Status of International Collaborations on Modeling the Bentonite Rock Interaction Experiment

Fuel Cycle Research & Development

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1. BACKGROUND

As part of the Crystalline Rock Disposal R&D work package in the Used Fuel Disposition Campaign (UFDC), Los Alamos National Laboratory is developing a new discrete fracture network (DFN) modeling capability (Painter et al., 2012; Hyman et al., 2013). DFN models depict the rock mass as an interconnected network of explicitly represented fractures. The approach is in the reductionist tradition, implicitly assuming that detailed statistical descriptions of small observable features will, once combined in numerical simulations, lead to understanding of the system as a whole. Networks of fractures are first stochastically generated using a stochastic model derived from site data. A computational mesh is placed on each fracture plane usually ensuring that the mesh on each of a pair of intersecting fractures matches along the intersection. Groundwater flow equations are then solved using this computational mesh. The final step is then to simulate radionuclide transport using the computed flow field, usually by particle tracking. DFN simulations were introduced first in theoretical studies; feasibility of detailed site-specific applications has also been clearly demonstrated (e.g. Cvetkovic et al. 2004, Svensk Kärnbränslehantering 2011).

The Swedish Nuclear Fuel and Waste Management Company (SKB) is currently conducting a multiyear flow experiment in the fractured crystalline rock at the Äspö Hard Rock Laboratory (Äspö HRL). The Bentonite Rock Interaction Experiment (BRIE, www.chalmers.se/en/projects/Pages/brie.aspx, Bockgård et al., 2010) is focused on the interaction between rock and bentonite in a borehole similar to those planned for emplacement of waste in the KBS concept for disposal in crystalline rock. The main objectives of the BRIE are better understanding of the movement of water across the bentonite-rock interface, better prediction of wetting of the bentonite, and better characterization methods for emplacement boreholes. The site selected for BRIE is located at 420 m depth in the TASO-tunnel of Äspö HRL.

Details of the BRIE can be found elsewhere (Bockgård et al., 2010). The main part of the experiment comprises two bentonite-filled boreholes that are monitored as water flows from the surrounding fracture network into the bentonite. The experiment involved several phases: characterization of the site, drawdown of the water table near the two emplacement boreholes, emplacement of the bentonite, wetting of the bentonite, and post-experiment recover and analyses of the bentonite. Tunnel and borehole geometry in the vicinity of the BRIE is shown in Figure 1. The two arrows indicate the positions of the boreholes in which bentonite was placed. Five pilot boreholes shown in Figure 1 were first drilled in the bottom of the tunnel. These boreholes and the nearby tunnels made it possible to infer the position of three major fractures, which are shown in Figure 2. The pilot boreholes were then pumped to draw down the water table. Two emplacement boreholes were then drilled to a diameter of 30 cm and the bentonite emplaced. The bentonite contained relative humidity sensors to allow the saturation of the bentonite to be monitored.

This report summarizes the status of the UFDC's efforts to model the BRIE experiment using the new DFN modeling capability. The main objective of the work is to trial and refine the DFN modeling capability using the BRIE site as a relatively well characterized demonstration site. This work is part of SKB's Task Force on Groundwater Flow and Transport Modeling (Bockgård et al., 2010, www.skb.se/templates/SKBPage____37222.aspx), which involves modeling teams from several countries.

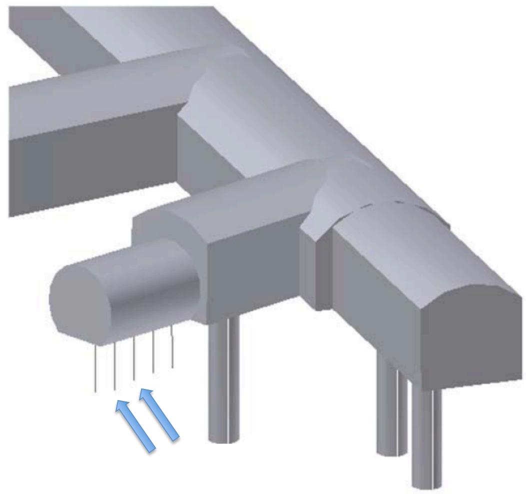

Figure 1. Tunnel geometry in the vicinity of the BRIE. The two arrows indicate the positions of the bentonite boreholes. Modified from Bockgård et al. (2010).

