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RESEARCH NOTES

PSRK模型的修正混合规则及其应用于聚合物溶液汽液平衡的预测

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摘要 To extend the PSRK (predictive Soave-Redlich-Kwong equation of state) model to vapor-liquid equilibria of polymer solutions, a new EOS-gE mixing rule is applied in which the term ∑xiln (b/bi) in the PSRK mixing rule for the parameter a, and the combinatorial part in the original universal functional activity coefficient (UNIFAC) model are cancelled. To take into account the free volume contribution to the excess Gibbs energy in polymer solution, a quadratic mixing rule for the cross co-volume bij with an exponent equals to 1/2 is applied [bij^1/2=1/2(bi1/2+bj1/2)]. The literature reported Soave-Redlich-Kwong equation of state (SRK EOS) parameters of i3 - 2- pure polymer are employed. The PSRK model with the modified mixing rule is used to predict the vapor-liquid equilibrium (VLE) of 37 solvent-polymer systems over a large range of temperature and pressure with satisfactory results.

关键词 PSRK模式 混合工艺 聚合物 计算方法 UNIFAC模式

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A Modified Mixing Rule for PSRK Model and Application for the Prediction of Vapor-Liquid Equilibria of Polymer Solutions

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Abstract To extend the PSRK (predictive Soave-Redlich-Kwong equation of state) model to vapor-liquid equilibria of polymer solutions, a new EOS-gE mixing rule is applied in which the term ∑xiln (b/bi) in the PSRK mixing rule for the parameter a, and the combinatorial part in the original universal functional activity coefficient (UNIFAC) model are cancelled. To take into account the free volume contribution to the excess Gibbs energy in polymer solution, a quadratic mixing rule for the cross co-volume bij with an exponent equals to 1/2 is applied [bij^1/2=1/2 (bi1/2+bj1/2)]. The literature reported Soave-Redlich-Kwong equation of state (SRK EOS) parameters of i3 - 2- pure polymer are employed. The PSRK model with the modified mixing rule is used to predict the vapor-liquid equilibrium (VLE) of 37 solvent-polymer systems over a large range of temperature and pressure with satisfactory results.

Key words predictive Soave-Redlich-Kwong equation of state mixing rule; vapor-liquid equilibrium; polymer solutions

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