Calibration and Reliability in Groundwater Modelling: From Uncertainty to Decision Making
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Palaeo-evolution and uncertainty analysis of regional groundwater flow in discretely fractured crystalline rock

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Abstract A detailed groundwater flow analysis of an 83 km^2 portion of a larger regional 5734 km^2 watershed situated on the Canadian Shield has been conducted to illustrate aspects of regional and sub-regional groundwater flow evolution since the retreat of the Laurentide ice-sheet approximately 11 000 years ago. Field investigations at the Underground Research Lab (URL) of the Whiteshell Research Area (WRA) near Lac du Bonnet, Manitoba, show evidence of anomalously high piezometric heads and high total dissolved solids (TDS) concentrations of 50 to 100 g L^{-1} in the deeper sparsely fractured rock (SFR). Elevated heads are a result of surface loading from the Laurentide Ice Sheet, while salinity of most of the fracture groundwaters and the pore fluids is derived from a marine source, likely as a result of infiltration during early Palaeozoic times. The hydrogeochemical data indicate that below 500 m at the URL, fracture hosted groundwaters are very saline, reducing, and old. The groundwater can be considered essentially stagnant for at least 1 000 000 years. The discrete-fracture dual continuum finite element model FRAC3DVS was used to investigate the importance of large-scale fracture zone networks on flow and particle migration. As part of the analysis, 100 complex irregular equally probable Fracture Network models were delineated from surface features and superimposed onto a 600 000 element flow domain mesh. Orthogonal fracture faces (between adjacent finite element blocks) were used to best represent the irregular discrete-fracture network. The crystalline rock between these structural discontinuities was assigned properties characteristic of the URL representing either SFR or moderately fractured rock (MFR). An uncertainty analysis of the 100 fracture realizations on flow system characteristics is provided herein.

Keywords Canadian Shield; fractures; FRAC3DVS; Laurentide Ice Sheet; over-pressures; regional scale; salinity; stochastic; sub-regional scale

INTRODUCTION

Work is being conducted to advance the understanding of groundwater flow and groundwater flow system evolution in Canadian Shield settings at time and space scales relevant to the safety of a deep geological repository for used nuclear fuel. A key aspect in this work relates to groundwater flow system behaviour and dynamics at regional and local scales. At these scales, assumed flow system dimensionality, fracture interconnectivity, site specific spatial distribution of physical and chemical properties coupled with transient boundary conditions occurring as a result of long-term climate change, may markedly affect concepts of flow system stability as related to groundwater flow paths, hydraulic gradients, velocity fields and residence times.

As part of the analysis, a descriptive conceptual model is derived based on field data gathered at the Atomic Energy of Canada Ltd (AECL) Whiteshell Research Area (WRA), and information available from international geoscience radioactive waste management programmes. The primary goal of the analyses is the prediction and illustration of the sensitivity of groundwater flow pathways and residence times to assumed flow domain boundary conditions and parameters. Of particular interest is the role of topographic and density (salinity) gradients at regional and repository scales on groundwater flow paths. In this study, ArcView Geographic Information System (GIS) is used to facilitate data and model output management and visualization. For the sub-regional scale analyses, the approach includes the explicit inclusion of a site-specific, field constrained Fracture Network Model (FNM).

The sub-regional scale model was implemented using the dual continuum model FRAC3DVS. FRAC3DVS (Therrien *et al.*, 2001) is a numerical algorithm for the solution of three-dimensional variably-saturated groundwater flow and solute transport in discretely-fractured porous media. The model includes a dual-porosity formulation, in which discrete fractures are idealized two-dimensional parallel plates. Versions of the model couple fluid flow with brine transport through the fluid density that is dependent on both pressure and brine concentration.

MODELLING DATABASE

The analyses presented in this paper are based on three-dimensional groundwater flow in a hypothetical watershed; however, the properties of the watershed and rock domain are representative of the characteristics of typical crystalline rock systems in the Canadian Shield. The predominant rock type within the watershed is massive to foliated granodiorite to granite. The surficial geology of the watershed is predominantly exposed granite with small till-covered areas.

