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Dynamical Capillary Network Model Built On Molecular Level Simulation at the Pore Scale

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As length scales grow smaller, the behavior of two fluids flowing through a porous media is more and more strongly affected by capillary pressure. The canonical Young-Laplace equation gives a good estimate of the pressure change across fluid interfaces, but it is technically valid only in equilibrium conditions. It is well-known that for two fluids flowing in capillaries, the interfacial pressure change depends on dynamics, such as flow velocity or, more directly, changes to the interface shape. In this work we investigate ways to represent the dynamical state of pore scale flow in a network model that tracks two-fluid interfaces as they move through a series of connected capillaries. The pore scale model consists of molecular level simulations of two fluids flowing through a single cylindrical capillary. The network model consists of a network of cylindrical capillaries of varying lengths and diameters, for which we combine the equations of motion for two fluids with continuity equations to derive a system of differential algebraic equations, which can be solved for the state of the network in time. To link the two simulations, from the pore scale results we extract the dependence of the capillary pressure on flow speed, which can enter in various ways into the equations of motion for the capillary network.

References

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Primary authors: Dr BRYANT, Peter (IBM Research); Dr GIRO, Ronaldo (IBM Research); NEUMANN, Rodrigo (IBM Research - Brazil); Dr ENGEL, Michael (IBM Research); Dr STEINER, Mathias (IBM Research)

Presenter: Dr GIRO, Ronaldo (IBM Research)

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