Phase equilibria modeling of methanol-containing systems with the CPA and sPC-SAFT equations of state

Proper representation at various conditions of phase equilibria of methanol-containing mixtures (with hydrocarbons, water, etc.) is important for oil flow assurance purposes. In this work, two association equations of state, CPA and sPC-SAFT, are applied to methanol-containing mixtures. The purpose of this work is to investigate which association schemes (e.g., two-site, three-site) should be used for methanol which will result in successful representation of methanol-water-hydrocarbon phase equilibria. Parameters from the literature as well as newly estimated parameters based on vapor pressure, liquid density, enthalpy of vaporization, and compressibility factor data at used. Methanol-alkane vapor-liquid equilibrium (VLE) and liquid-liquid equilibrium (LLE) data, water-methanol VLE as well as water-methanol-hydrocarbon LLE are considered.

It is concluded that the two association equations of state perform overall similarly, with the two-site association scheme being a better choice than the three-site scheme, for phase equilibrium calculations. Use of the additional properties (enthalpy of vaporization and compressibility factor) in the parameter estimation has a larger effect on the performance of sPC-SAFT compared to CPA (C) 2009 Elsevier B.V. All rights reserved.

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