Excerpt from the Proceedings of the 2011 COMSOL Conference in Stuttgart

Verification and validation of flow and transport in cracked saturated porous media

Janez Perko*, Suresh Seetharam and Dirk Mallants
Belgian Nuclear Research Centre SCK·CEN, Institute for Environment, Health and Safety
*Corresponding author: Boeretang 200, B-2400 Mol, Belgium, jperko@sckcen.be

Abstract: Study of presence of cracks in porous media and their effect on fluid flow and mass transport is of great interest in many fields including geotechnical, petroleum or civil engineering. In radioactive waste disposal there is considerable interest in crack behaviour in concrete structures for the following reasons: (i) open cracks are more permeable than the concrete matrix and may lead to increasing and unwanted water fluxes into the disposal facility, (ii) when water-filled there is little or no sorption in cracks and hence they could present preferential pathways for contaminant migration from the disposal facility to the environment and (iii) long-term chemical concrete degradation owing to e.g. carbonation could progress faster in the presence of cracks. Assessment of long-term behaviour of concretes and the wastes for which they provide containment, is feasible only by numerical modelling. This is even more true when cracks are considered and evaluated in the concrete degradation and mass transfer models. However, before the model is deemed suitable for assessments of real engineered structures, it should be thoroughly verified and if possible validated.

Keywords: Cracks, saturated porous media, model verification, numerical modeling of flow and transport

1. Introduction

Flow and transport phenomena in fractured porous media have been thoroughly studied, theoretically, experimentally and numerically, mostly because cracks are commonly present in rocks, bricks, or concrete. In this paper we focus on numerical evaluation of flow and transport in fractured man-made porous media (i.e. concrete structures), constructed to contain contaminants such as radioactive waste. Concrete is the most used material for encapsulation of radioactive waste, especially for near-surface disposal facilities. Concrete is preferred over other materials mainly due to its favourable chemical properties resulting in a high chemical retention capacity, and owing to its good hydraulic isolation properties. Presence of cracks may change the containment ability in terms of increase in hydraulic conductivity and decrease in overall sorption (or increase in contaminant mobility).

Cracks in a concrete disposal facility exist in many sizes, locations and time of formation. However, it is extremely difficult to predict formation and propagation of cracks within the various components of such facility. One approach to tackle the issue of cracks is to study different contrasting and possibly enveloping theoretical cases by which it is possible to gain an insight into system behaviour. Before such study can be carried out, it is inevitable to make extensive verifications and, if possible, validations of the model used.

Several modelling approaches have been proposed to model flow and transport through cracked porous media. In hydrogeology, mathematical models for flow and transport through cracked porous media fall into one of three broad classes, either characterized as equivalent continuum models, discrete network simulation models, or by using hybrid techniques [1]. The models differ in their representation of the heterogeneity of the cracked medium. They may be cast in either a deterministic or stochastic framework.

In a conventional equivalent continuum model, the heterogeneity of e.g. fractured rock is modelled by expressing the volume-averaged behaviour of many fractures in some form of effective properties such as permeability and porosity. Equivalent continuum models cover several variants [2,3,4].

Discrete network models, on the other hand, are predicated on the assumption that fluid flow behaviour can be predicted from knowledge of the fracture geometry and data on the transmissivity of individual fractures. The fractures are realized as the conductive elements in a fracture network flow or transport model [1,5,6].

The latter approach will be carried forward in the present paper. Discrete cracks can be modeled in two ways. The first way, most commonly used in such analyses, is to explicitly express cracks as a geometrical property. This approach is intuitively easier to capture, because material properties, geometry and corresponding results are as seen in reality. Numerically, the approach is viable if the crack is relatively wide relative to the overall domain. By contrast, many thin cracks in a large domain would result in an enormous computational demand owing to the fine discretization to represent the cracks.

The discretization problem can be alleviated by a mathematical translation of the crack domain into boundary elements by using Stoke's (Green's) theorem [7]. As a result, the dimension of modelled cracks is lower that the one of the actual problem solved. Consequently, the domain around the crack need not to be too finely discretized. The advantages of the *implicit formulation* are easier discretization, better stability, computational efficiency and easy adaption to different crack dimension. On the other hand, the *explicit crack modelling* offers straight-forward formulation and consequently more transparent implementation.

