

# Comments on “Solubility of CO<sub>2</sub>, N<sub>2</sub>, and CO<sub>2</sub> + N<sub>2</sub> 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.<sup>1</sup> reported the solubility, at three temperatures, of CO<sub>2</sub> in isooctane and of N<sub>2</sub> in isooctane. The equilibrium compositions of CO<sub>2</sub> and N<sub>2</sub> 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.<sup>2–6</sup> Recently, we extended our approach to systems containing CO<sub>2</sub><sup>5</sup> and N<sub>2</sub>.<sup>6</sup> To do so, we built a huge databank containing all the VLE data for CO<sub>2</sub>–hydrocarbon and N<sub>2</sub>–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.<sup>1</sup> 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 N<sub>2</sub> and CO<sub>2</sub> in isooctane”. This is incorrect, as literature data are in fact available<sup>7–12</sup> for the two binary mixtures. Between 1959 and 2005, four papers<sup>7–10</sup> were published regarding the solubility of CO<sub>2</sub> 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<sup>7,11,12</sup> were published concerning the binary mixture N<sub>2</sub> + 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,<sup>7–12</sup> Zhang et al. would have been able to compare their measured values with literature data for the two studied binary systems (CO<sub>2</sub> + isooctane and N<sub>2</sub> + isooctane) instead of checking the validity of their experimental setup with a binary system (CO<sub>2</sub> + water) which has no evident link with the subject of their paper.

3. Concerning the test run, the authors write that “The solubility of CO<sub>2</sub> 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.

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