

New Mixing Rules for High-Pressure Equilibrium Calculation of Water + Ethylene Glycol + Methane, Ethane and Acid Gases systems using EOS/GE

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Vapor-liquid equilibrium (VLE) modeling of natural gas at high pressure is essential in design of many processes such as dehydration and natural gas treatment. The EOS/GE models have been applied using several cubic equation of state (CEOS) and excess Gibbs energy functions for equilibrium calculation of natural gas which consists of light to heavy hydrocarbons with water and acid gases, i.e., H₂S and CO₂. The various mixing rules using local composition models have been developed such as Huran-Vidal, MHV2, Wong-Sandler etc. These mixing rules are widely applied for modeling variety of systems using energy interaction parameters which should be adjusted by optimization of VLE data. In addition, application each of these mixing rules limited to some binary systems. In this work using EOS/GE, a new local composition-equation of state model (LCEOS1) was developed in which the energy interaction parameters were expressed in terms of attractive and repulsive parameters of the cubic equation of state. Applying this new mixing rule, the bubble point pressure and vapor phase compositions at the condition of 100-400 bars were simulated. The binary parameters of coupling and a lumped nonrandomness for binary systems containing CO₂, H₂S, H₂O, CH₄, C₂H₆, EG, TEG have been obtained. Using the binary parameters, solubility of CH₄ and C₂H₆ in ternary systems CH₄ EG (TEG) H₂O and C₂H₆ EG (TEG) H₂O were predicted, respectively. In addition, a modification of Wong-Sandler-NRTL mixing rule (LCEOS2) was expressed and results obtained for the same binary and ternary systems. Comparison of these two new mixing rules with experimental data, Wong-Sandler (WS) and Van der Waals (VdW) mixing rules showed that both LCEOS1 and LCEOS2 demonstrate better accuracy.