The aim of the paper is to present the efforts to verify discrete crack models integrated in water flow and contaminant transport simulations by using implicit cracks implemented in COMSOL multiphysics.

2. Mathematical Description and Use of COMSOL Multiphysics

Modelling of advective transport in fractured porous media requires solution of at least two coupled or uncoupled partial differential equations, depending on the problem being solved. In case of contaminant transport, the assumption that the contaminants do not affect water flow is mostly justified. Consequently water flow can be calculated separately before applying the Darcy velocity to the advective–dispersive equation.

Water flow in non-fractured porous media is described by Darcy's equation [8].

$$S\frac{\partial p}{\partial t} = \nabla \cdot \left(\frac{K_{mat}}{\rho_w \cdot g} \cdot \nabla p \right) \tag{1}$$

where S, p, K_{mat}, ρ_{w}, and g are, respectively storage coefficient [1/Pa], fluid pressure [Pa], saturated hydraulic conductivity of the matrix domain [m/s], water density [kg/m^3] and the gravitational acceleration constant [m/s^2]. The Darcy velocity vector $\vec{u}$ is then calculated as

$$\vec{u} = -K_{mat}\frac{\nabla p}{\rho_w \cdot g} \tag{2}$$

As explained above, the cracks are modeled implicitly. The so-called implicit formulation is based on including a 1D (line) element into a 2D model. In this way, the discretization of the crack is only made in one dimension, whereas the majority of the remaining matrix domain does not need to be too finely discretized.

Flow in cracks are modelled similarly to modelling flow in a porous matrix based on equation **(1)**. Because cracks are modelled as 1D elements, crack dimension d_{crack} is added to ensure dimensional consistency between the porous matrix and the cracks:

$$S \cdot d_{crack} \cdot \frac{\partial p}{\partial t} = \nabla \cdot \left(d_{crack} \cdot \frac{K_{frac}}{\rho_w \cdot g} \cdot \nabla p \right) \tag{3}$$

The storage coefficient S in both equations **(1)** and **(3)** is put to a very low number representing water compressibility, which makes both equations represent almost steady-state with respect to p. The Darcy velocity in the crack is calculated as in equation **(2)**, but by using tangential derivatives on the boundary instead of field pressure derivatives. Equation **(3)** is implemented in a weak form, which transforms domain integrals to the boundary ones by multiplication with a test function T*and integration by parts:

$$\begin{aligned}
&\int_\Omega T^* \cdot S \cdot d_{crack} \cdot \frac{\partial p}{\partial t} = -\int_\Omega T^* \cdot \nabla \cdot \left(-d_{crack} \cdot \frac{K_{frac}}{\rho_w \cdot g} \cdot \nabla p \right) \\
&\int_\Omega T^* \cdot S \cdot d_{crack} \cdot \frac{\partial p}{\partial t} d\Omega = \\
&\int_\Gamma \left(T^* \cdot d_{crack} \cdot \frac{K_{frac}}{\rho_w \cdot g} \cdot \nabla p \right) \cdot \vec{n}\, d\Gamma - \\
&\int_\Omega \nabla T^* \cdot d_{crack} \cdot \frac{K_{frac}}{\rho_w \cdot g} \cdot \nabla p d\Omega
\end{aligned} \tag{4}$$

where *Ω* and *Γ* represent domain and boundary, respectively and $\vec{n}$ is outward normal to the boundary. The hydraulic conductivity K_{frac} of cracks is approximated by the formulation of Walton and Seitz [9] which assumes Poiseuille flow between two parallel plates. The derivation results in the following notation for hydraulic conductivity of a single crack:

$$K_{frac} = \frac{\rho_w \cdot g \cdot b^2}{12\mu}. \tag{5}$$

The crack aperture is denoted by b [m] and dynamic viscosity of water by μ [Pa·s]. Studies showed that the actual hydraulic conductivity is one- to two-thirds of the one based on equation **(5)**. Similarly to the procedure in Walton and Seitz [9] one half is of the value from equation **(5)** is therefore used here:

$$K_{frac} = \frac{\rho_w \cdot g \cdot b^2}{24\mu}. \qquad (6)$$

The advective-dispersive transport equation has to be rewritten in the non-conservative form when dealing with implicit cracks. Because the field variables interpret cracks as a source/sink boundary line, the velocity divergence is not zero which leads to spurious mass generation. Forcing the velocity divergence in the last – advective – term to zero ($\nabla \cdot \vec{u} = 0$) as written in equation (7) solves this problem:

$$\frac{\partial(\theta \cdot c)}{\partial t} + \frac{\partial(\rho_b \cdot K_d \cdot c)}{\partial t} = \nabla \cdot \left(\theta \cdot \xi \cdot D_p \nabla\right) + \vec{u} \nabla c \cdot \qquad (7)$$

The transport equation for cracks is then derived from equation **(7)** in a similar way as was done for equation **(4)**.

