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热力学

超临界丙烷分级聚苯乙烯

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摘要 利用超临界流体的溶剂强度随温度、压力的变化而变化和超临界流体泄压至常压时溶质完全析出的特点，采用超临界丙烷取代常规溶剂对聚苯乙烯进行分级研究，以期柔性地调节操作温度和压力，获得分子量分布较窄的聚合物级分.结果表明，对多分散系数为4.225的聚苯乙烯进行等温超临界分级和等压超临界分级实验能够得到多分散系数分别为1.0～2.0和1.3～2.0的级分.并且发现，压力和温度越高，溶剂的溶解能力越大，分级得到的级分分子量越大.同时，从高聚物溶液理论出发，结合超临界溶液的溶解特性，建立了超临界流体分级高聚物的级分分子量的预测模型.利用实验数据对模型参数优化结果表明，当压力大于25 MPa时，超临界等温分级模型的平均相对误差为5.32%；当温度大于413.15 K时，超临界等压分级模型的平均相对误差为18.03%.

关键词 超临界流体 丙烷 聚苯乙烯 分级 模型

分类号

POLYSTYRENE FRACTIONATION WITH SUPERCRITICAL PROPANE

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Abstract

Polystyrene can be fractionated with supercritical propane.The main advantage of supercritical fluid fractionation is that large polymer fractions with a narrow molecular mass distribution can be obtained without using hazardous organic solvent.Isothermal fractionation was performed using increasing pressure profiling that provided milligram-size fractions with M_w distribution of 1.0—2.0 as compared to parent polymer with polydispersity 4.225.At the same time,isobaric fractionation was performed using increasing temperature profiling that provided fractions with M_w distribution of 1.3—2.0 from the same parent polymer.The molecular mass of fraction increases with increasing operating pressure and temperature as the solvent power of SCF increases.The major benefit of SCF solvent relative to a liquid solvent is that the solvent power of SCF can be finely tuned by controlling operating conditions.It is recommended that pressure should be controlled to tune the solvent power of SCF effectively.With a SCF solvent, the solubility of a polymer drops to essentially zero if the pressure is reduced to near ambient condition,thus facilitating the recovery of a solvent-free polymer fraction.
A model relating the molecular mass of fraction to operating variables was deduced on the basis of the theory of polymer solution.The model parameters were estimated by using experimental data.The average relative deviation was below 18%.

Key words supercritical fluid propane polystyrene fractionation model

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