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论文

超临界CO<sub>2</sub>与叔丁醇二元系统高压相平衡研究

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摘要:

采用固定体积可视观察法测量装置测定了CO<sub>2</sub>与叔丁醇在323.2~353.2 K温度范围内于不同压力下的平衡数据, 并运用Peng-Robinson状态方程(PR)和Van der Waals-2混合规则建立了相平衡模型, 通过非线性最小二乘法优化计算得到了不同温度下的模型参数, 并得到了模型参数与温度的表达式, 分别为 $k_{12} = -199.2066 + 1.81367 - 0.00548T^2 + 5.50 \times 10^{-6} T^3$ ;  $n_{12} = -384.5626 + 3.49607 - 0.01056T^2 + 1.06 \times 10^{-5} T^3$ . 获得了此体系在不同组成下的临界压力、临界温度、临界摩尔体积、临界压缩因子和临界密度等临界性质. 研究表明, CO<sub>2</sub>与叔丁醇二元体系的临界温度、临界压力和临界压缩因子均随着临界CO<sub>2</sub>组成的增加而降低.

关键词: 超临界二氧化碳; 叔丁醇; 相平衡模型; 临界性质

Studies on Phase Equilibrium of Tertbutanol in Supercritical CO<sub>2</sub>

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Abstract:

Vapor-liquid phase equilibrium data of tertbutanol in the SC-CO<sub>2</sub> from 323.2 K to 353.2 K were determined by constant-volume visual method. The phase equilibrium model was established by Peng-Robinson equation of state and Vander Waals-2 mixed regulation. Model parameters were obtained by nonlinear least square method optimization calculation. Furthermore, the correlation equations of model parameters vs. temperature were obtained:  $k_{12} = -199.2066 + 1.81367 - 0.00548T^2 + 5.50 \times 10^{-6} T^3$ ,  $n_{12} = -384.5626 + 3.49607 - 0.01056T^2 + 1.06 \times 10^{-5} T^3$ . Critical properties of critical pressure, critical temperature, critical molar volume and critical density were deduced. The results showed that critical temperature, critical pressure and critical compressibility factor of CO<sub>2</sub>-tertbutanol system would decrease with the increasement of critical CO<sub>2</sub> content.

Keywords: Supercritical carbon dioxide; Tertbutanol; Phase equilibrium model; Critical property

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