The hypothetical sub-regional model domain was chosen from several candidate sites within the regional watershed shown in Fig. 1 (Sykes *et al.*, 2003). The hypothetical regional model domain contains two major rivers, a northern and a southern, each draining their respective portion of the larger watershed. Criteria such as the range in topographic relief, as well as, the areal extent, shape, and location of boundary conditions (rivers, lakes, and wetlands) were considered. The chosen domain has an area of approximately 83 km^2, an easting extent of 10.8 km and a northing extent of 12 km as shown in Fig. 2. As can be seen in Fig. 1, the northern topographic divide of the modelled area is coincident with the watershed divide between the northern and southern rivers.

The FRAC3DVS model was applied to the hypothetical sub-regional site. Various GIS data sources were used to facilitate the development of the sub-regional model: (1) Digital Elevation Model (DEM) with a planimetric resolution of 3 arc seconds and a vertical resolution of 1.0 m; (2) Digital NTS (National Topographic Service) maps at a scale of 1:50 000 to represent contours, lakes, rivers, wetlands, dams, and other features found on the NTS maps; and (3) Aerial photography at a scale of 1:60 000 from the National Air Photo Library (NAPL). The aerial photography was digitized, orthorectified, and mosaiced to the Digital NTS GIS files.

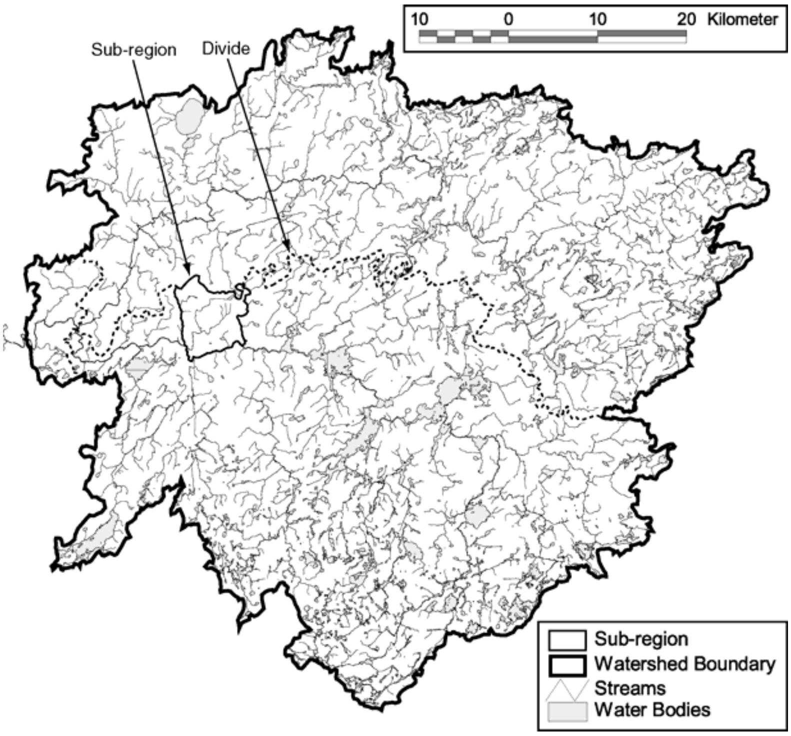

Fig. 1 Location of sub-regional model within regional domain.

