Application of GC-PC-SAFT EoS to Organic Sulfur Compounds

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Introduction

Design and optimization of separation processes require accurate knowledge of the thermodynamic properties and phase equilibria of involved pure compounds and mixtures. Thermodynamic models are thus needed to determine these properties. Model development relies on not only appropriate theory but also experimental data. However, for the organic sulfur compounds which are commonly found in diverse industrial sectors, few or even no experimental data exist in the literature. Therefore, models with predictive features may act as an alternative to handle engineering purposes.

Statistical Associating Fluid Theory (SAFT) equation of states (EoS) has been proved to be a powerful tool for modeling phase equilibria, as statistic mechanics and molecular theory were incorporated into the development. In this work, the Perturbed-Chain SAFT (PC-SAFT) EoS [1] was combined with the Group Contribution method proposed by Tamouza et al. [2]. The predictive model (named GC-PC-SAFT) was applied to investigate two series of typical organic sulfur compounds: sulfide (R-S-R’) and 1-thiol (R-SH). The group parameters of (S) and (SH) were fitted to vapor pressure and liquid density data (from [3]) of 9 sulfides and 7 1-thiols, respectively. The regression results show that the average deviations on vapor pressure are generally lower than 5%, while those on liquid density are generally lower than 2%.

GC-PC-SAFT EoS

Hard spherical segment

PC-SAFT EoS [1]

Segment number m

Association

CH3 CH3

S

SH

Pure compound parameters

\( m_{\text{molecule}} = \sum N_i m_i \frac{\sigma_{ij}}{\sum N_i} \)

Group parameters

\( (\sigma_{ij}, \epsilon_{ij}) \)

\( \epsilon_{molecule} = \left( \prod \epsilon_{ij} \right)^{\frac{1}{m}} \)

Dipole term from Jog and Chapman [4]

Dipole moment \( \mu \)

Dipolar segment number \( x_m \)

Results

Prediction of vapor pressure data (from [5])

Prediction of saturated liquid density data (from [5])

Prediction of enthalpy of vaporization data (from [5])

Prediction of heat capacity data (from [5])

Conclusion & Perspective

Application of GC-PC-SAFT EoS with a dipolar term to investigate the sulfides and 1-thiols

Good correlation and prediction of pure compound properties (AAD generally less than 5%)

Satisfactory prediction of mixture VLE and h^liq data without any binary interaction parameters (k = 0)

Prediction for multi-compound systems

Improvement in representing the solvation

Extension to other organic sulfur compounds

Reference