MoMaS benchmark

February 2017

1 Introduction

The background of this benchmark is the production of hydrogen gas due to the corrosion of the metallic container in the nuclear waste repository. Numerical model is built to illustrate such gas appearance phenomenon. The model domain is a two dimensional horizontal column representing the bentonite backfill in the repository tunnel, with hydrogen gas injected on the left boundary. This benchmark was proposed in the GNR MoMaS project by French National Radioactive Waste Management Agency. Several research groups has made contributions to test the benchmark and provided their reference solutions Neumann et al. (2013); Bourgeat et al. (2009); Marchand and Knabner (2014); Ben Gharbia and Jaffré (2014). Here we adopted the results proposed in Marchand’s paper Marchand and Knabner (2014) for comparison.

1.1 Physical scenario

Here a 2D rectangular domain $\Omega = [0, 200] \times [-10, 10]$ m (see Figure 1) was considered with an impervious boundary at $\Gamma_{imp} = [0, 200] \times [-10, 10]$ m, an inflow boundary at $\Gamma_{in} = \{0\} \times [-10, 10]$ m and an outflow boundary at $\Gamma_{out} = \{200\} \times [-10, 10]$ m. The domain was initially saturated with water, hydrogen gas was injected on the left-hand-side boundary within a certain time span ($[0, 5 \times 10^4 \text{ century}]$). After that the hydrogen injection stopped and no flux came into the system. The right-hand-side boundary is kept open throughout the simulation. The initial condition and boundary conditions were summarized as

- $X(t = 0) = 10^{-5}$ and $P_L(t = 0) = P_{out}^{L} = 10^{6}[\text{Pa}]$ on $\Omega$.
- $q^w \cdot \nu = q^h \cdot \nu = 0$ on $\Gamma_{imp}$.
- $q^w \cdot \nu = 0, q^h \cdot \nu = Q_{d}^{h} = 0.2785 \text{ [mol century}^{-1}\text{m}^{-2}]$ on $\Gamma_{in}$.
- $X = 0$ and $P_L = P_{out}^{L} = 10^{6}[\text{Pa}]$ on $\Gamma_{out}$. 
1.2 Model parameters and numerical settings

The capillary pressure $P_c$ and relative permeability functions are given by the van-Genuchten model Van Genuchten (1980).

$$P_c = P_r \left( S_{le}^{\frac{1}{m}} - 1 \right)^{\frac{1}{m}}$$

$$K_{rl} = \sqrt{S_{le} \left( 1 - \left( S_{le}^{\frac{1}{m}} \right)^{m} \right)^2}$$

$$K_{rg} = \sqrt{1 - S_{le} \left( 1 - S_{le}^{\frac{1}{m}} \right)^{2m}}$$

where $m = 1 - \frac{1}{n}$, $P_r$ and $n$ are van-Genuchten model parameters and the effective saturation $S_{le}$ is given by

$$S_{le} = \frac{1 - S_g - S_{lr}}{1 - S_{lr} - S_{gr}} \quad (1)$$

here $S_{lr}$ and $S_{gr}$ indicate the residual saturation in liquid and gas phases, respectively. Values of parameters applied in this model are summarized in Table 1.

Table 1: Fluid and porous medium properties applied in the H$_2$ migration benchmark.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intrinsic Permeability</td>
<td>$K$</td>
<td>$5 \times 10^{-20}$</td>
<td>[m$^2$]</td>
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<tr>
<td>Porosity</td>
<td>$\phi$</td>
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<td>-</td>
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<td>Residual Saturation of liquid phase</td>
<td>$S_{lr}$</td>
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<td>[-]</td>
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<td>Residual Saturation of gas phase</td>
<td>$S_{gr}$</td>
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<td>[-]</td>
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<td>Viscosity of liquid</td>
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<td>[Pa·s]</td>
</tr>
<tr>
<td>Viscosity of gas</td>
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<td>$9 \times 10^{-6}$</td>
<td>[Pa·s]</td>
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<td>van Genuchten parameter</td>
<td>$P_r$</td>
<td>$2 \times 10^6$</td>
<td>[Pa]</td>
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<tr>
<td>van Genuchten parameter</td>
<td>$n$</td>
<td>1.49</td>
<td>-</td>
</tr>
</tbody>
</table>
1.3 Results and analysis

The results of this benchmark are depicted in Figure 2. The evolution of gas phase saturation and the gas/liquid phase pressure over the entire time span are shown. In addition, we compare results from our model against those given in Marchand’s paper Marchand and Knabner (2014). In Figure 2, solid lines are our simulation results while the symbols are the results from Marchand et al. It can be seen that a good agreement has been achieved.
References


