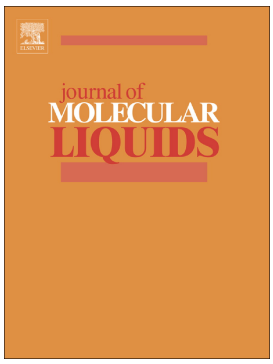

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Study on the solubility parameter of supercritical carbon dioxide system by molecular dynamics simulation

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Abstract

The enhancement of the solubility parameter of supercritical carbon dioxide plays pivotal role in the application of extraction operation. The solubility parameter of supercritical CO_2 solvent (SC-CO_2) and supercritical CO_2 with cosolvent (SC-CO_2-cosolvent) system have been studied using the molecular dynamics simulations (MD). The calculated results reveal that the solubility parameters of pure SC-CO_2 solvent and SC-CO_2-cosolvent both reduce with the raising of temperature, enhance with the raising of pressure, and boost linearly with the raising of their density. The adding of the cosolvent (methanol, ethanol, acetone and cyclohexane) into the SC-CO_2 system can enhance the solubility parameter of SC-CO_2 solvent significantly, and the solubility parameter boosts with the raising of the cosolvent concentration. The cosolvent effect on solubility parameter of SC-CO_2 solvent decreases in the order: methanol, ethanol, acetone, cyclohexane. The hydrogen bonding ability of the cosolvent has significant effect on solubility parameter of SC-CO_2 solvent via the strengthening of the interactions among the CO_2 and cosolvent molecules.

Key words: supercritical carbon dioxide; solubility parameter; cosolvent; molecular dynamics simulation

1. Introduction

As a flexible and practical chemical engineering technology, the supercritical carbon dioxide fluid (SC-CO_2) technology has been applied as an industrial technology in the extraction process for its wide supercritical operation conditions and the strong dissolving capacity of nonpolar and weak polar molecules [1-6]. The extraction of essences, heavy metal cations, hops and the active ingredients of Chinese herbal medicines using SC-CO_2 solvent have been applied in the industry [7]. However, the lower solubility of high polymer with strong polar functional group in SC-CO_2 solvent is a critical factor in hindering the application of SC-CO_2 extraction technology in more fields [2, 3]. There are two pathways proposed to improve the solubility of high polymers in the SC-CO_2 solvent. In one of the pathways, higher pressure and temperature are adopted in the extraction operation process to enhance the solubility of high polymers in SC-CO_2 solvent. In the other pathway, The cosolvents, such as methanol, ethanol and acetone, are added into the SC-CO_2 solvent to improve the solubility of polar solutes under lower temperature and pressure. Mobbs [8] et al. pointed out that the cosolvents (methanol, ethanol, acetone etc.) added into the SC-CO_2 system (SC-CO_2-cosolvent system) can improve the solubility