3. Numerical examples

The conceptualisation of a problem and demonstration of adequacy of the model used, its correctness and accuracy of the results is built in several steps. Firstly, the model has to undergo a qualification process, where the conceptual model is set up on the basis of adequate knowledge of the interacting processes involved. This step involves argumentation about the hypotheses, assumptions, and parameters used when building the model. Model qualification is followed by model verification, where the latter can be performed in several ways. Either the results are compared to an analytical solution if the problem is relatively simple, or an alternative numerical solution of the same conceptual model is tested (benchmarking). Initial model verification was done by comparing the implicit crack implementation to the comprehensive explicit crack formulation as shown in Fig. 1. This approach gives very simple visual and numerical confirmation of proper numerical implementation of implicit (weak-form) cracks. However, this verification does not confirm correct solution of the physical model. For this purpose more sophisticated test cases should be used. Many different analytical models are available [10,11] related to advection-dispersion transport in fractured porous media. One example is shown in Fig. 2. The analytical solution of Sudicky and Frind [11] is based on a 2D problem representing porous media with planar vertical cracks. A decaying contaminant is injected on the top, directly into the cracks vith prescribed velocity. Cracks are distributed equidistantly in the domain with a distance 2B between them. The domain is initially solute free.

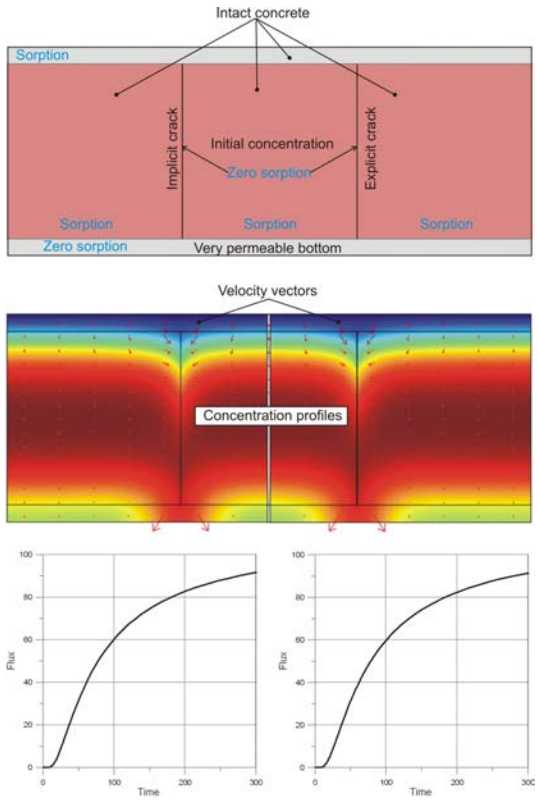

Figure 1. Comparison of contaminant flux (bottom) through implicit (top) and explicit (middle) crack representation for an initial value problem.

The entire bottom boundary is defined as a zero concentration Dirichlet boundary, while side boundaries assume zero flux.

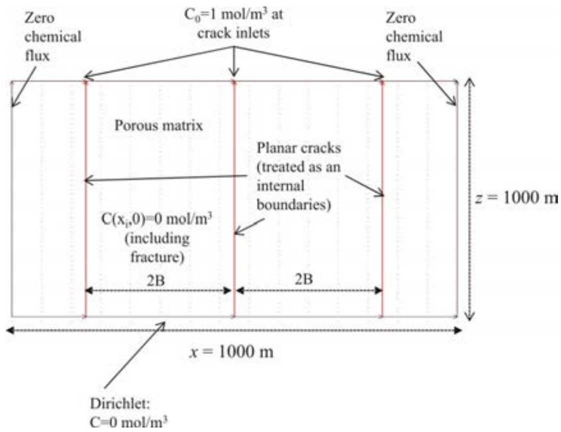

Figure 2. Transport through Multiple Parallel Cracks for a boundary value problem; model description with boundary and initial conditions.

