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Micro-Scale Simulation of Water Evaporation, Condensation and Transport in Multi-mineral Porous Media

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Summary

Fluid phase changes is one of the challenging concepts in micro-scale simulation of transport phenomena in porous media. Conservation of mass and energy combined with an approperiate phase change model and fluid interface tracking scheme are simultaneously considered to capture complexities involved in the evaporation and condensation processes. We implement a numerical algorithm based on the Volume-of-Fluid method using the OpenFOAM open-source CFD package along with four phase change models. In this paper, steam-saturated multi-mineral porous media are used to simulate evaporation and condensation phenomena at a liquid-vapor interface in non-isothermal boundary conditions. Results demonstrate that the nucleation site locations and numbers as well as condensation film formation are strongly dependent on the solid surface quality in terms of roughness and minerology.

Introduction

As the demand for pore scale physics modeling increases, methods following Eulerian viewpoints have become more attractive, given their feasibility of tracking multiple interfaces and virtual simplicity of implementation into CFD packages such as OpenFOAM. The Level-Set (LS) and the Volume-of-Fluid (VOF) methods are two popular techniques based on the Eulerian perspective. LS tracks the interface by a smooth function $\boldsymbol{u}$, where $\boldsymbol{u} = \boldsymbol{0}$ represents the interface and is called the zero level set. $\boldsymbol{u}$ is positive for one phase and negative for the other. In this method, interfacial topologies such as curvatures and sharp interfaces can be easily captured. However, the drawback of this method is its inability to handle mass conservation as it results in mass loss when solving the advection equation [1]. VOF tracks an interface based on the phase volume fraction, $\boldsymbol{\alpha}$, of each fluid where $\boldsymbol{0} \leq \boldsymbol{\alpha} \leq \boldsymbol{1}$. So, the sum of volume fractions of vapor and liquid in a cell is equal to unity. VOF is one of the most actively researched methods for evaporation and boiling problems[2], which garantees mass conservation. However, it compromises estimation of the interface topology compared to LS. Thus, we use coupled Level Set/Volume of Fluid (CLSVOF) which integrates the the LS dvantages in tracking the fluid interface and VOF mass conservation when the interface is formed [3].

Phase change processes are numerically captured using various methods including widely used Lee, Merkle, Knuz and Schnerr-Sauer techniques. The Lee model assumes that mass is transferred at a constant pressure and a quasi-thermo-equilibrium state while the following three models take the pressure into account in an isothermal state. In this work, these approaches are modified to respond to both pressure and temperature gradients.

Theory

We adopt the three available cavitation models, i.e. Merkle, Knuz and Schnerr-Sauer, to take the temperature into account. Also, the Lee model is implemented in the solver "multiphasecmpressibleinterFoam" to consider phase change phenomena in the presence of three phases such as oil, water and its vapour. Grain surface is inherently rough, hence accurate pore scale physics simulations require considering rough surfaces.

In all our simulations, the medium of interest initially consists of vapor and grains. We initialize the medium at zero fluid velocity. We assume that the medium is surounded by an infinite source of vapour with constant pressure from all its boundaries (top, bottom, left, right). So, from this surfaces, there is an influx of vapour for the case of condensation. No-slip condition has been imposed for solid wall surfaces. Grains remain at costant tempertaure of 330 K while steam at 400 K enters the medium.

