Pore scale multiphase flow simulation in low permeable porous media by LBM and SPH methods.

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Introduction
Sedimentary formations of Callovo-Oxfordian (COx) clay are projected to be used as a host site for a long term radioactive waste repository. Characterized by low permeability, these media can serve as a natural barrier against radioactive materials. During the storage phase, certain amount of gas (mostly hydrogen) will be released due to corrosion of iron components of the facility. Increased pressure causes the gas migration through the highly water saturated sedimentary material. Therefore, a good understanding of this complex process is of a high interest.

Generally, the clayey material has a complex porous structure with the total porosity of order of 20% where the most of the pores smaller than 100 nm. At this scale, multiple phenomena unusual for transport in macro pores may take place, such as slippage phenomenon due to large Knudsen number values (Klinkenberg effect). Accounting for these effects can modify predictions of the transport properties such as permeability.

Due to recent advances in digital rock imaging, it is now possible to obtain real samples images with pixel size of order of 5 nm, such as one displayed in Figure 1. This provides the opportunity to perform numerical simulations using these digital images obtained by FIB-SEM, in order to better understand the gas transport in saturated low permeable porous media. Various numerical methods can be employed to calculate capillary pressure, absolute and relative permeabilities. In our study, we focus on using LBM [1] and SPH [3] with the principal objective to improve the description of gas transport in highly water saturated clays. The obtained numerical results for liquid/gas permeability are then confronted with experimental data.

Numerical Modelling
Multiphase flow can be described by various computational fluid dynamics (CFD) methods. Recently, non-conventional numerical methods such as LBM and SPH received a lot of attention for multiphase flow modelling.
in porous media since they permit to cope naturally with fluid-fluid interface and complex fluid-solid boundary conditions. Various physical phenomena can be relatively easily incorporated in these numerical methods. Finally, possessing a high level of intrinsic parallelism, these methods can easily profit from parallel computing on CPU and GPU clusters, which is important when dealing with prohibitively large samples.

The SPH model employed in our study, is a Lagrangian mesh free method. It is based on the idea that function value at a point can be approximated by the function values in close proximity of that point as

\[ f(x) = \int f(x')W(x - x', h)dx' + \text{err}_{\text{smoothing}} \] (1)

where \( W(x - x', h) \) is a smoothing function, \( h \) is a smoothing length, and \( \text{err}_{\text{smoothing}} \) is the approximation error. Generally, SPH can be successfully applied to discretize various partial differential equations in multiple areas of physics. Here, it is used to numerically solve the Navier-Stokes equations for liquid/gas phase. The surface tension effects as well as contact angle are described in terms of continuum force model, i.e., via a volumetric force normal to the interface and proportional to its local curvature.

Originally derived as a generalization of lattice gas automata, LBM can be also obtained by discretizing the continuous Boltzmann equation in space, time, and particle velocity space. Unlike the classical CFD methods, the LBM describes fluid state by the probabilistic particle distribution function. The macroscopic fluid velocity and density are calculated as moments of the distribution function. The distribution function evolution is described by the collision operator. In our model, a multiple-relaxation-time (MRT) operator is used along with pseudo-potential Shan-Chen model [4] employed to simulate surface tension and wetting effects. The Klinkenberg effect is incorporated by proper modification of fluid-solid boundary conditions and relaxation rates of the collision operator [1].

Both LBM and SPH are applied to simulate single- and multiphase flow inside the digital image of the real clay sample. The obtained results will be presented and discussed.

References