Material and crack properties are given in Table 1.

Table 1: Material properties used for the solution of transport through multiple parallel cracks.

Crack aperture	100 μm
Porosity of the matrix, θ	0.01
Tracer half life, $T_{1/2}$	12.35 years
Velocity in the crack, v	0.01 and 0.1 m/day
Tortuosity, ξ	0.1
Free Diffusion coefficient (for matrix), D_0	1.38x10^{-4} m^2/day
Longitudinal dispersivity in the crack, α_L	0.1 m
Dispersion coefficient in the crack, D	$\alpha_L v + D_0$
Retardation coefficient, R	1
Crack spacing, $2B$	0.1 and 0.5 m

Details of the analytical solution of Sudicky and Frind can be found in [11]. Figures 3 and 4 give the graphical results of concentration profiles along the cracks for two respective fluid velocities in cracks given in Table 1.

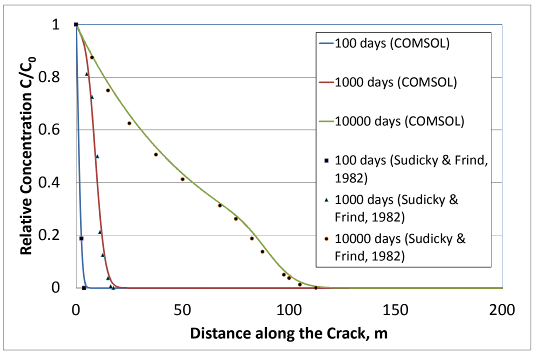

Figure 3. Relative concentration along the crack length; crack spacing *2B* = 0.1 m, velocity = 0.1 m/d.

Results show good agreement between analytical and numerical solution and this proves adequate solution of a well defined and simplified physical model.

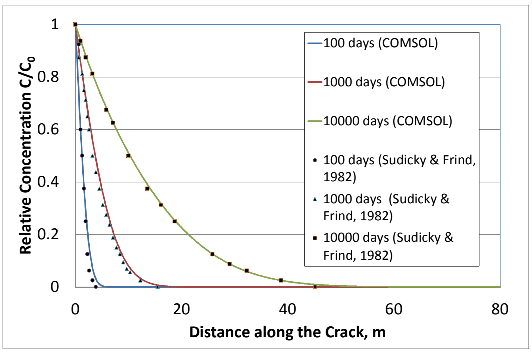

Figure 4. Relative concentration along the crack length; crack spacing *2B* = 0.1 m, velocity = 0.01 m/d.

The most valuable information for model validation can be obtained by comparison with experimental data. One of the main problems of validation is in a proper definition of initial and boundary conditions and material properties. Few small scale experiments related to flow and transport in fractured porous media are available in the literature. We use the experiment of Hull and Clemo [20] for model validation; the test was performed for the purpose of the validation of dual permeability models and is therefore also fit for our purpose. The 2D experiment is made in porous 2-cm thick polyethylene (PE) plates of dimension 81.3cm×40.6cm. The PE has well defined pores and the hydraulic conductivity can be easily measured. The fractures were generated by milling the PE into various shapes and combining them like pieces in a jigsaw puzzle as shown in Fig. 5. Fracture aperture ranges from 50 to 1520 µm.

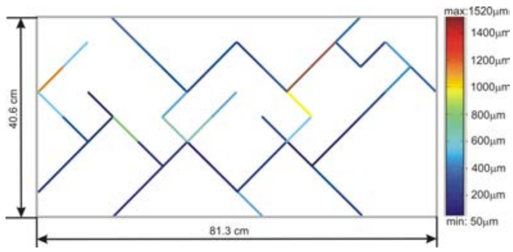

Figure 5. Configuration of cracks with the thickness of evaluated fracture apertures.

Hydraulic conductivity of porous media was estimated to 0.53 cm/min, porosity to 37.7% and dispersivity to 0.366 cm. Pressure head in the red nodes denoted in Fig. 6 is kept constant. Tracer is injected in the blue point for 76 minutes.

