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Effects of molecular details on two-phase flows through nanopores

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Geological storage of carbon dioxide and spent nuclear fuel are topics of huge significance for our societies. This motivates an improved understanding of fluid transport of gases through partially saturated porous networks such as clay materials or caprock. However, this is a complicated problem spanning length scales from nano- to millimeter sized channels. To fully model drying, evaporation and diffusion through these networks we need to understand the dominating physics at all scales. At nanometer scales the molecular nature of fluids becomes apparent. For multiphase fluid systems this involves fluid–fluid interfaces, which have explicit widths of several molecules across and physical properties separate to those of the bulk phases. Physical modeling of multiphase flows must include these effects when applied to systems of sizes approaching the nanoscale [1].

We present our work on resolving these molecular details of fluid–fluid interfaces in two-phase systems. Since it is inherently difficult to study nanoscale behavior in laboratory experiments, our approach is by the use of molecular dynamics (MD) simulations of gas/liquid flows through nanopores. MD simulations are fully atomistic and so include realistic molecular effects by its nature. However, molecular simulations of multiphase flows at the nanoscale are still challenging and should be achieved with care and adequate methodology, as proposed in this work, to avoid unphysical behavior. These numerical experiments give us physical insight in how molecular interfaces affect two-phase flows in nanochannels. We also show how these effects can be included as effective quantities or boundary conditions in continuum physical models of similar systems.

Participation

In-Person

References

[1] Johansson, Galliero, Legendre. How molecular effects affect solutal Marangoni flows. *Physical Review Fluids* 7: 064202, 2022.

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