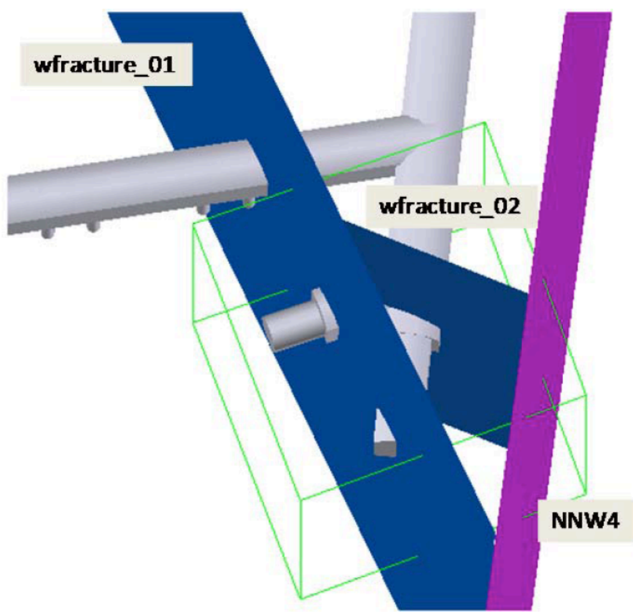

Figure 2. Location of known fractures near the BRIE. The green box shows the location of the modeling domain. Modified from Bockgård et al (2010).

2. MODEL DEVELOPMENT REQUIRED TO SUPPORT THE BRIE MODELING EFFORT

The scope of the modeling task is to model wetting of the bentonite in the emplacement boreholes. This requires that flow in the fracture network near the boreholes also be modeled. The DFN grids are locally two-dimensional whereas the emplaced bentonite requires a conventional three-dimensional space-filling grid. As preliminary step in the BRIE modeling, the UFDC's DFN modeling capability needed to be extended to allow for hybrid DFN/volume grids.

The procedure used to create hybrid DFN/volume meshes is illustrated in Figure 3. In this example, the interior of a cylinder is to be meshed and merged with a DFN grid in the nearby rock volume. A DFN is first generated using the procedures described previously (Painter et al. 2012, Hyman et al. 2013). The generated DFN ignores the volume to be meshed. However, before the DFN is meshed, interfaces between fractures and the cylinder to be meshed are identified. A two-dimensional mesh is then created on each fracture in a way that conforms to the fracture intersections and to the fracture-volume interfaces (Figure 3a). The fracture grids are then merged, as described previously and in Hyman et al. (2013). In the second step, nodes on the fractures within the volume to be meshed are removed (Figure 3b). A tetrahedral mesh that conforms to the fracture intersection is then created within the cylinder. In the final step, the tetrahedral mesh and the DFN mesh are merged and duplicate nodes removed (Figure 3c). The LaGriT software (Los Alamos Grid Toolbox, 2013) was used to execute the meshing calculations.

