研究论文

利用统计缔合流体理论状态方程预测混合气体水合物的平衡形成条件

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摘要 利用统计缔合流体理论(SAFT)状态方程结合van der Waals-Platteeuw统计力学模型用于预测含有甲烷、乙烷、丙烷、乙烯、丙烯、 H_2S , CO_2 , N_2 和 H_2 二元气体水合物的平衡形成条件. 对于气相和液相,应用SAFT方程来描述. 在气相和液相相平衡的模拟过程中, SAFT方程考虑了硬球斥力、成链力、色散力以及缔合相互作用. 对于水合物相, 采用van der Waals-Platteuw模型来计算. 该方法的预测结果与实验数据吻合.

关键词 <u>气体水合物</u> <u>统计缔合流体理论</u> <u>状态方程</u> <u>平衡形成条件</u> 分类号

Prediction of Equilibrium Hydrate Formation Conditions for Gas Mixtures Using the Statistical Associating Fluid Theory Equation of State

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Abstract The statistical associating fluid theory (SAFT) equation of state in conjunction with the statistical model of van der Waals and Platteeuw was employed to predict the formation equilibrium conditions of binary gas mixtures containing methane, ethane, propane, ethylene, propylene, H_2S , CO_2 , N_2 and H_2 in the presence of aqueous solutions. The SAFT equation was used to describe the vapor and liquid phases. In calculation, the SAFT took into account hard sphere repulsion, hard chain formation, dispersion and association interactions. The van der Waals and Platteeuw model was applied to calculate the hydrate phase. The predictions were found to be in quite good agreement with the experimental data.

Key words gas hydrate the statistical associating fluid theory equation of state equilibrium formation condition

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