A Simple Group Contribution Method for Predicting Binary Interaction Parameters of Cubic Equations of State for Glycol-Hydrocarbon Systems

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Objectives and Challenges Design and Optimization of upstream processes require accurately predicting phase equilibria of mixtures of water, hydrocarbons, and glycols which are injected as hydrate inhibitors at elevated pressures. It is known that cubic equations of state (CEoS) with an empirical mixing rule proposed by Cunningham et al. [1] work well for correlating the equilibria. However, the challenge is that even experimental data are missing for many of the binary pairs to determine values of the binary interaction parameters (BIPs).

Proposed Approach This work establishes a simple and practical group contribution method for predicting the BIPs for pairs of hydrocarbon and each of mono-ethylene glycol (MEG), diethylene glycol (DEG), and triethylene glycol (TEG), based on numbers of saturated carbons, aromatic carbons, and saturated carbons directly connected to aromatic carbons. A simple linear formula is applied. Moreover, for petroleum pseudo-components, we roughly estimate the numbers of the carbons based on the Watson K-value of each petroleum component even when the exact molecular structure is not known. A simple sigmoid function is applied to estimate the ratio between the carbon number of saturates and that of aromatics.

Results At first, we determined BIPs for around 20 glycol-hydrocarbon pairs for which experimental data were available with respect to vapor-liquid equilibrium and/or liquid-liquid equilibrium. The hydrocarbon components were in the range of carbon numbers of 1-9, including paraffinic and aromatic components. The proposed method successfully correlated the BIPs. It was also demonstrated that the method was applicable to petroleum pseudo-components, when combined with the procedure using the Watson K-value.

Conclusions A simple and practical group contribution method was established to predict BIP values of CEoS for glycol-hydrocarbon pairs. The method was applicable to pairs of glycol-petroleum pseudo-components also using Watson K-value.

References:

[1] J.R. Cunningham, J.E. Coon, and C.H. Twu; “Estimation of Aromatic Hydrocarbon Emissions from Glycol Dehydration Units using Process Simulation” Presented at 72nd Annual GPA Convention, March 15-17 (1993)