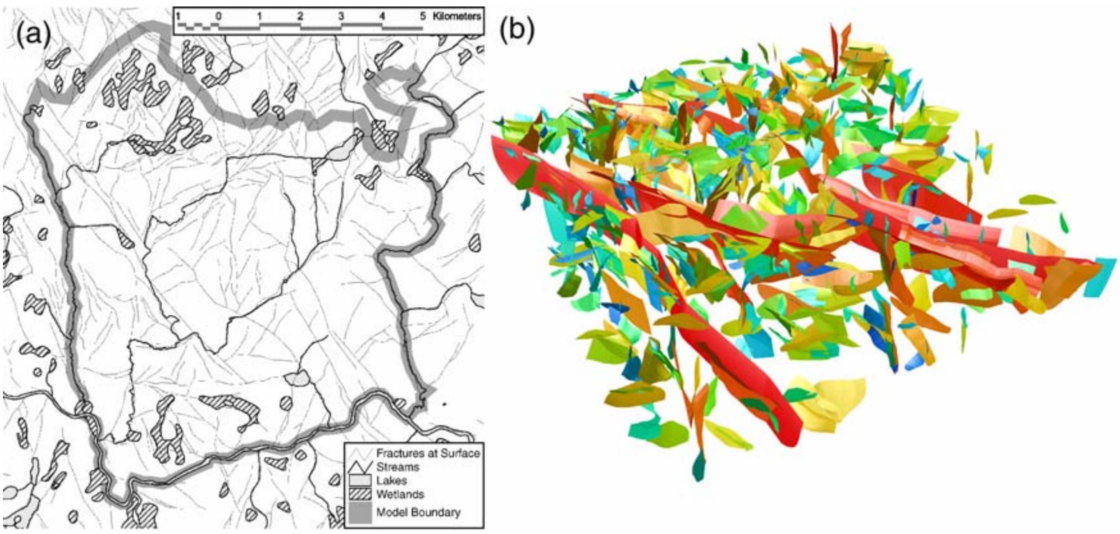

Fig. 2 (a) Sub-regional model domain with water features and fractures that intersect ground surface, and (b) 3-D view of a single fracture network realization.

Conceptual model development

Surface water features such as wetlands, lakes and rivers are defined as Dirichlet (Type I) boundary conditions. A Digital Elevation Model (DEM) was used to establish the elevation of these water features, and consequently the top layer of the numerical model. A recharge boundary condition (Type II or Neumann) was not used to represent infiltration from precipitation for the top surface of the model, but rather the Dirichlet boundary condition of fixed piezometric head was applied. This application is based on the fact that the water table is typically a subdued representation of surface topography. The northern model boundary was chosen based on a topographic divide, while the eastern, southern, and western model boundaries were chosen coincident with rivers. An implied assumption, consistent with regional scale simulations, was that such rivers create flow divides beneath which groundwater cannot flow.

The three-dimensional sub-regional domain is discretized into 610 320 nodes, and 568 442 brick elements. The grid is orthogonal with each matrix element having the same planimetric dimensions of 50 × 50 m. The model is vertically discretized into 19 layers; each layer containing the same number of elements. The vertical thicknesses of the layers are presented in Table 1.

Table 1 Model properties by layer.

Layer	Thickness (m)	Bottom elev. (m)	Hydraulic conductivity ($m\ s^{-1}$): Case 1	Case 2	Case 3
19	10	Var.	7.0×10^{-8}	7.0×10^{-7}	7.0×10^{-7}
18	20	Var.	7.0×10^{-9}	7.0×10^{-8}	7.0×10^{-8}
17	40	Var.	7.0×10^{-9}	7.0×10^{-8}	7.0×10^{-8}
16	80	Var.	6.0×10^{-11}	8.0×10^{-10}	5.0×10^{-9}
15	100	Var.	4.0×10^{-12}	7.0×10^{-11}	1.0×10^{-9}
14	100	0	4.0×10^{-12}	7.0×10^{-11}	1.0×10^{-9}
13	100	–100	1.0×10^{-12}	3.0×10^{-11}	5.0×10^{-10}
12	100	–200	1.0×10^{-12}	3.0×10^{-11}	5.0×10^{-10}
11	75	–275	8.0×10^{-13}	7.0×10^{-12}	5.0×10^{-11}
10	50	–325	8.0×10^{-13}	7.0×10^{-12}	5.0×10^{-11}
9	50	–375	8.0×10^{-13}	7.0×10^{-12}	5.0×10^{-11}
8	50	–425	2.0×10^{-13}	1.0×10^{-12}	1.0×10^{-11}
7	50	–475	2.0×10^{-13}	1.0×10^{-12}	1.0×10^{-11}
6	50	–525	2.0×10^{-13}	1.0×10^{-12}	1.0×10^{-11}
5	75	–600	2.0×10^{-13}	1.0×10^{-12}	1.0×10^{-11}
4	100	–700	2.0×10^{-13}	1.0×10^{-12}	1.0×10^{-11}
3	150	–850	2.0×10^{-13}	1.0×10^{-12}	1.0×10^{-11}
2	200	–1050	2.0×10^{-13}	1.0×10^{-12}	1.0×10^{-11}
1	200	–1250	2.0×10^{-13}	1.0×10^{-12}	1.0×10^{-11}