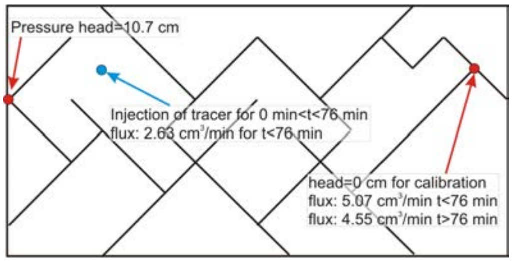

Figure 6. Points of water and tracer injection.

Pressure heads are measured in several points along fractures and in the matrix as denoted in Fig. 7.

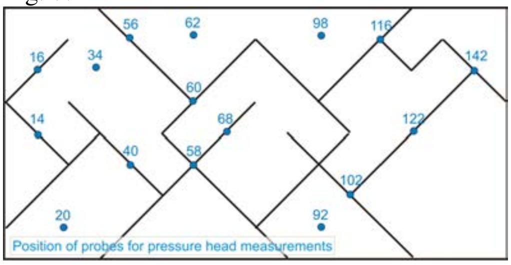

Figure 7. Position of probes for pressure head measurements.

At this point we needed to determine the crack apertures, because epoxy resin used in the construction of the experiment shrinks when curing and the fractures compress. Consequently crack apertures become unknown. Hence, the hydraulic characteristics of the completed fracture network had to be evaluated to determine the effective fracture apertures for the dual permeability model. Fracture apertures were determined by forcing a match between the head distribution in the experiment and the one of the model. A comparison of experimental and simulated pressure heads is shown in Fig. 8. Fitted apertures in [12] and in the present work are similar, but not exactly the same.

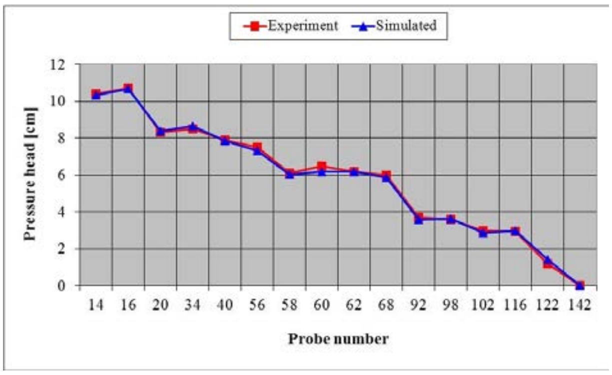

Figure 8. Comparison between observed [12] and COMSOL simulated pressure heads.

In the numerical model of advective-dispersive transport of a tracer the same crack apertures were used as defined for the flow model. The tracer was selected such that it could be recorded visually and also by electrical probes due to its lower specific electrical conductance. Snapshots of the tracer plume at various times during the test are produced. These maps provide a qualitative means to model validation; at the edge of the plume the diffuse boundary is replaced by a single line on the map. This is particularly true for the trailing edge of the plume, where significant dispersion was occurring. The drawings were taken from the top surface of the physical model, but there was a slight difference from the bottom plume due to some density effects. Selected plumes characteristic for different times are shown in Fig. 9. The figures are made on the basis on the original b/w drawings of Hull and Clemo [12] overlain with coloured numerical results obtained by COMSOL Multiphysics.

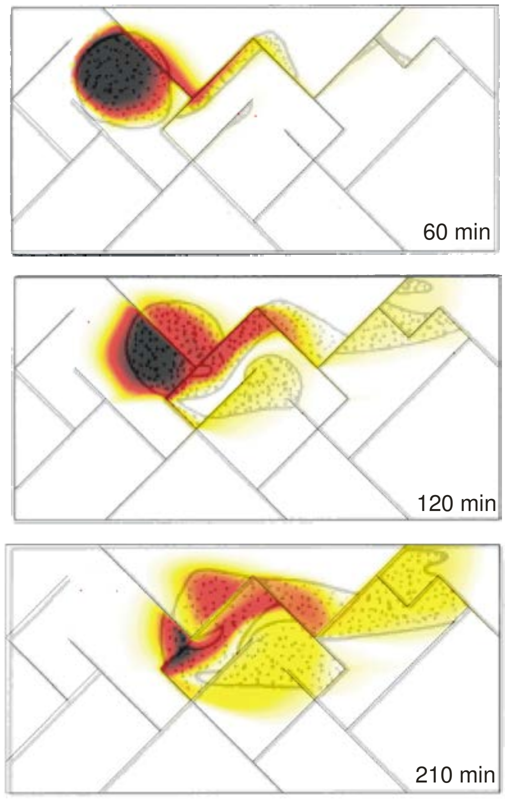

Figure 9. Tracer plumes from Hull and Clemo at 60 min (top), 120 min (middle) and 210 min (bottom) are overlain with COMSOL numerical results.

