

Accepted Manuscript

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PII: S0140-7007(17)30355-9

DOI: <http://dx.doi.org/doi: 10.1016/j.ijrefrig.2017.09.008>

Reference: IJIR 3748

To appear in: *International Journal of Refrigeration*

Received date: 16-6-2017

Revised date: 10-9-2017

Accepted date: 12-9-2017

Please cite this article as: Hamidreza Soltani Panah, Modeling binary vapor-liquid equilibrium data containing perfluorocarbons using the Peng-Robinson and the PC-SAFT equations of state, *International Journal of Refrigeration* (2017), <http://dx.doi.org/doi: 10.1016/j.ijrefrig.2017.09.008>.

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Modeling Binary Vapor-Liquid Equilibrium Data Containing Perfluorocarbons using the Peng-Robinson and the PC-SAFT Equations of state

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Highlights

- Thermodynamic modeling of 24 binary systems containing PFC compounds is studied.
- The PC-SAFT pure parameters for R-1216 and HFPO are obtained.
- Interaction parameters of binary systems are estimated for PR and PC-SAFT EoS.
- A solution for VLE calculations near critical zone using cubic EoS is suggested.

Abstract

In this communication, thermodynamic modeling of twenty four binary systems containing perfluorocarbon compounds is studied using the Peng-Robinson and the PC-SAFT equations of state. Interaction parameters of binary systems were estimated through fitting to experimental equilibrium pressures and vapor phase compositions. Very good results were obtained through using temperature-independent interaction parameter for both equations of state. According to the results, percent deviations in pressure were varying between 0.5 and 7.7 for the PR EoS and 0.2 and 6.5 for the PC-SAFT EoS. Also, percent deviations in vapor phase composition were varying between 0.1 and 6.6 for the PR EoS and 0.1 and 7.4 for the PC-SAFT EoS. Furthermore, when binary system has critical point, phase equilibrium calculations using the PR EoS do not converge through common methods. For solving this problem, a solution is suggested that was absolutely effective on all the studied systems.

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