The aerial photography served as a basis for developing the various fracture features. A surface lineament analysis was conducted by Srivastava (2002) to define the major fracture features. These fracture features are primarily coincident with surface drainage features that exhibit linearity. Additional surface lineaments were created to account for the extension of existing major lineaments, and to preserve site-specific fracture density in areas where overburden cover would have obscured the surface lineaments or where the aerial photograph had weak contrast. The resulting surface fracture features are shown in Fig. 2(a). The surface traces are then propagated to depth. The resulting discrete fracture network contains a high degree of realism that honours many geological, statistical, and geomechanical constraints (Srivastava, 2002). A three-dimensional view of the discrete-fracture network is shown in Fig. 2(b).

The geometry of individual curve-planar fracture surfaces in the discrete fracture model is described by an interconnected network of triangular facets as depicted in Fig. 3(a). Because an orthogonal brick finite element mesh was used, software was developed to create orthogonal fractures that best represents each fracture feature. The resulting orthogonal fracture representation is shown in Fig. 3(b). The stepped nature of the orthogonal fracture accommodates both the dip and orientation of the original fracture feature.

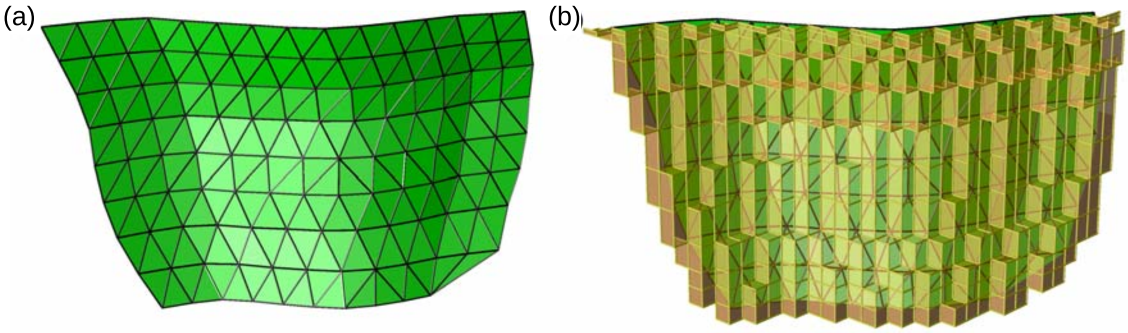

Fig. 3 (a) A single triangulated fracture, and (b) an orthogonal fracture representation of the single triangulated fracture, seen in the background.

Model properties

The FRAC3DVS sub-regional model is comprised of 19 layers. The porosity throughout the modelling domain is assumed to be 0.002. Table 1 lists the layer thickness, the bottom elevation, and the hydraulic conductivity for three cases representing different hydraulic conductivities for the deeper rock. Case 1 represents a low conductivity deep rock, while Case 3 represents a higher conductivity. Case 2 represents an intermediate hydraulic conductivity of 10^{-12} m s^{-1} for the deeper rock, midway between Case 1 and Case 3. The hydraulic conductivities listed in Table 1 are isotropic with respect to the three principal axes for all layers and all cases. Fracture properties are uniform with a hydraulic conductivity of 10^{-6} m s^{-1} and a 1 m width. Layers 1 through 14 inclusive have a constant thickness, while Layers 15 through 19 have a variable thickness which depends on the elevation of the ground surface.

100 fracture network realizations

One hundred fracture network realizations were generated and used in steady-state flow analyses to determine the influence of stochastic fracture geometry on the groundwater flow system. Each fracture network model uses the same surface lineaments shown in Fig. 2(a). A plot of the probability of intersecting a fracture at a depth of 720 m is shown in Fig. 4. This figure shows the regions of unfractured rock that would be suitable for the siting of a hypothetical waste repository.

