MoMaS benchmark

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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 ($[0, 5 \times 10^4$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 $P_L(t=0) = P_L^{out} = 10^6$ [Pa] on Ω.
- $q^w \cdot \nu = q^h \cdot \nu = 0$ on Γ_{imp}.
- $q^w \cdot \nu = 0, q^h \cdot \nu = Q_d^h = 0.2785$ [mol century^{-1}m^{-2}] on Γ_{in}.
- $X = 0$ and $P_l = P_L^{out} = 10^6$ [Pa] on Γ_{out}.

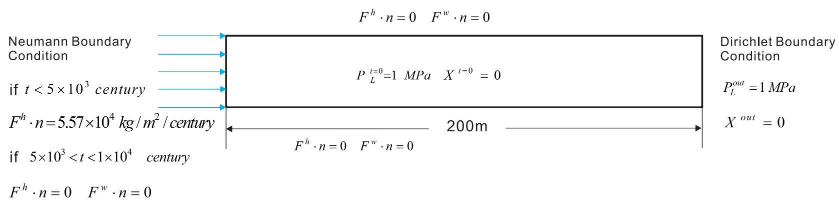

Figure 1: Geometry and boundary condition for the H_2 injection benchmark.

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).

$$P_c = P_r \left(S_{le}^{-\frac{1}{m}} - 1\right)^{\frac{1}{n}}$$
$$K_{r_L} = \sqrt{S_{le}} \left(1 - \left(1 - S_{le}^{\frac{1}{m}}\right)^m\right)^2$$
$$K_{r_G} = \sqrt{1 - S_{le}} \left(1 - S_{le}^{\frac{1}{m}}\right)^{2m}$$

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

$$S_{le} = \frac{1 - S_g - S_{lr}}{1 - S_{lr} - S_{gr}} \tag{1}$$

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.

Parameters	Symbol	Value	Unit
Intrinsic Permeability	K	5×10^{-20}	[m^2]
Porosity	Φ	0.15	-
Residual Saturation of liquid phase	S_{lr}	0.4	[-]
Residual Saturation of gas phase	S_{gr}	0	[-]
Viscosity of liquid	μ_l	10^{-3}	[Pa·s]
Viscosity of gas	μ_g	9×10^{-6}	[Pa·s]
van Genuchten parameter	P_r	2×10^6	[Pa]
van Genuchten parameter	n	1.49	-

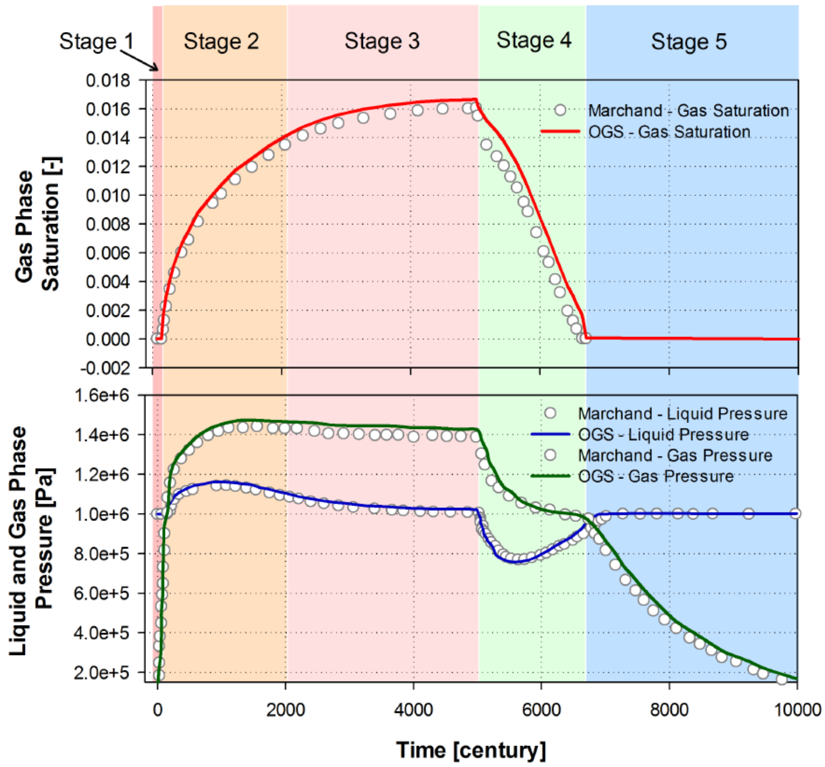

Figure 2: Evolution of pressure and saturation over time.

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 additional, 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

Ben Gharbia, I., Jaffré, J., 2014. Gas phase appearance and disappearance as a problem with complementarity constraints. Mathematics and Computers in Simulation 99, 28–36.

Bourgeat, A., Jurak, M., Smaï, F., 2009. Two-phase, partially miscible flow and transport modeling in porous media; application to gas migration in a nuclear waste repository. Computational Geosciences 13 (1), 29–42.

Marchand, E., Knabner, P., 2014. Results of the momas benchmark for gas phase appearance and disappearance using generalized mhfe. Advances in Water Resources 73, 74–96.

Neumann, R., Bastian, P., Ippisch, O., 2013. Modeling and simulation of two-phase two-component flow with disappearing nonwetting phase. Computational Geosciences 17 (1), 139–149.

Van Genuchten, M. T., 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil science society of America journal 44 (5), 892–898.