in a given geological setting (Sudicky et al., 1998). Therefore statistical representations of fracture parameters are used simulate real geological environments, thereby incorporating uncertainty, which is inherent in the fractured rock-mass characterisation approach.

Figure 1. An aquifer analogue and the typical range of data scales required for characterising fractured rock aquifers.
APPROACHES

Estimates of DNAPL penetration depth are derived in a tiered approach: 1) a stochastic discrete fracture network model is utilized to generate statistically representative realisations of the fractured rock mass; 2) a fully 3-D invasion percolation model describing quasi-equilibrium 2-phase flow is employed to derive a distribution of bulk retention capacity for a given DNAPL for each of the DFNM realisations; and 3) the bulk retention values are then applied to a given aquifer geometry and spill scenario to estimate a distribution of DNAPL penetration depths.

Fractured rock mass characterisation should be undertaken at a range of scales (Figure 1): Regional scale lineaments (faults) mapped at the sedimentary basin scale indicate the potential influence of basinal scale features on the heterogeneity of fracturing, particularly adjacent to basin margins, and Regional scale lineaments (faults) mapped at the sedimentary basin scale indicate the potential influence of basinal scale features on the heterogeneity of fracturing, particularly adjacent to basin margins, and fracture orientations measured at outcrops across a sedimentary basin provide the regional context for fracture network characteristics observed at the outcrop and borehole scales; Outcrop scale mapping involves 1-D scanline and 2-D tracemap surveys and provide the input data to the to the discrete fracture network model; Borehole scale studies focus on characterising the hydraulic properties of the fracture network, and confirming fracture trends observed at outcrop.

The successful interpretation of fracture data is an iterative process that progresses by data collection and synthesis, the development of a conceptual model, and construction of a numerical model (Jones et al. 1999). Description of the fracture parameters for fracture network analysis is based on the separation of data into discrete sets, which are described by their statistical properties and by approximation to theoretical distributions.

Results from the numerical model are subject to potential biases both from i) the capability of the numerical model to represent geological reality and, ii) our ability to measure fractures and fracture networks at the scales of interest. It is the potential bias resulting from the ability to characterise fractured rocks that is the focus of the following discussion. Uncertainty in the representation of the principal fracture network properties may result from a number of sources (Table 1).

<p>| Table 1. Sources of potential bias for the principal fracture network parameters |</p>
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Derived fracture network property</th>
<th>Potential bias</th>
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<tbody>
<tr>
<td>Fracture spacing</td>
<td>Fracture intensity and block size</td>
<td>• Spacing, and hence block size, may be overestimated if values are not corrected for scanline orientation</td>
</tr>
<tr>
<td>Fracture orientation</td>
<td>Fracture inclination, strike and fracture set</td>
<td>• Outcrops subject to weathering and stress relief may lead to inaccurate measurement of fracture orientation</td>
</tr>
<tr>
<td>Fracture trace length</td>
<td>Apparent fracture size</td>
<td>• Fractures commonly censored due to scale of observation (outcrop or borehole) it is therefore difficult to constrain true fracture size</td>
</tr>
<tr>
<td>Fracture termination mode</td>
<td>Fracture connectivity</td>
<td>• Poor representation of 3D connectivity based on termination percentage measured in 2D tracemaps</td>
</tr>
<tr>
<td>Fracture aperture</td>
<td>Apparent fracture aperture</td>
<td>• Hydraulic apertures underestimate aperture; mass balance aperture (from tracer tests) may be more representative for predicting fracture porosity</td>
</tr>
<tr>
<td>Fracture infill</td>
<td>Percentage open fracture for fluid flow</td>
<td>• Calculating hydraulic aperture by assigning equal transmissivity to each of the fractures in a hydraulic test zone assumes an unlikely hydrogeological model</td>
</tr>
<tr>
<td>Fracture aperture</td>
<td>Percentage open fracture for fluid flow</td>
<td>• Are fractures open or filled (e.g., with sediment)?</td>
</tr>
<tr>
<td>Fracture infill</td>
<td>Percentage open fracture for fluid flow</td>
<td>• How are the effects of sediment filled fractures incorporated in contaminant transport models?</td>
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</tbody>
</table>
Measurement error, whether intentional or not, is accommodated in the stochastic modelling approach by the process of iteratively sampling the distribution functions which describe the given parameters. Where the stochastic realisations form the input to a two-phase model, the rules for preserving uncertainty are obeyed. This uncertainty is then propagated through to estimates of DNAPL penetration depth.

**ESTIMATING DNAPL PENETRATION DEPTHS**

A fully 3D macroscopic-scale invasion-percolation model, which utilises the output from the fracture network simulator, is being developed. The model will test the hypothesis of DNAPL connectivity, by predicting penetration depths based on spill volume and available fracture porosity. The model incorporates some of the physics of two-phase flow, but assumes that the capillary forces are dominant and that viscous forces are negligible. Invasion is initiated from a non-wetting NAPL discrete volume source with a given density and interfacial tension (IFT). The invasion front progresses by successively invading connected fractures where the capillary pressure ($P_c$) of the invading fluid exceeds the threshold (entry) pressure ($P_e$) of the given fracture (Kueper & McWhorter 1991). The capillary pressure

$$P_c = (\rho_{nw} - \rho_w)gh$$

(1)

where $\rho_{nw}$ is the non-wetting phase density; $\rho_w$ is the wetting phase density; g is the gravitational constant; and h is the height of the pool of DNAPL.

$$P_e = \frac{2\sigma \cos \theta}{e}$$

(2)

where $\sigma$ = interfacial tension between the DNAPL and water; $\theta$ = contact angle on the fracture walls; and $e$ = fracture aperture.

At present the fractures are represented by homogenous 2D planes, based on a parallel-plate model assuming constant aperture, with an inter-model aperture distribution which is a function of the statistical input parameters of the fracture network simulator.

The non-wetting phase residual saturation ($S_{NWr}$) is determined as a function of dip (Longino and Kueper 1999) for individual pathway fractures. End-members for residual saturation are: dip $0^\circ$ $S_{NWr} \approx 21\%$, and dip $90^\circ$ $S_{NWr} \approx 3.2\%$. The derived bulk retention capacity (a function of $S_{NWr}$) is then used to estimate DNAPL penetration depths by comparison with given spill volumes. The bulk retention values are then applied to a given aquifer geometry and spill scenario to estimate a distribution of DNAPL penetration depths (Figure 2).

A number of modelling scenarios are envisaged based on spill volume, spill area, and variable fluid properties. Future developments aim to include accessibility of the resident fluid through the fracture walls to the matrix, applying aperture distributions to individual fractures, and a visual model output.
DISCUSSION

This approach provides a methodology for estimating DNAPL penetration depths in fractured aquifers, based on parameters that can be measured at most sites which have been impacted by DNAPLs. The approach to estimating penetration depths, based on bulk retention capacity, gives an indication of the likely impact of DNAPL spills, and will aid risk assessment.

Reducing uncertainty in modelling the migration of limited volume DNAPL spills in fractured systems requires detailed representation of the fracture system. Clearly, this cannot be achieved through the use of REVs or equivalent porous media approaches. Therefore, a stochastic fracture network model is employed to provide discrete representation of the characteristics of heterogeneity in the fractured rock mass.

The invasion percolation model is based on the output from the fully 3D fracture network simulator. Estimation of DNAPL penetration depth is subject to the limiting assumptions of both models, but does accommodate the uncertainties resulting from our abilities to both measure and represent geological reality in numerical models.

REFERENCES


