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聚合物-溶剂体系中能量对溶剂扩散的影响

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摘要 The Vrentas-Duda free-volume theory has been extensively used to correlate or predict the solvent diffusion coefficient of a polymer/solvent system. The energy term in the free volume diffusion equation is difficult to estimate, so the energy term was usually neglected in previous predictive versions of the free volume diffusion coefficient equation. Recent studies show that the energy effect is very important even above the glass transition temperature of the system. In this paper, a new evaluating method of the energy term is proposed, that is, the diffusion energy at different solvent concentrations is assumed to be a linear function of the solvent diffusion energy in pure solvents and that in polymers under the condition that the solvent in infinite dilution. By taking consideration of the influence of energy on the solvent diffusion, the prediction of solvent diffusion coefficient was preformed for three polymer/solvent systems over a wide range of concentrations and temperatures. The results show an improvement on the predictive capability of the free volume diffusion theory.

关键词 [solvent diffusion in polymer](#) [prediction](#) [energy effect](#)

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Influence of Energy on Solvent Diffusion in Polymer/Solvent Systems

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Abstract The Vrentas-Duda free-volume theory has been extensively used to correlate or predict the solvent diffusion coefficient of a polymer/solvent system. The energy term in the free volume diffusion equation is difficult to estimate, so the energy term was usually neglected in previous predictive versions of the free volume diffusion coefficient equation. Recent studies show that the energy effect is very important even above the glass transition temperature of the system. In this paper, a new evaluating method of the energy term is proposed, that is, the diffusion energy at different solvent concentrations is assumed to be a linear function of the solvent diffusion energy in pure solvents and that in polymers under the condition that the solvent in infinite dilution. By taking consideration of the influence of energy on the solvent diffusion, the prediction of solvent diffusion coefficient was preformed for three polymer/solvent systems over a wide range of concentrations and temperatures. The results show an improvement on the predictive capability of the free volume diffusion theory.

Key words [solvent diffusion in polymer](#); [prediction](#); [energy effect](#)

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