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Modeling bubble flow in fracture with Lattice Boltzmann model

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Abstract. *In the framework of radioactive waste disposal studies, behavior of hydrogen produced through anaerobic corrosion of the steel canisters is a key point. At the near and far field scale, the migration process of hydrogen is modelled using macroscopic two-phase flow models requiring macroscopic data like relative permeability curves. As relative permeability curves for very low permeable media are difficult to measure experimentally, two-phase flow modelling at the pore scale appears as an interesting tool. The objective of this paper is to present a Lattice Boltzmann approach used to model two-phase flow in fractures with apertures of a few micrometers in aperture and some elementary simulations of bubble flow allowing to understand the behavior of two-phase flow in very low gas saturation context.*

1 Introduction

In the context of radioactive waste disposal in deep geological media, hydrogen generation due to anaerobic corrosion of the waste containers steel is expected. The behavior of the produced hydrogen is a key point because of the possible increase of the gas pressure inside of disposal cells and consequently of the possible degradation of the confinement properties of the host rock and of the plugs and seals of the system.

At the near and far field scale, the modeling of the hydrogen migration is performed through numerical tools using macroscopic two-phase flow equations requiring macroscopic data like relative permeability curves [1]. For very low permeable media such as radioactive waste disposal host rocks, the experimental measurements of these relative permeability curves is difficult, especially for very low gas saturations where gas phase is expected to be discontinuous. Tools allowing two-phase flow modelling at the pore scale like Lattice Boltzmann models appear thus as an interesting approach to complete the required data sets.

We choose to use a Lattice Boltzmann model based on the color gradient method mixed with a Two Relaxation Time collision operator. The LB model was successfully validated through classical tests and then used to simulate a single bubble displacement across a fracture presenting a restriction aperture.

2 Lattice Boltzmann model

We choose to use the the color-gradient approach that defines two species, the red and blue populations, representing in our case water and hydrogen, f_q^w and f_q^{nw} respectively.

Each iteration of the LBM consists in two steps: computing the new distributions $\left(\Omega_q^k(f_q^k)\right)$, and streaming to the neighboring nodes:

$$f_q^k(\boldsymbol{x} + \boldsymbol{c_q},\, t + \delta t) = f_q^k(\boldsymbol{x},\, t) + \left(\Omega_q^k(f_q^k)\right)(\boldsymbol{x},\, t) \tag{1}$$

where t is time, δt is the time step and superscript $k = w$ or $k = nw$. The new distributions are obtained by successive application of three operators:

$$\Omega_q^k = (\Omega_q^k)^{(3)} \left[(\Omega_q^k)^{(1)} + (\Omega_q^k)^{(2)}\right] \tag{2}$$

- the collision operator $(\Omega_q^k)^{(1)}$ relaxes the distributions to their equilibrium state. The TRT scheme was used to relax the populations f_q^k to an equilibrium state defined by the equilibrium populations $f_q^{k\,eq}$ [3].

- The perturbation operator $(\Omega_q^k)^{(2)}$ adds an anisotropic perturbation to the populations near the interface creating an anisotropic pressure field generating the surface tension [2],

- the recoloring operator $(\Omega_q^k)^{(3)}$ redistributes the phases in the interface region such that the diffusion of color across the interface is minimized and then controls the interface sharpness [4].

The populations are then propagated to neighbor nodes.

In order to validate the chosen model and its implementation, successful tests through classical Laplace law for static behaviour and through classical three layers two-phase Poiseuille flow for dynamic behaviour were conducted.

3 Application

Our LB model was then used to simulate the displacement of a single hydrogen bubble inside a simple fracture geometry with a narrowing aperture in order to evaluate if hydrogen bubbles can be trapped inside complex fracture geometry or not (see Figure 1).

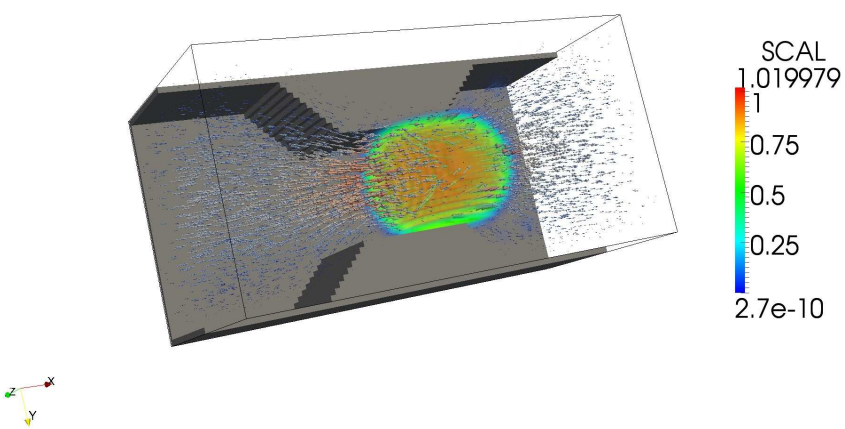

Figure 1: Bubble displacement across a fracture geometry with a narrowing aperture.

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