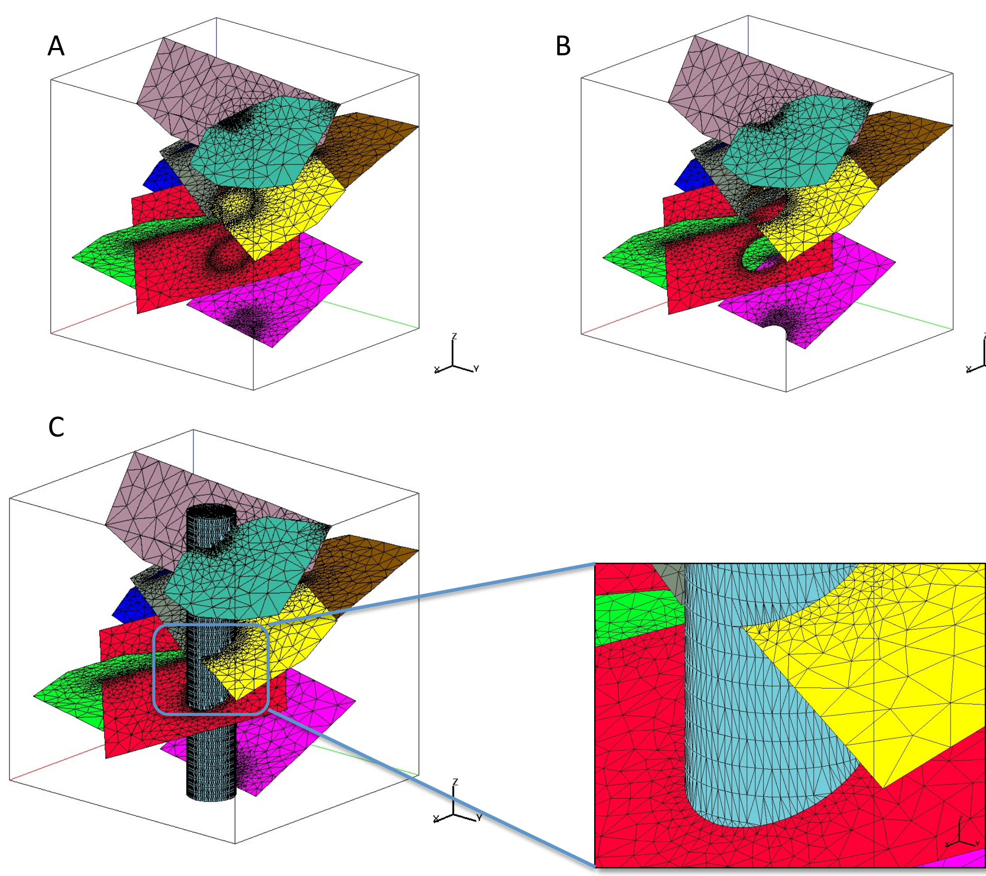

Figure 3. Example showing the creation of a hybrid tetrahedral/DFN mesh. Such hybrid meshes were required to model the rewetting of bentonite in the BRIE.

3. SCOPING CALCULATIONS

A set of scoping calculations were first performed to test the capability to solve for flow in hybrid tetrahedral/DFN grids. Those scoping calculations used a single fracture intersecting the bentonite volume. The FEHM software was used (Zyvolosky, 2007). FEHM has an option for defining the same node multiple times. It then imposes a constraint that the unknowns be the same for a multiply defined node. That capability simplifies the construction of the mesh because it avoids having to merge control volumes at the interface between the three-dimensional and two-dimensional meshes, which would create issues with property assignments at the merged control volumes.

The van Genuchten model (van Genuchten, 1980) was used for both the bentonite and the rock fracture. In the van Genuchten model, liquid saturation s_l is related to capillary pressure as

$$s_l = \left[1 + \left(\frac{P_g - P_l}{P_0}\right)^{\frac{1}{1-\lambda}}\right]^{-\lambda} \qquad (1)$$

where P_g is gas pressure, P_l is liquid pressure, and P_0 and λ are empirical parameters. The reference case parameters used for the fracture and bentonite are provided in Table 1. The initial saturation of the bentonite was specified as 36%. The fracture was initially saturated with water. The boundary conditions on the fracture edges were specified at 2 MPa. Richards model was used for the reference case.

Table 1. Parameter Values Used in the Scoping Calculations (Bockgård et al., 2010).

Parameter	Bentonite	Fracture
van Genuchten pressure parameter P_0 [MPa]	9.23	1.74
van Genuchten shape parameter λ [–]	0.3	0.6
Hydraulic conductivity [m/s]	6.4×10^{-14}	Not applicable
Porosity [-]	0.44	Not applicable
Transmissivity [m^2/s]	Not applicable	5×10^{-10}
Transport Aperture [m]	Not applicable	10^{-4}

Results for the reference case at 10 days, 6 months and 1 year are shown in Figure 4. The top row of images shows the liquid saturation in three-dimensional view. The bottom row shows the saturation at a horizontal cut at the fracture plane. After about 1 year, enough water has been imbibed into the bentonite to raise the saturation in the bentonite at the location of the fracture to approximately 65%. Water is also starting to migrate upward in the bentonite.