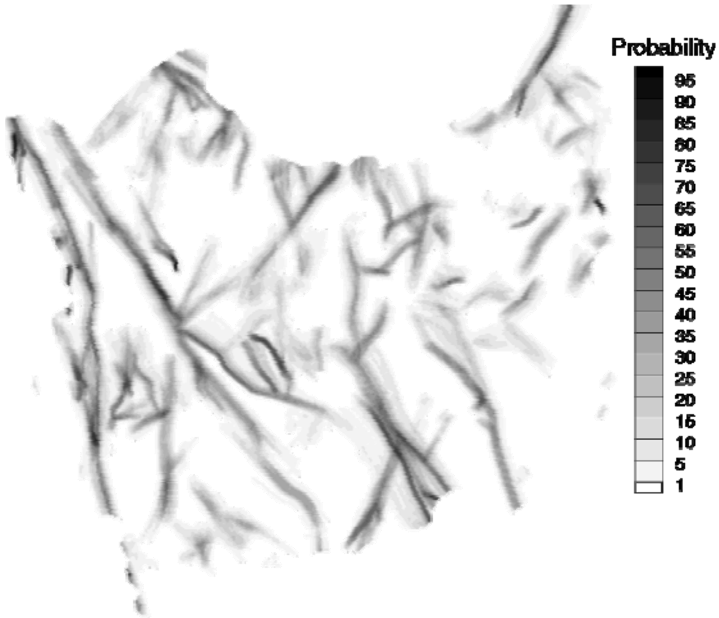

Fig. 4 Probability of fracture intersection at a depth of 720 m.

RESULTS AND CONCLUSIONS

Steady-state groundwater flow and transient 10 000 year brine migration simulations were performed. First and second moments for the 100 Monte Carlo flow and brine migration simulations were calculated to determine the extent to which the 100 realizations for fracture geometry would affect either set of simulations. Only the standard deviation for both sets of simulations are shown in Fig. 5. As can be seen, fracture variability can markedly affect not only piezometric heads, but primarily solute migration. Fractures represent high conductivity pathways, and hence are able to transmit fluids at much greater velocities than is typical of the rock matrix. The locations of these fractures will naturally control solute migration in a fractured rock setting.

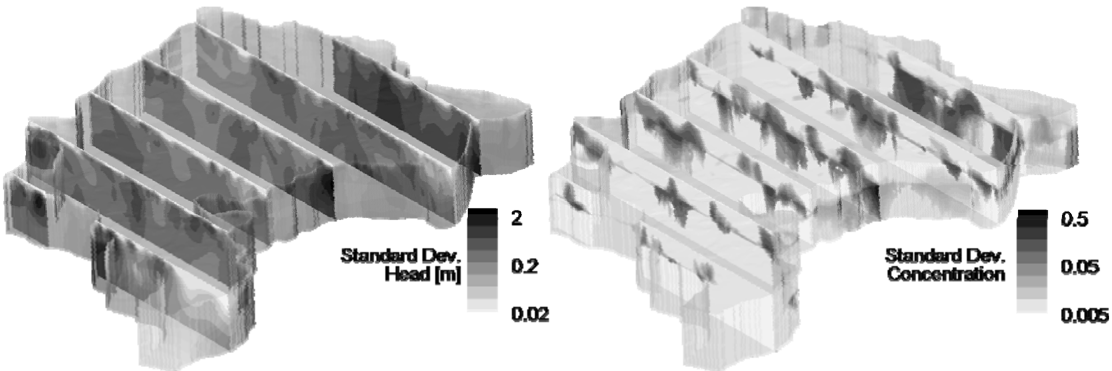

Fig. 5 Standard deviation of piezometric head and of brine concentration.

Further numerical experiments are underway to determine the influence of variable surface lineaments along with variable fracture propagation with depth, and the role of spatially variable fracture properties such as porosity, permeability, and width on these and other performance measures, including various percentile based travel times, and groundwater ages.

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