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Use of molecular simulations to fit EOS in confined space in order to perform large scale tight oil and shale gas reservoir simulations

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Unlike conventional reservoirs where pore size distribution has a micrometer scale (Nelson 2009), tight oil and shale gas reservoirs have predominantly mesopores (between 2 and 50 nm) and micropores (below 2 nm). Volume fraction of micropores is not negligible and can be as high as 20% (Kuila et Prasad 2011). As hydrocarbon molecules range between 0.5 and 10 nm (Nelson 2009), interaction forces between confined fluid and pore wall molecules become as significant as inter molecular interactions within the confined fluid. That is why nanofluidic experiments (Wang et al. 2014) and bubble point measurement on hydrocarbon mixture in mesoporous materials (Cho, Bartl et Deo 2017) have demonstrated that confinement considerably changes fluid phase behavior. Consequently the commonly-used equation of state (EOS) such as Peng-Robinson EOS is not able to describe the confined fluid phase behavior. A pore radius dependent EOS is therefore needed in reservoir simulators for accurate large scale tight oil and shale gas production forecast simulations.

The idea of this work is to integrate first the capillary pressure effect into the classical Peng-Robinson EOS and then to calibrate EOS parameters function of pore radius to fit molecular simulations. The capillary pressure which depends on pore radius adds pressure difference between vapor and liquid phase in the equilibrium computation. It is calculated using the Young-Laplace equation. Molecular simulation is performed using Monte Carlo method in the grand canonical and in the NVT Gibbs ensemble with anisotropic volume change in order to calculate equilibrium properties of several pure hydrocarbon components and mixtures in confinement. Kerogen pores are modelled by graphite slit pores and fluid/wall interaction potential is added. For a given pore radius, the critical temperature and pressure are determined for pure components, and liquid and vapor pressures, densities and molar fractions of components are calculated for both pure components and mixtures at different temperatures for calibration. These values are used as reference fitting data for the Peng-Robinson EOS with capillary pressure. The optimization parameters are the Peneloux volume correction constant, the acentric factor and the binary interaction coefficients. The calibration of these parameters allows getting correlations versus pore radius that will be used to model the confined fluid thermodynamic behavior.

The pore radius dependent EOS calibrated with molecular simulation data can therefore be used in reservoir simulators to accurately forecast tight oil and shale gas production. However the grid cells in a dynamic flow simulation is usually in order of several meters to 100m. Such a cell includes a large pore size distribution, the pore radius value used in the EOS is therefore an issue. In order to consider the pore size variability within a simulation cell, an effective radius function of oil saturation is taken. It is determined from the distribution function of pore size volume. Assuming oil is the wetting phase, during a flow simulation, oil is present in small pores and gas appears in larger pores, then the effective pore radius decreases. Oil and gas production simulations with a dual porosity model for a fractured tight-oil reservoir show that this methodology gives more reasonable results than using an average pore radius and of course than a bulk approach.

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