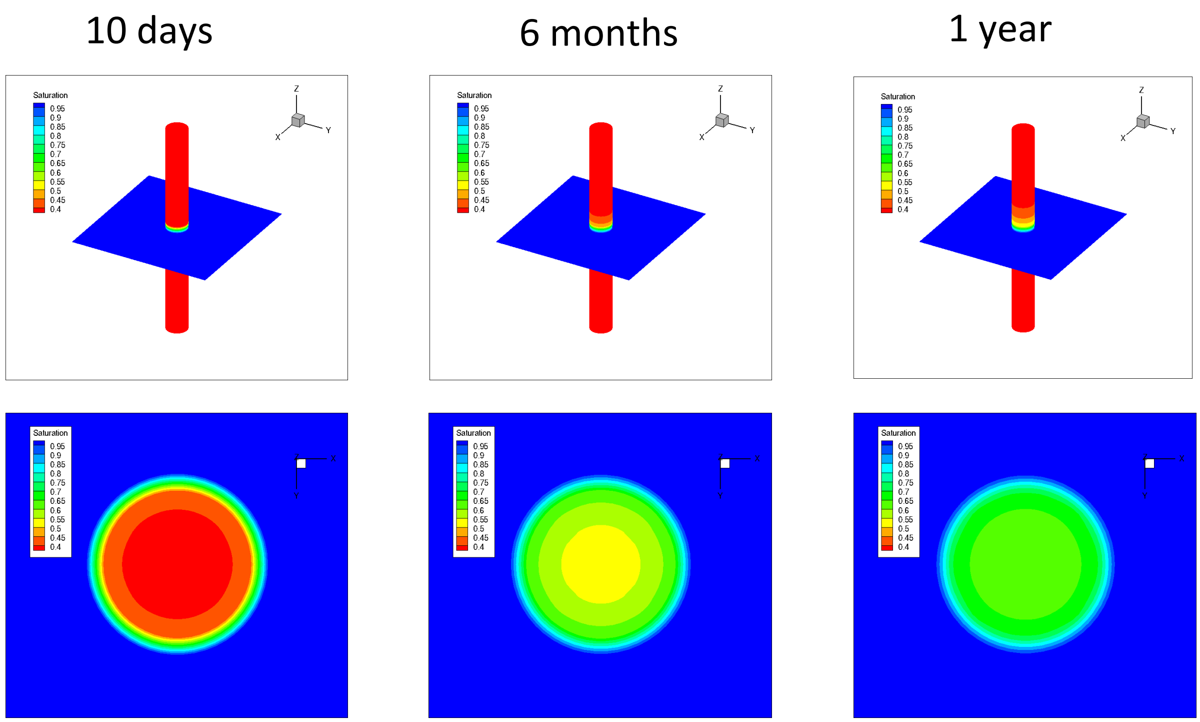

Figure 4. Liquid saturation for a scoping calculation using a single fracture and a bentonite cylinder representing one of the BRIE boreholes. The images in the bottom row are at the plane of the fracture.

A comparison between the Richards equation representation, which treats gas as a passive phase and ignores the conservation equation for air, and a more complete representation that solves the two-component system is shown in Figure 5. There is no significant difference between the two representations at 1 year, which suggests that the Richards equation representation is adequate for representing the rewetting process. This comparison would need to be revisited for longer simulation times, however.

Liquid saturation at 1 year for the reference case is compared to two variant cases in Figure 6. The images on the left show liquid saturation for a variant case in which bentonite permeability is higher by an order of magnitude. The images on the right are for the case with an annular gap at the outer edge of the bentonite cylinder. The effect of the annular gap is represented by increasing vertical permeability in the outermost ring of cells. In both variant cases, the bentonite wetting progresses faster than in the reference case. A variant case with higher fracture permeability was also run. That result was not significantly from the reference case and is not shown.

