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Modeling of Supercritical Carbon Dioxide Extraction of Andrographolide from *Andrographis paniculata* Leaves

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Mathematical modeling is necessary for the optimization and design of any separation process, such as the extraction of bio-molecules from their natural resources. The objective of this work is to obtain a quantitative description of the supercritical carbon dioxide extraction (SCDE) of andrographolide from Andrographis paniculata *leaves through the development of a mathematical model based on first-order desorption rate of solute into supercritical solvent. Numerical calculations to obtain the adjustable parameter of the model, using experimental data obtained from the SCDE of andrographolide at different solvent flow rates and particle sizes, were done using MATLAB software. The results showed that this model agrees well with the experimental data. Therefore, this model is useful for the optimization and design of SCDE of andrographolide from* Andrographis paniculata *leaves.*

Keywords *Andrographis paniculata*; Andrographolide; Extraction; MATLAB; Modeling; Supercritical carbon dioxide

Introduction

Andrographis paniculata Nees, locally known as hempedu bumi, grows widely in the tropical area of Southeast Asia, India, and China, with an annual growth of 30–70 cm in height. In Malaysia, this plant has been extensively used in traditional medicine for treating fever, dysentery, diarrhea, inflammation, and sore throat. Furthermore, it is a promising new treatment for many diseases, including HIV, AIDS, and numerous symptoms associated with immune disorders (Calabrese et al., 2000). Based on medicinal activities, there are three main diterpenoid lactones identified in *Andrographis paniculata* leaves, namely andrographolide, neo-andrographolide, and deoxy-andrographolide (Choudhury et al., 1987; Wongkittipong et al., 2000; Rajani et al., 2000). Andrographolide, which is grouped as an unsaturated trihydroxy lactone, has a molecular formula of $C_{20}H_{30}O_5$. The molecular structure of andrographolide is shown in Figure 1. Andrographolide can be easily dissolved in methanol, ethanol, pyridine, acetic acid, and acetone, but only slightly dissolved in ether and water. The melting point of this substance is 228°–230°C, and its ultraviolet
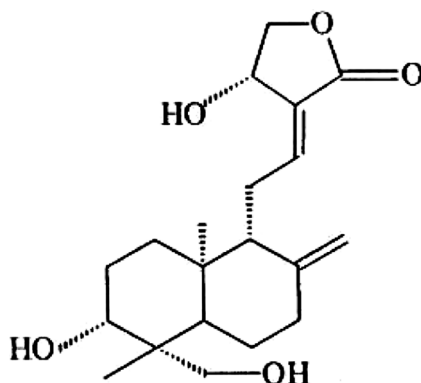
Figure 1. Molecular structure of andrographolide (Rajani et al., 2000).

spectrum in ethanol, $\lambda_{\max}$, is 223 nm (Rajani et al., 2000). There are some techniques that can be used for the analysis of andrographolide, such as thin-layer chromatography (TLC) (Choudhury et al., 1987; Wongkittipong et al., 2000), high-performance liquid chromatography (HPLC) (Wongkittipong et al., 2000; Tang et al., 2000; Li and Fitzloff, 2004), and crystallization techniques (Rajani et al., 2000).

Extraction using an organic solvent is the most common method of separating bioactive components from their natural hosts. However, since these organic solvents are not able to be completely removed by existing separation techniques, and their traces may remain in the final product, extraction using only organic solvents is no longer attractive from the clinical, environmental, energy, and time-consumption points of view (Luque de Castro and Garcia-Ayuso, 1998; Kolar et al., 2002). Therefore, supercritical fluid extraction is a better alternative method to extract andrographolide from *Andrographis paniculata* leaves, since this method offers shorter extraction times, cheaper operating cost, higher extraction selectivity, safer conditions (nontoxic, nonflammable, nonhazardous), and adjustable solvating power (Taylor, 1996).

The objective of this work is to obtain a quantitative description of the supercritical carbon dioxide extraction (SCDE) of andrographolide from *Andrographis paniculata* leaves through the development of a mathematical model based on first-order desorption rate of solute into supercritical solvent.

Mathematical Model Development

Consider a fixed bed of *Andrographis paniculata* leaf particles with an initial concentration of solute, $S = S_0$. Fresh supercritical solvent is introduced into the bed, which is operated isothermally. The total mass balance of this condition can be represented by the following equation:

$$\alpha \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial z} - \alpha \left(D_z \frac{\partial^2 C}{\partial z^2} + D_x \frac{\partial_2 C}{\partial x^2} \right) = -(1 - \alpha) \frac{\partial S}{\partial t} \tag{1}$$

Although several bio-components exist in the leaf particle matrix, the fitting parameter is accounted just as a single parameter, called the solute. This is a pseudo