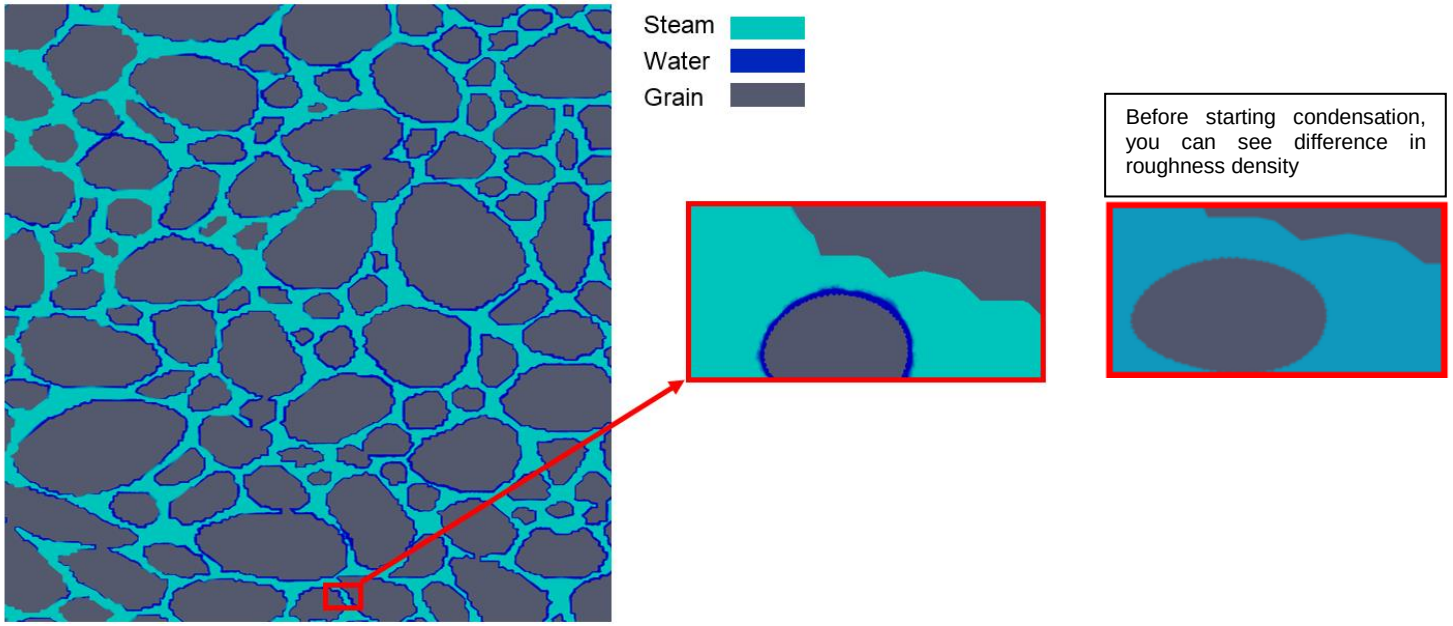

Figure 1 Synthetic 2D porous media including single mineral (water wet)

Examples

Figure 1 depicts the first set of simulations representing condensation in porous media. The medium is initially saturated with steam at the temperature of $\mathbf{400}\boldsymbol{k}$ while the grain tempertaure is $\mathbf{300}\boldsymbol{k}$. Condensation occurs as a result of heat transfer from steam to grains. It was intersting to report that condensation film is first formed on the grain surfaces with high specific surface area, i.e. high roughness density (Figure 1).

We also examin the effect of solid surface mineralogy. Figure 2 shows a medium composed of water–wet minerals (grey color) and oil-wet minerals (red color). Simulation results reveal that nucleation sites and condensation film first occur in the water wet area.

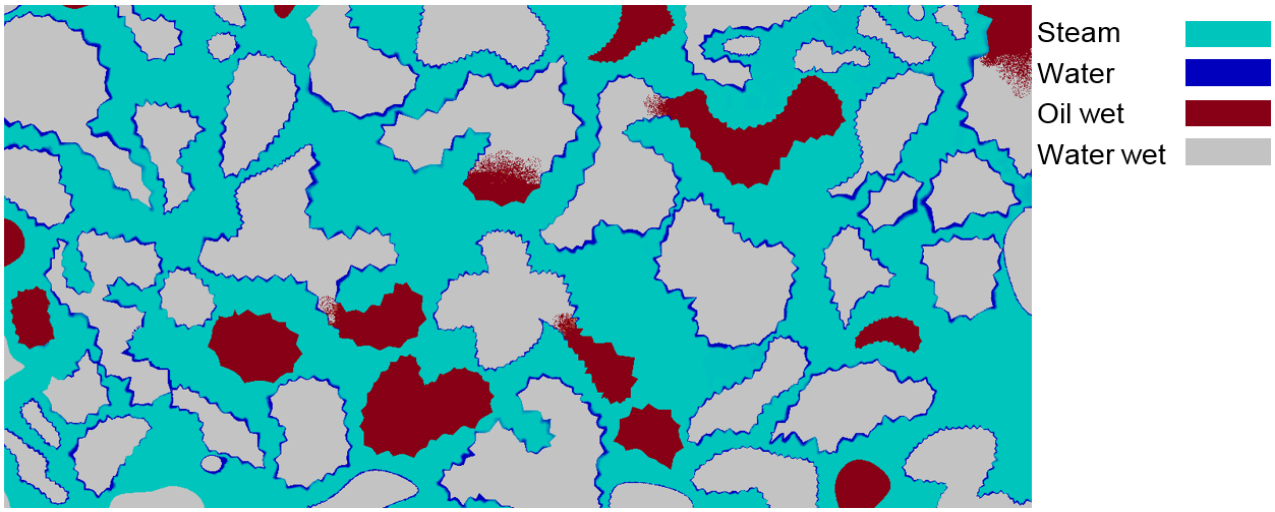

Figure 2 Alpha function distribution in a typical 2D multi-mineral porous medium

We further examine the errect of surface roughness using a 3D porous medium, as presented in Figure 3. Similat to the 2D example, the first nucleation sites occur in the zones with high density roughness.