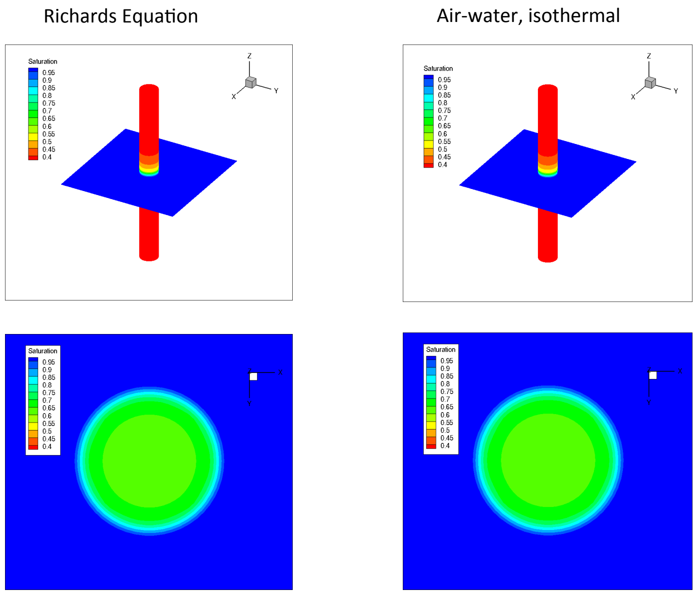

Figure 5. Comparison between the Richards equation representation and a more complete two-component representation. Shown is liquid saturation at 1 year.

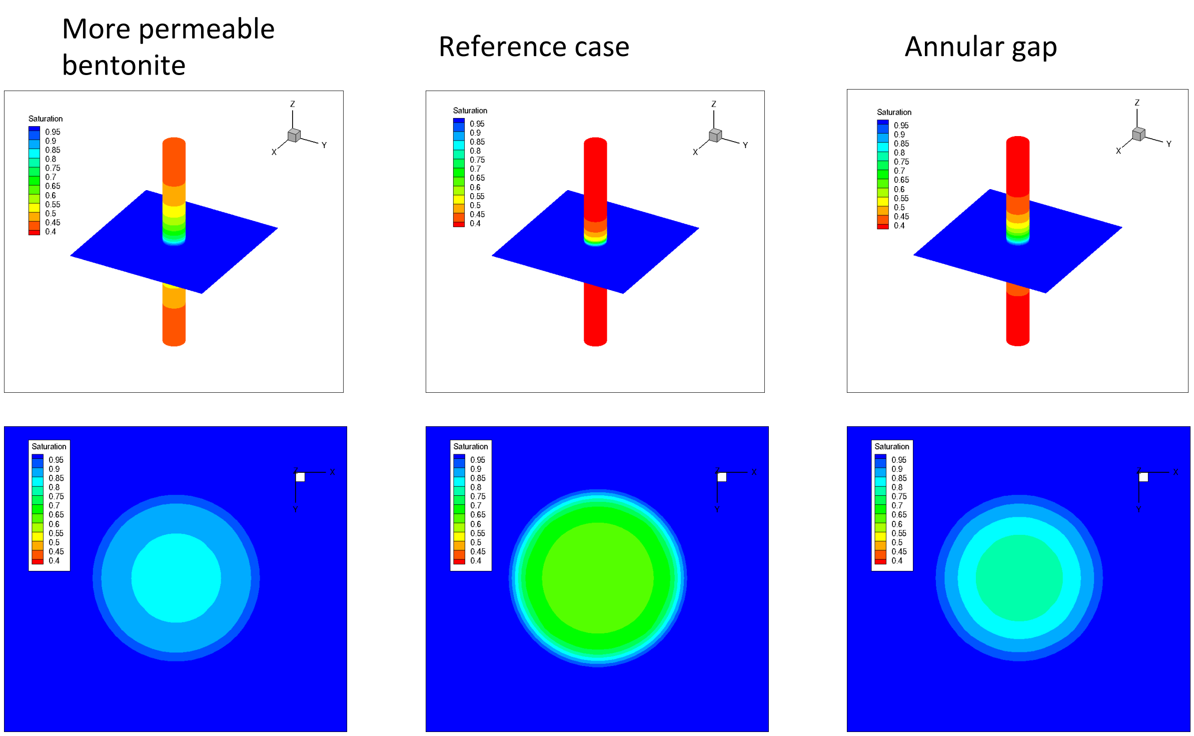

Figure 6. Comparison between the reference case scoping run and two variant cases. Shown is liquid saturation at 1 year.

4. MODEL SETUP FOR HYBRID DFN/BENTONITE SIMULATIONS

A primary goal of this work is to gain experience in applying advanced DFN models in practical applications that involve complicated geometries and boundary conditions. Task 8d of SKB's Task Force on Groundwater Flow and Transport Modeling is a valuable application for that purpose. In Task 8d, flow in the fractured granite surrounding the two BRIE boreholes as well as flow in the boreholes themselves are being modeled. This section describes preliminary model setup for Task 8d.

