Optimization of the Reduced Temperature Associated with Peng-Robinson Equation of State to Improve Vapour Pressure Prediction for Heavy Hydrocarbon Compounds

Zehua Chen[1] and *Daoyong Yang*[1]

Abstract

In general, a good representation of vapour pressures of pure substances leads to a good saturation pressure prediction for their mixtures. As for the Peng-Robinson equation of state (PR-EOS), the Pitzer acentric factor is originally defined at reduced temperature of 0.7 and subsequently redefined at 0.5 and 0.6, respectively. Such definitions have been found to impose a significant impact on the accuracy of the vapour pressure prediction for both pure heavy compounds and their mixtures. In this study, a pragmatic technique has been developed to optimize the reduced temperature for acentric factor associated with the PR-EOS by minimizing the deviation between the measured and calculated vapour pressures for non-hydrocarbon compounds and hydrocarbon including heavy alkanes up to n-tritetracontane (n-$C_{43}H_{88}$) under different conditions. All the compounds are divided into four categories, i.e., light-saturated hydrocarbons, heavy-saturated hydrocarbons, aromatic compounds, and other compounds, among which heavy-saturated hydrocarbons and aromatic compounds are found to be more sensitive to the predicted vapour pressures for heavy oil components. By redefining the reduced temperature, four different alpha functions are then used to evaluate their respective accuracy of predicting vapour pressures for pure substances. For the existing database with 1164 data points, the reduced temperature is found to have its optimum value of 0.62 for the acentric factor corresponding to a minimum AARD of 1.87%. For the newly expanded database with 2046 data points, the reduced temperature has its optimum value of 0.57 for the acentric factor for calculating the vapour pressures with a minimum AARD of 7.35%. Such a larger difference from the latter is mainly due to the fact that it is composed of more data points that are deviated from the optimum reduced temperature of 0.57. Therefore, it is recommended that reduced temperature of 0.6 shall be used for predicting the vapour pressure of heavy hydrocarbon compounds and their mixtures.

[1]Petroleum Systems Engineering, Faculty of Engineering and Applied Science, University of Regina, Regina, Saskatchewan S4S 0A2, Canada

Zehua Chen is a Ph.D. graduate student in petroleum systems engineering in the Faculty of Engineering and Applied Science at the University of Regina. His Research interests include thermodynamics and phase behavior, CO_2 and chemical enhanced oil recovery, and reservoir modeling and simulation. Chen holds a B.Sc. degree and a M.A.Sc. degree in petroleum engineering from the China University of Petroleum (East China).