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Determination of saturated vapor pressure of aromatic compounds based on experimental data on their solubility in supercritical carbon dioxide

© **Timur R. Bilalov***+ and **Farid M. Gumerov**
Kazan National Research Technological University. K. Marx St., 68. Kazan, 420015. Tatarstan Rebublic. Russia. E-mail: t.bilalov@yandex.ru

*Supervising author; +Corresponding author

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Abstract

The paper presents a method to describe the solubility of various substances in supercritical carbon dioxide, based on the Peng-Robinson's equation of state of real gases, as well as M. Mukhopadhyay, G.V.R. Rao's one-parameter mixing law. The calculation algorithm includes an unknown binary interaction parameter, determined by the method of minimizing the root mean square deviation of the calculated solubility values from the experimental ones on the described isotherm, as well as the saturated vapor pressure of the soluble substance at the process temperature. In the presence of experimental data of saturated vapor pressure, the accuracy of the description is primarily affected by the correctness of the experimental technique and its accuracy. In the absence of reliable experimental data, this value is determined by different calculation methods. Most of the calculation methods are based on the Clausus-Clapeyron equation and use the critical parameters of the test substance as the initial data, as well as the normal boiling point. Different authors have proposed unique calculation methods for determining the saturated vapors pressure, the results of calculations on which differ sometimes by several orders. The paper presents the results of the study of the influence of the method for determining the saturated vapors pressure of the substance soluble in supercritical carbon dioxide on the accuracy of the description of solubility. The list of calculation methods for establishing the value of the saturated vapor pressure includes methods: Clayperon, Lee-Kesler, Riedel, Frost-Kalkwarf-Todos and Riedel-Plank-Miller. It is shown that in most cases these methods do not allow describing experimental data of solubility of substance in SC-CO_2 with acceptable accuracy (up to 10-12%). The paper also suggests the use of saturated vapor pressure as a second adjustable parameter in the description of solubility in addition to the traditionally accepted binary interaction parameter. This significantly increases the accuracy of the description of the solubility of substances in supercritical carbon dioxide. The significantly greater convergence of the saturated vapor pressure values established in this way with the values obtained in the framework of the experimental methods is shown.

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