Model geometry is shown in Figure 2. The domain of interest is a 40 m × 40 m × 40 m cube. The model domain contains multiple tunnels, the two BRIE boreholes, and three deterministic fractures. For this work, the task description (Bockgård et al., 2010) specified a DFN model for stochastically simulating unobserved fractures (Table 2). This model used the isotropic Fisher distribution (Fisher, 1953) for fracture orientation

$$f(\theta) = \frac{\kappa \sin\theta \, \mathrm{e}^{\kappa\cos\theta}}{e^{\kappa} - e^{-\kappa}} \qquad (2)$$

where t is the deviation of the fracture pole orientation from the mean orientation and the parameter $\kappa > 0$ is the concentration parameter. The concentration parameter quantifies the degree of clustering; values approaching zero represent a uniform distribution on the sphere and large values imply small average deviations from the mean direction.

Table 2. DFN Parameters for the Fractured Rock Mass Near the BRIE Boreholes (Bockgård et al., 2010)

	Orientation Distribution: Fisher			**Size Distribution: Power Law**		**Fracture Density**
Set	**Mean Trend**	**Mean Plunge**	**Concentration Parameter**	**Lower Cutoff r_0**	**Exponent k_r**	**Area per Volume P_{32}**
1	280º	20º	10	0.25 m	2.6	1.1 m^{-1}
2	20º	10º	15	0.25 m	2.6	2 m^{-1}
3	120º	50º	10	0.25 m	2.6	0.75 m^{-1}

A workflow was developed for modeling the BRIE experiment. The major steps are:

1. A realization of the DFN model is created using stochastic simulation. The stochastically generated fractures are combined with the three deterministic fractures.
2. Two meshes are created. In the first, the DFN model is meshed without the boreholes. In the second, the DFN is meshed in combination with at tetrahedral mesh for the interior of the boreholes using the methods described in Section 3. These two meshes do not include tunnels.
3. The tunnel is represented in both meshes by specifying all nodes that fall inside the tunnel as boundary nodes with pressure specified as atmospheric.
4. Boundary conditions are mapped to the faces of the cube in both meshes. Pressure results from a larger simulation were provided for that purpose.
5. A steady-state flow simulation is performed without the boreholes to establish pre-experiment conditions in the fracture network.

6. The result of Step 5 is used as initial condition for a transient flow simulation with the BRIE boreholes represented. The liquid saturation index in the bentonite is initially 36%. Of interest is the rewetting of the bentonite.

The result of Step 2, a meshed realization of the DFN with the three deterministic fractures and the two BRIE boreholes is shown in Figure 7. For this preliminary simulation the lower cutoff was increased to 1.0 m to reduce the size of the network, with appropriate adjustments to the fracture density. The network contains approximately 3500 stochastically generated fractures.

The result of Step 3, a computational mesh with tunnel nodes identified is shown in Figure 8. The tunnel nodes are blue and green. Non-tunnel nodes are shown in red.

5. SUMMARY AND STATUS OF THE WORK

Refinement and extension of the DFN modeling capability was undertaken to enable representation of the tetrahedral mesh within the DFN mesh. That development work is largely complete and initial computational meshes for the DFN and BRIE boreholes have been generated. The work is continuing in FY2014. The next steps are to apply boundary conditions and perform the flow simulations (Steps 4-6 in Section 5). Comparisons to data on moisture content in the bentonite will then be undertaken.