More quantitative comparisons can be obtained from the electrode responses. Electrodes were located at different locations, within the porous matrix and on the cracks in the experimental setup as shown in Fig. 10.

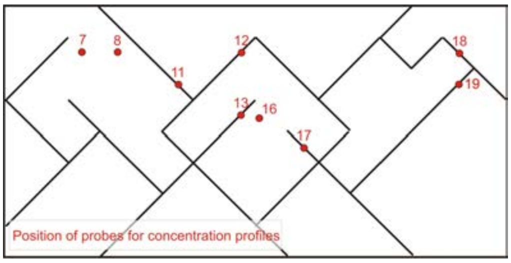

Figure 10. Location of electrodes for tracer concentration measurements.

Results from selected probes are shown in Fig. 11.

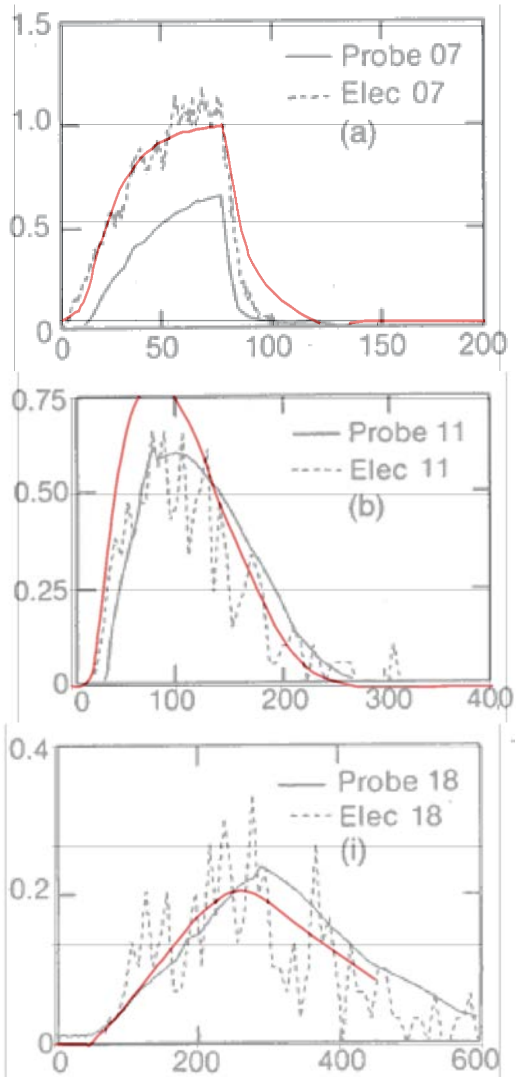

Figure 11. Concentration records at different locations. Dashed line represents measurements, full black line is the numerical solution by Hull and Clemo and the red line is from COMSOL Multiphysics.

Dashed lines display measurements, the full black lines are results of previous numerical calculations by Hull and Clemo [12], and the red line is based on COMSOL. Generally, the shape of the breakthrough curve and timing of the peak agree well with measurements. The magnitude of the response, however, varies more than both simulations, especially when electrodes are located in the porous matrix farther from the source.

4. Discussion

In this paper we presented examples of numerical model verification and validation. All cases shown consider the system being fully saturated. Partial desaturation of the cracked porous media could have several consequences, including cracks would desaturate first and consequently hydraulic conductivity of desaturated cracks could be much lower than the one of the matrix. In other words, the cracks would act as a hydraulic barrier rather than a conductor. Hence, the behaviour of fluid flow and transport in cracked porous media depends strongly on the saturation degree of our system.

Model verification requires thorough analysis of processes involved. The most reliable way is the comparison of a numerical model with an appropriate analytical solution. Analytical solutions, however, are usually based on simplified initial and boundary conditions and regular geometries. Therefore, the correctness of the solution can be proven only partially. A further acknowledged way of verification is benchmarking with other numerical models.

