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Title: Mesoscale Modeling of Fluid Displacement Through Bundle of Capillary Tubes Using Dissipative Particle Dynamics
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It is crucial to understand how one fluid is displaced by another through a capillary, as many industrial and recovery methods from petroleum reservoirs fall into this category including displacement of in-situ fluids by injected CO_2. The dissipative particle dynamics (DPD) method has been successfully applied to model mesoscale behaviours of many processes. The mesoscopic regime corresponds to small length scales where, although the fluid is still well represented by, the molecular nature of the fluid is already appreciable and it is modelled through the inclusion of random noise terms in the hydrodynamic equations. Molecular dynamics (MD) and lattice Boltzmann method (LBM) are two well known methods for simulation at atomistic and mesoscopic regimes, respectively. DPD combines feature of MD and LBM while avoids the artefacts of LBM and captures much larger spatio-temporal hydrodynamics scales compared to MD. In DPD, (like MD), a system is simulated using a set of interacting particles. However, unlike MD, each particle is a coarse-grained entity representing a cluster of molecules instead of a single molecule or atom. The particles are off-lattice (unlike LBM) and follow a set of velocity dependent forces.

In our study, a 'bundle of tubes' model has been used to represent a reservoir and DPD particles are used to model displacing and displaced fluids to capture the mesoscale flow pattern. Validation of the in-house computer code written in C# is carried out by modeling isothermal no-slip fluid flow. Simulation of non-isothermal fluid displacement using energy conserving DPD gives insight about the parameters affecting the flow.