

Comments on “Solubility of CO₂, N₂, and CO₂ + N₂ Gas Mixtures in Isooctane” (Zhang, J. S.; Lee, S.; Lee, J. W. *J. Chem. Eng. Data* 2008, 53, 1321–1324)

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In a recent paper in this journal, Zhang et al.¹ reported the solubility, at three temperatures, of CO₂ in isooctane and of N₂ in isooctane. The equilibrium compositions of CO₂ and N₂ binary mixtures in isooctane at 273.8 K were also determined.

In 2004, we started to develop a group contribution method aimed at predicting the binary interaction parameter k_{ij} for the Peng–Robinson equation of state.^{2–6} Recently, we extended our approach to systems containing CO₂⁵ and N₂.⁶ To do so, we built a huge databank containing all the VLE data for CO₂–hydrocarbon and N₂–hydrocarbon binary systems. Then, group interaction parameters have been determined to minimize the deviations between calculated and experimental VLE data from the databank. We are thus extremely interested by new experimental data, such as those published by Zhang et al.¹ Indeed these data allow us to test the accuracy and the predictive capacities of our model. Nevertheless, we would like to make the following comments on the content and conclusions reported in their paper.

1. In the Introduction, it is said that “At present, no reports can be found on the solubility of N₂ and CO₂ in isooctane”. This is incorrect, as literature data are in fact available^{7–12} for the two binary mixtures. Between 1959 and 2005, four papers^{7–10} were published regarding the solubility of CO₂ in 2,2,4-trimethylpentane (isooctane). For this binary system, more than 180 experimental points (bubble points and dew points) are available at temperatures ranging from (277.63 to 393.15) K. The corresponding pressures vary between (0.1 and 11.1) MPa.

Three papers^{7,11,12} were published concerning the binary mixture N₂ + isooctane, and more than 60 experimental points are thus available at temperatures ranging from (323.15 to 452.95) K. The corresponding pressures vary between (2.0 and 63.0) MPa.

2. With the previously mentioned papers,^{7–12} Zhang et al. would have been able to compare their measured values with literature data for the two studied binary systems (CO₂ + isooctane and N₂ + isooctane) instead of checking the validity of their experimental setup with a binary system (CO₂ + water) which has no evident link with the subject of their paper.

3. Concerning the test run, the authors write that “The solubility of CO₂ in water under this condition is (1.20 ± 0.09) %, very close to the value of 1.27 predicted by CO2SOL, which

confirms the validity of our method”. From our point of view, it is questionable to assert that an experimental method is valid because the obtained result is close to a calculated value.

Literature Cited

- (1) Zhang, J. S.; Lee, S.; Lee, J. W. Solubility of CO₂, N₂, and CO₂ + N₂ Gas Mixtures in Isooctane. *J. Chem. Eng. Data* **2008**, *53*, 1321–1324.
- (2) Jaubert, J. N.; Mutelet, F. VLE predictions with the Peng–Robinson equation of state and temperature dependent k_{ij} calculated through a group contribution method. *Fluid Phase Equilib.* **2004**, *224*, 285–304.
- (3) Jaubert, J. N.; Vitu, S.; Mutelet, F.; Corriou, J. P. Extension of the PPR78 model (predictive 1978, Peng–Robinson EOS with temperature dependent k_{ij} calculated through a group contribution method) to systems containing aromatic compounds. *Fluid Phase Equilib.* **2005**, *237*, 193–211.
- (4) Vitu, S.; Jaubert, J. N.; Mutelet, F. Extension of the PPR78 model (predictive 1978, Peng–Robinson EOS with temperature dependent k_{ij} calculated through a group contribution method) to systems containing naphthenic compounds. *Fluid Phase Equilib.* **2006**, *243*, 9–28.
- (5) Vitu, S.; Privat, R.; Jaubert, J. N.; Mutelet, F. Predicting the phase equilibria of CO₂ + hydrocarbon systems with the PPR78 model (PR EOS and k_{ij} calculated through a group contribution method). *J. Supercrit. Fluids* **2008**, *45*, 1–26.
- (6) Privat, R.; Jaubert, J. N.; Mutelet, F. Addition of the Nitrogen Group to the PPR78 Model (Predictive 1978, Peng–Robinson EOS with Temperature-Dependent k_{ij} Calculated through a Group Contribution Method). *Ind. Eng. Chem. Res.* **2008**, *47*, 2033–2048.
- (7) Prausnitz, J. M.; Benson, P. R. Solubility of liquids in compressed hydrogen, nitrogen, and carbon dioxide. *AIChE J.* **1959**, *5*, 161–164.
- (8) Hiraoka, H.; Hildebrand, J. H. The Solubility and Entropy of Solution of Certain Gases in (C₄F₉)₃N, CCl₂F₂, CClF₂, and 2,2,4-(CH₃)₃C₅H₉. *J. Phys. Chem.* **1964**, *68*, 213–214.
- (9) Han, B.; Yan, H.; Hu, R. Solubility of CO₂ in a mixed solvent of n-octane and i-octane at elevated pressures. *Thermochim. Acta* **1990**, *169*, 217–221.
- (10) Mutelet, F.; Vitu, S.; Privat, R.; Jaubert, J. N. Solubility of CO₂ in branched alkanes in order to extend the PPR78 model (Predictive 1978, Peng–Robinson EOS with temperature-dependent k_{ij} calculated through a group contribution method) to such systems. *Fluid Phase Equilib.* **2005**, *238*, 157–168.
- (11) Graham, E. B.; Weale, K. E. The solubility of compressed gases in nonpolar liquids. In *Progress in International Research on Thermodynamics of Transport Properties*, ASME Proceedings from the 2nd Symposium on Thermophysical Properties, Princeton, NJ, 1962; American Society of Mechanical Engineers (ASME): New York, 1962; pp 153–158.
- (12) Peter, S.; Eicke, H. F. Phase equilibrium in the systems nitrogen-n-heptane, nitrogen-2,2,4-trimethylpentane, and nitrogen-methylcyclohexane at higher pressures and temperatures. *Ber. Bunsen-Ges.* **1970**, *74*, 190–194.

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