材料化学工程与纳米技术

超临界二氧化碳溶胀聚甲基丙烯酸甲酯的在线可视测量及热力学模拟计算

陈力骅，曹贵平，张人瀚，何峰，刘涛，赵玲，袁渭康，George W.Roberts

华东理工大学联合化学反应工程研究所，化学工程联合国家重点实验室; Department of Chemical and Biomolecular Engineering, North Carolina State University

摘要

采用高压视窗釜配合高清晰相机研究了聚甲基丙烯酸甲酯(PMMA)在超临界二氧化碳(scCO$_2$)中溶胀行为，得到了PMMA在scCO$_2$中的平衡溶胀率。Sanchez-Lacombe(S-L)状态方程对于高压气体和聚合物系统的热力学性质有着很强的预测能力。将PMMA的PVT数据使用S-L状态方程进行拟合，得到压力、温度和密度的特征参数分别为：212.38 MPa、898.04 K以及1206.7 kg·m^{-3}（8～25 MPa，305～350 K），类似地可以得到二氧化碳(CO$_2$)的特征参数541.56 MPa、313.38 K以及1502.1 kg·m^{-3}（8～25 MPa, 305～325 K）。将实验得到的PMMA平衡溶胀率使用S-L状态方程拟合，可得二元相互作用参数为1.0671，结果表明在超临界区域，S-L状态方程模拟溶胀率与实验值吻合较好。

关键词

聚甲基丙烯酸甲酯　 超临界二氧化碳　 溶胀　 在线可视测量　 Sanchez-Lacombe状态方程

分类号

In-situ visual measurement of poly(methyl methacrylate) swelling in supercritical carbon dioxide and interrelated thermodynamic modeling

CHEN Lihua, CAO Guiping,ZHANG Renhan, HE Feng, LIU Tao, ZHAO Ling, YUAN Weikang, George W.Roberts

Abstract

A visual measurement apparatus was applied to monitor *in-situ* the swelling behavior of poly(methyl methacrylate) (PMMA) in supercritical carbon dioxide(scCO$_2$).This work presents the swelling data of PMMA over a useful range of processing conditions (temperature from 305 K to 325 K, and pressure up to 24 MPa).The Sanchez-Lacombe equation of state (S-L EOS) is suitable to describe low molecular weight solvent-polymer systems.Through fitting the *PVT* data into S-L EOS, the characteristic pressure, temperature and density of PMMA were regressed as 212.38 MPa, 898.04 K and 1206.7 kg·m^{-3} (8—25 MPa,305—350 K), respectively.Similarly, the characteristic parameters for carbon dioxide (CO$_2$) were 541.56 MPa, 313.38 K and 1502.1 kg·m^{-3} (8—25 MPa,305—325 K), respectively.The equilibrium swelling data of PMMA in scCO$_2$ were correlated with S-L EOS, the binary interaction parameter was obtained as 1.0671.These results indicated that the S-L EOS can be used to predict the solubility of CO$_2$ and the swelling of PMMA over a wide range of pressure.The S-L EOS modeled values agreed well with the experimental data in supercritical region.

Key words

poly(methyl methacrylate)　 supercritical carbon dioxide　 swelling　 *in-situ* visual measurement　 Sanchez-Lacombe equation of state

通讯作者 曹贵平 gpcao@ecust.edu.cn