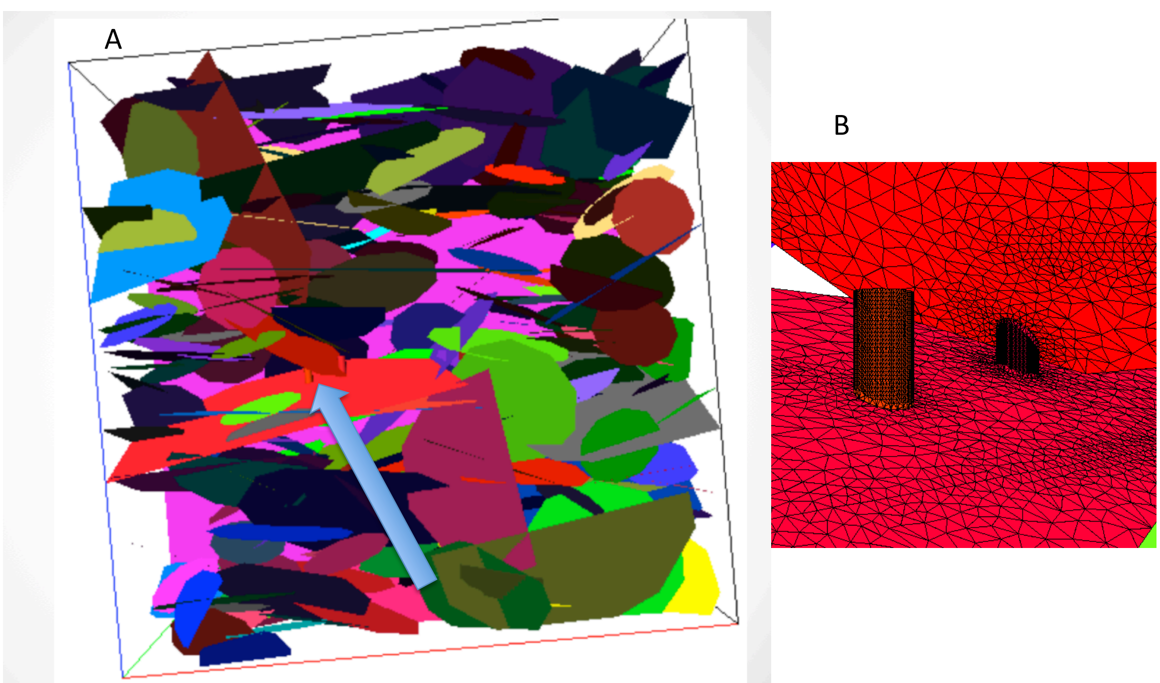

Figure 7. Computational mesh for the three-dimensional model of the BRIE experiment. The DFN and boreholes are shown in A. The arrow indicates the position of the boreholes. A detail from the computational mesh showing the merged DFN and tetrahedral mesh is shown in B.

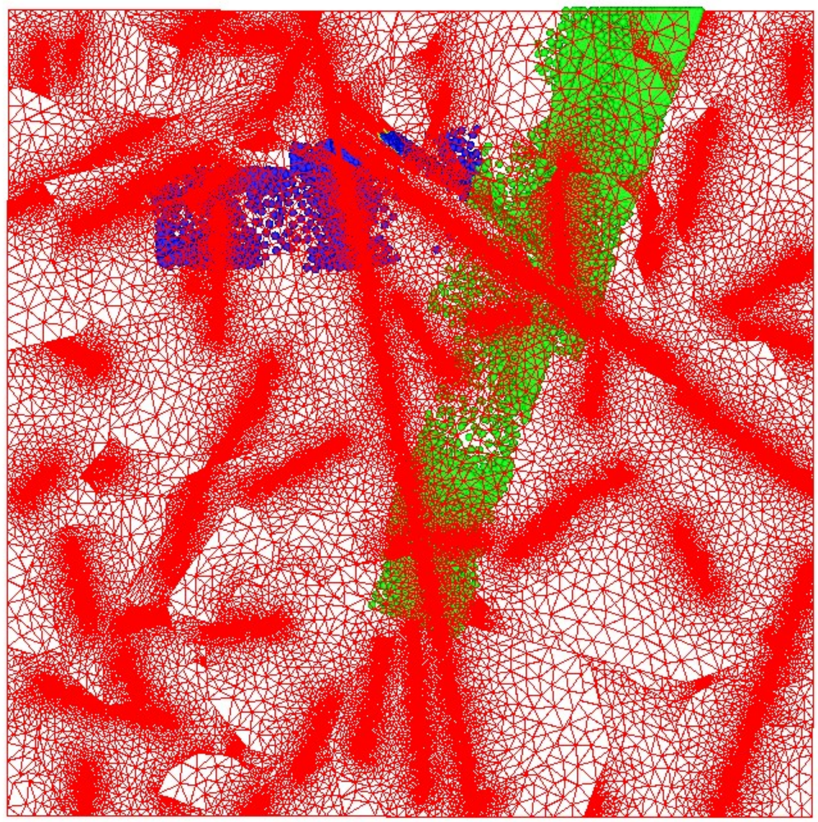

Figure 8. Computational mesh with tunnel nodes tagged (blue and green).

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