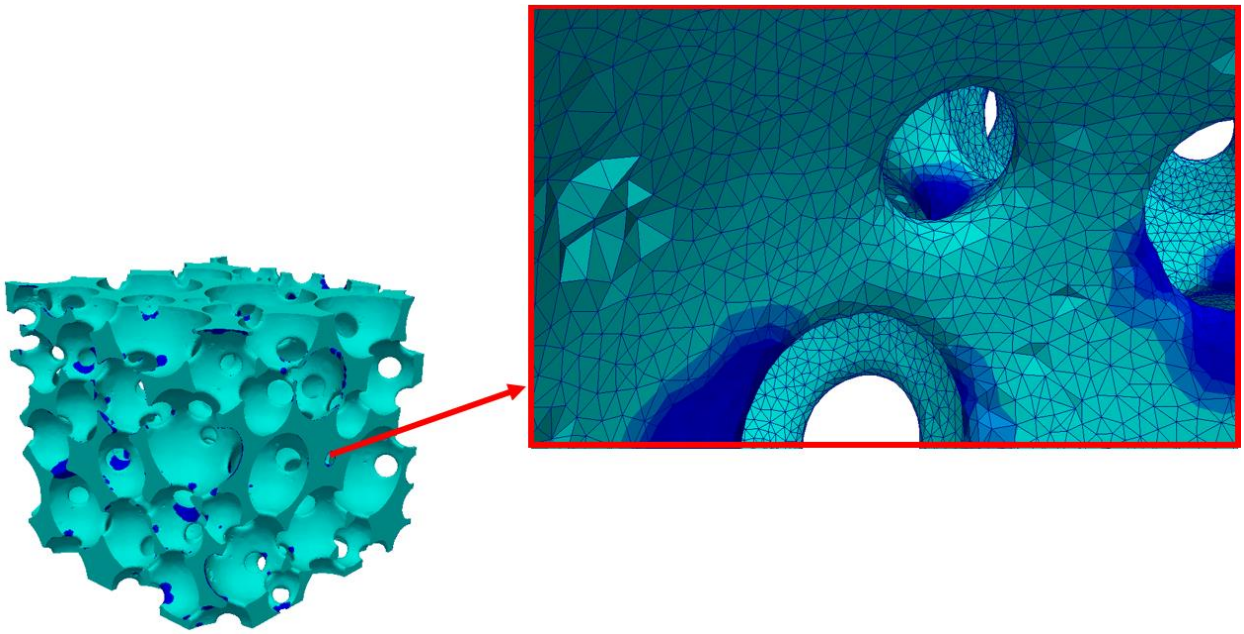

Figure 3 Alpha function distribution in a 3D porous medium

We should note on the importance of porous medium discritization in the above cases. To capture all rough surfaces efficiently, particularly in 3D geometries in the present study, we discretize the grain surface much finer than the pore body not close to the walls. Another approach is using dynamic mesh refinement in which a fine discretized region moves along the interface to capture liquid/vapor interface physics. However, in evaporation/condensation cases, interface is created on the solid surface and curvature calculation is very sensitive to the type of discretization. The most challenging problem is to optimize the total mesh number with a trade-off between resolution requirements for accuracy of the results and computational time. The way-out is adaptive grid meshing but it is not as much efficient to resolve the issue, especially in more complex configurations such as three phase systems.

Conclusions

Multi-physics modelling was used to study water evaporation and condensation phenomena in micro-scale porous media. Mineral heterogeneity was taken into the account by defining minerals with different wettabilities. The main observations are as follows:

- Number and location of nucleation sites and condensation film occurrence depend on the mineralogy, surface roughness and the thermodynamic conditions of the system.
- Contact angle on the surface has significant effect on the results.
- In all configurations, the temperature profile is consistent with the corresponding saturation profile.
- High density of roughness exacerbates the problem in calculation of curvature-based parameters.
- Fine meshing compromises stability, consistency, and convergence of numerical discretization.

References

1. T. Menard , S. Tanguy and A. Berlemont, “Coupling level set/VOF/ghost fluid methods: Validation and application to 3D simulation of the primary break-up of a liquid jet”, International Journal of Multi-Phase. 2006
2. Gueyffier, D., J. Li, A. Nadim, R. Scardovelli and S. Zaleski, “Volume-of-Fluid interface tracking with smoothed surface stress methods for three-dimensional flows”, Journal of Computational Physics, 152(2), 1999, 423-456.
3. Sun D.L., J. L Xu and L. Wang, “Development of a vapor–liquid phase change model for volume-of-fluid method in FLUENT”, International Communications in Heat and Mass Transfer, 39(8), 2012, 1101-1106.
4. Hirt, C. W. and B. D. Nichols, “Volume of Fluid (VOF) method for the dynamics of free boundaries”, Journal of Computational Physics, 39(1), 1981, 201–225.
5. Lee, H., C. R. Kharangate, N. Mascarenhas, I. Park and I. Mudawar, “Experimental and computational investigation of vertical down flow condensation”, International Journal of Heat and Mass Transfer, 85, 2015, 865-879.
6. Jones, S.F., G.M. Evans and K.P. Galvin, “The cycle of bubble production from a gas cavity in a supersaturated solution”, Advances in Colloid and Interface Science, 80(1), 28, 1999, 51-84.
7. Nicol, A. A. and J. O. Medwell. “The effect of surface roughness on condensing steam” The Canadian Journal of Chemical Engineering, 44(3), 1966, 170-173.