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Simulation of transition flows and phase changes in porous media using modified equations of state to obtain the correct surface tension

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The phenomena of phase change and coexistence of two phases of a substance are of great interest in engineering. The two most widespread ways of describing these phenomena numerically are the sharp interface [1] and phase field [2] numerical models. The former assume that there is an abrupt transition at the interface between the two fluid phases while the latter propose a smooth transition with a thickness greater than zero. The latter approach takes advantage of the same equation of state (EoS) to describe the thermodynamic properties of both phases. The most widely used EoS, the Van der Waals EoS [3], while obtaining reasonable results for a wide set of substances, in the case of water is quite far from the experimental results. The major current challenge for the simulation of multiphase and multicomponent pore-scale flow in permeable media is the effect that EoS has on the effective surface tension. In the present work it is shown that multiphase flow simulations based on traditional equations of state (e.g. cubic EoS) result in surface stresses that are several orders of magnitude larger than the actual ones, when intended to simulate problems of interest in geosciences and engineering where the characteristic length of the problem is much larger than the physical width of the interface (on the order of nm). A modification of the Van der Waals EoS is proposed by applying the methodology proposed in [4] with applications to numerical modeling of phase changes in porous media.

Participation

In-Person

References

[1] Luis Cueto-Felgueroso et al., Phys. Rev. Fluids 3, 084302, 2018
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[3] J.D. van der Waals, J. Stat. Phys. 20, 197–244, 1979
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Primary author: Dr FERNÁNDEZ-FIDALGO, Javier (Universidade da Coruña and Universidad Politécnica de Madrid)

Co-authors: Dr CUETO-FELGUEROSO, Luis (Universidad Politecnica de Madrid); Dr RAMÍREZ, Luis (Universidade da Coruña); Dr MARTÍNEZ, Abel (University College Cork); Dr NOGUEIRA, Xesús (Universidade da Coruña)

Presenter: Dr FERNÁNDEZ-FIDALGO, Javier (Universidade da Coruña and Universidad Politécnica de Madrid)

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