Contribution ID: **382** Type: **Poster Presentation**

A Robust Vapor-liquid-liquid Equilibrium Calculation Algorithm Considering Capillary Pressure and Critical Shift in Nanopores

Monday, 13 May 2024 09:55 (1h 30m)

Porous media contains a huge amount of nanopores, and the behavior of confined fluid phases in nanopores will be affected by significant interfacial effects between the fluids and the walls. A large number of publications have recently investigated the influence of interfacial effects on the phase behavior of confined fluids in nanopores. Many influences such as adsorption, critical shift, capillary pressure have been discussed. However, most of these studies have focused only on vapor-liquid equilibrium (VLE), and few attempts have been made to generalize these influences to vapor-liquid-liquid equilibrium (VLLE) in nanopores. In this work, a robust and efficient algorithm for the calculation of VLLE is proposed. The algorithm can simultaneously consider the influences of capillary pressure and critical shift on VLLE in nanopores. In order to be able to accurately and efficiently calculate each of the possible phases, the algorithm adjusts some of the steps in the conventional VLE calculation and improves the solution methodology.

The results of VLLE in this algorithm are obtained from three-phase flash calculations. It is well known that three-phase flash calculations are extremely dependent on initial guess and have poor convergence properties. In order to solve this problem, this work couples the successive substitution iteration with the Newton-Raphson iteration and builds a joint solver. The results show that this coupled joint solver not only improves the computational efficiency, but also enhances the stability of the flash calculations.

The robustness of the present algorithm is verified by several computational examples, and influences of capillary pressure and critical shift on VLLE in nanopores are investigated. In this work, mixtures of hydrocarbons with water and carbon dioxide were calculated and several possible fluid distribution scenarios were considered. The computational results show that both capillary pressure and critical shift can change the phase distribution of the confined fluid in nanopores.

1. The effect of capillary pressure on phase behavior is determined by the wettability between nanopores and the confined fluids. When the nanopores have a higher affinity for the vapor phase than the liquid phase, the generation of the bubble point will be advanced and the generation of the dew point will be lagged. If wettability is reversed, the effect of capillary pressure on phase behavior of the system is also reversed at the same time.
2. Critical shift affects the phase behavior of confined fluids more than capillary pressure for a certain range of pore sizes. However, the critical shift is independent of the wettability. Regardless of the pore size, the effect of critical shift on phase behavior has the same trend.
3. The effect of pore size on the behavior of confined fluids is nonlinear. In other words, there is an inflection point in the trend of pore size versus the phase behavior, and when the pore size is higher than this inflection point, the effect of capillary pressure or critical shift can be neglected when calculating the VLLE. Based on the findings of this work, we believe that this inflection point lies around 100 nm.

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Session Classification: Poster

Track Classification: (MS13) Fluids in Nanoporous Media