

## A Novel Semi Empirical Equation for Prediction the Solute Solubility in Supercritical Carbon Dioxide

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**Abstract:** Supercritical fluid carbon dioxide with very favorable critical properties has been so important in the recent two decades as an alternative to organic solvent. In the past two decades, researchers presented many semi empirical equations for solubility prediction in supercritical carbon dioxide. In this paper, accuracy of seven semi empirical equation (consist of Chrastil, Dell Valle, Mendez, Yu, Gordillo, Jouyban, Jafari Nejad) was calculated using 26 published solubility data sets. Results showed Jouyban's equation has less mean ARD (about 14.92%) than other equations. In the next step a modified form of Jouyban's equation proposed. The proposed equation is  $\ln y_2 = B_0 + B_1 P + B_2 P^2 + B_3 P \cdot T + B_4 T/P + B_5/T + B_6 \ln \rho$  where  $B_0$ - $B_6$  are the coefficients of equation calculated by least square method,  $P$ (bar) is pressure of process,  $T$ (Kelvin) is temperature of process,  $\rho$  is density of supercritical fluids and  $y_2$  is mole fraction of solute in supercritical fluid. The mean ARD of proposed equation is 11.34%. The proposed model presents more accuracy than previously published semi empirical equation.

**Key word:** Solubility; Supercritical carbon dioxide; Semi empirical equation; ARD.