Gaining confidence in simulation models is further enhanced by doing model validation. Model validation is aimed at reproducing processes in nature. Experiments carried out to validate numerical models must have clear boundary and initial conditions, geometry and well defined material properties. As concerns the experiment of Hull and Clemo, all such requirements are met except for the physical properties of cracks. Cracks should have a well defined aperture in order to be able to validate the assumption of Poiseuille's flow in cracks. Now, the crack aperture was fitted on the basis of the model. Hence, the mathematical description was validated in terms of ability to reproduce natural processes, but exact constitutive relations were not validated.

5. Conclusions

In this paper we presented several cases which cater to increase confidence in the simulations of fractured porous media fluid flow and mass transport.

Explicit and implicit fracture representation in COMSOL gave identical results for the relatively simple 2D initial value problem at hand. Comparison between an analytical solution and numerical simulations for a boundary value problem with multiple parallel cracks gave excellent results. A model validation exercise based on a 2D laboratory tracer test gave convincing results in terms of reproducing plume spreading (qualitative comparison) and breakthrough curves (quantitative comparison).

We have thus demonstrated that implementing cracks in COMSOL for flow and transport simulations produces adequate results and is fit for purpose for use in the analysis of saturated fractured porous media.

6. References

1. Committee on fracture characterization and fluid flow et al. Rock fractures and fluid flow, contemporary understanding and applications, National Academy Press, (1996)
2. Davison, C. C. URL Drawdown Experiment and comparison with models. TR 375, Atomic Energy of Canada Ltd., Pinawa, Manitoba. (1985)
3. Pruess, K., and Narasimhan, T. N.. Numerical modeling of multiphase and nonisothermal flows in fractured media. In Proceedings of the Symposium Conference on Fluid Flow in Fractured Rocks, May 15-18. (1988)
4. Mallants, D., D. Jacques, M. Vanclooster, J. Diels and J. Feyen. A stochastic approach to simulate water flow in a macroporous soil. Geoderma, Volume 70, Issues 2-4, Pages 299-324. (1996)
5. Herbert, A., Gale, J., Lanyon, G., MacLeod, R., Modeling for the STRIPA site characterization and validation drift inflow: prediction of flow through fractured rock. SKB Report 91-35. Swedish Nuclear Power and Waste Management Co., Stockholm. (1991)
6. Dershowitz, W., Wallmann, P., Kindred, S., Discrete Fracture Modeling for the Stripa Site Characterization and Validation Drift Inflow Predictions. SKB Report 91-16. Swedish Nuclear Power and Waste Management Co., Stockholm. (1991)
7. COMSOL Model library, Earth science module, (2008)
8. J.C. Walton and R.R. Seitz, Fluid Flow Through Fractures in Below Ground Concrete Vaults, Waste Management, 12, pp. 179-187 (1992).
9. Mallants, D., van Genuchten, M. Th., Simunek, J., Jacques, D., Seetharam, S., 2011. Leaching of contaminants to groundwater (2011)
10. Chiou, S-L., Li, S-H, Migration of radionuclides in fractured porous rock: Analytical solution for a flux-type boundary condition. Nuclear Technology, vol.101, pp.92-100, (1992)
11. Sudicky,E.A., Frind,E.O., Contaminant transport in fractured porous media:Analytical solutions for a system of parallel fractures. Water Resources Research, Vol. 18(6), pp. 1634-1642 (1982)
12. L.C. Hull and T.M. Clemo, Dual-Permeability model: Laboratory and FRACSL validation studies. In Geothermal Injection Technology Program Annual Progress Report FY-86, EGG-2511, Idaho National Engineering Laboratory, Idaho Falls (1987)

7. Acknowledgements

This work has been performed as part of the project on disposal of category A waste – short-lived low and intermediate level waste (LILW-SL) – that is carried out by ONDRAF/NIRAS, the Belgian Agency for Radioactive Waste and enriched Fissile Materials. The findings and conclusions in this paper are those of the authors and do not necessarily represent the official position of ONDRAF/NIRAS. The work presented in this paper was more particularly carried out as preparatory work to a future license application file for a near surface disposal facility at Dessel to be submitted by ONDRAF/NIRAS to the FANC. Therefore, the results in this paper have not yet undergone regulatory review nor approval by the FANC. Furthermore, it is not excluded that further developments and refinements of the work presented in this paper will be included in the future license application file.