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Prediction of solubility of biomolecules in supercritical solvents

Ratnawati Hartono [1], G. Ali Mansoori *, Aryadi Suwono

Thermodynamics Research Laboratory, Department of Chemical Engineering, The University of Illinois at Chicago, 202 CEB, M/C 110, 810 S. Clinton Street Chicago, IL 60607-7000 USA

Abstract

The supercritical fluid extraction (SFE) is considered an appropriate alternative for separation of biomolecules from food and pharmaceutical products. A major difficulty in utilizing the SFE for biomolecules has been the difficulty in measurement and prediction of their solubilities in supercritical solvents at various pressures and temperatures for process optimization. Lack of data for intermolecular energy parameters and/or critical properties, acentric factors, and molar refractions limits us to the use of the simple equations of state for prediction of their solubilities in supercritical solvents. In this report, six different cubic equations of state are used to predict the solubility of cholesterol and β-carotene, as two representative biomolecules, in supercritical fluids. They are the van der Waals, Redlich–Kwong, Mohsen-Nia–Moddaress–Mansoori (MMM), Peng–Robinson (PR) and Patel–Teja and modified PR equations. It is shown that the two-parameter MMM equation is more accurate than five of the other equations and comparable to the modified PR equation in predicting the solubility of cholesterol and β-carotene in supercritical fluids.

Keywords: Prediction; Solubility; Biomolecule; Supercritical solvent

1. Introduction

The advantages of utilizing supercritical solvents for extraction have been well documented (Park, Kwak, & Mansoori, 1987; Schulz, Martinelli, & Mansoori, 1991; Ekhtera, Mansoori, Mensinger, Rehmat, & Deville, 1997). The supercritical fluid extraction (SFE) has interested investigators during the past few decades. Unlike the conventional extraction process which uses liquids, the SFE process uses a supercritical fluid as the solvent. In comparison with conventional solvents, a supercritical fluid has high diffusivity and low viscosity, thus allowing rapid extraction and phase separation. Another attractive feature of supercritical solvents is the fact that their isothermal compressibility is several orders of magnitude greater than that of liquids while their density is the same as liquids. The relatively high supercritical fluid density gives it a good solvent power. As a result a sudden reduction in temperature or pressure often causes the loss of these special characteristics of the supercritical solvent. Therefore, a solute can be extracted at supercritical condition of the solvent, and separated from the solvent by reducing pressure or temperature below the critical condition of the solvent, yielding a solvent-free extract (Schulz et al., 1991). By using supercritical solvents having low critical temperatures, it is possible to extract thermally labile compounds, especially the pharmaceutical and food products. As an example, cholesterol can be removed from food products using supercritical solvents resulting in minimal protein degradation (Chao et al., 1991). Valuable thermal-labile compounds, such as β-carotene can also be extracted using supercritical solvents without any degradation observed (Skerget, Knez, & Habulin, 1995). Carbon dioxide is the most widely used gas as the supercritical solvent because it is non-toxic, nonflammable, inexpensive, abundantly available, and has low critical temperature (Schulz et al., 1991).

Cholesterol is a sterol that can be found in many animal tissues, but not in plant tissues. It is the most abundant sterol in human tissues. It is a component of all cell membranes and functions as a precursor of bile acids, steroid hormones, and vitamin D. The

* Corresponding author. Tel.: +1-312-996-5592; fax: +1-312-996-0808.

E-mail address: mansoori@uic.edu (G. A. Mansoori).

[1] Permanent address: Jurusan Teknik Kimia Fakultas Teknik Universitas Diponegoro Kampus Tembalang, Semarang, Indonesia.

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