DETERMINATION OF SATURATED VAPOR PRESSURE OF AROMATIC HYDROCARBONS ON EXPERIMENTAL DATA OF THEIR SOLUBILITY IN SUPERCRITICAL CARBON DIOXIDE

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The paper presents a method for describing the solubility of various substances in supercritical carbon dioxide, based on the equation of state of real gases penga-Robinson, as well as the one-parameter mixing law Muhopadhyaya and Rao. The calculation algorithm includes an unknown binary interaction coefficient determined by the method of iteration and minimization of 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 experiment methodology and its accuracy. In the absence of reliable experimental data, this value is determined by different calculation methods [1]. Most of the calculation methods are based on the Clausius-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 pressure of saturated vapors. Results of calculations with the use of these methods sometimes differ by several orders for one and the same substance. The paper presents the results of a study of the influence of the method for determining the pressure of saturated vapors of a substance dissolved 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 on substance solubility in supercritical carbon dioxide with acceptable (up to 10-12%) accuracy. 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 coefficient. This significantly increases the accuracy of the description of the solubility of substances in supercritical carbon dioxide. The substantially 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. Experimental data on solubility of various substances used in the

work were taken from [2].

1. R. Reid Properties of Gases and Liquids, McGraw-Hill publisher, New York, (1987). Khimiya publisher, Leningrad, (1982) 592 p.
2. Solubility in Supercritical Carbon Dioxide, Ram B. Gupta, Jae-Jin Shim, CRC press, ISBN: 0849342406, 960p.