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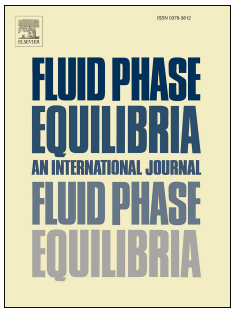

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Solubility of CO_2 in triglycerides using Monte Carlo simulations

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Abstract

The knowledge of solubility of different gases in triglycerides is required to design efficient cell disruption processes for biodiesel production from wet biomass. In this combined experimental and simulation study, we determine carbon dioxide solubility in long (C18) and short (C4) chain triglycerides, and provide microscopic picture of CO_2–triglyceride interaction. The solubility of CO_2 in tributyrin (a small chain triglyceride) was determined using a pressure drop gas apparatus at P = 800 to 1700 kPa and T = 283.2 to 303.2 K. Gibbs ensemble Monte Carlo simulations with configurational biased Monte Carlo algorithm were used to compute the solubility of CO_2 in both a long chain triglyceride (to mimic canola oil) and tributyrin at different pressures and temperatures. The transferable potentials for phase equilibria force field was used for modeling triglycerides and CO_2. Predicted densities and viscosities of both canola oil and tributyrin were in good agreement with the experimental data. We find that the computed solubilities are in excellent agreement with the experimental results for both CO_2–canola oil and CO_2–tributyrin where the mean deviation were 2.85% and 9.51%, respectively. The structural analysis of liquid phase indicates that CO_2 has slightly higher preference to bind with carbonyl group than the nonpolar segments.

Keywords: Gas solubility, Monte Carlo, microstructure, transfer free energy, carbon dioxide

1. Introduction

Oil extraction from wet biomass consisting of oleaginous yeast is a promising technique to produce biodiesel at a lower cost compared to the traditional lipid extraction methods that require energy intensive drying of the biomass [1, 2, 3, 4, 5]. To extract the lipid from biomass, the wet cell must be disrupted

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