Supercritical Extraction of ***Valeriana Officinalis* L.** Roots; Mathematical Modeling and Experiments

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Summary

The extraction of essential oil from valerian (*Valeriana Officinalis* L.) roots using supercritical carbon dioxide (SC-CO_2) as the solvent was modeled mathematically. Several parameters influencing extraction model basing on mass transfer balance for solid and supercritical fluid phases have been identified and studied such as: pressure (15.2-36.4 MPa), temperature (37-61 ^{o}C), solvent flow rate (0.5-1.5 ml/min) and particle size (2.5-19$\times 10^{-4}$ m) at the fixed static extraction time (20 min) in order to state the process behavior mathematically. Effective diffusivity (D_{eff}), axial dispersion coefficient (D_L), film mass transfer coefficient (k_i) and equilibrium coefficients were the model parameters. Linear, Langmuir, Freundlich-Langmuir and Toth adsorption isotherm were used to describe the equilibrium state of solid to fluid phase. Using method of line, the proposed model was numerically solved and using Nelder-Mead method, the parameters of the model was estimated.

Keywords: Mathematical modeling; Supercritical Fluid Extraction; *Valeriana Officinalis* L.*;* Mass transfer model.

Extended Abstract

The extraction of essential oil from valerian (*Valeriana Officinalis* L.) roots using supercritical carbon dioxide (SC-CO_2) as the solvent was modeled mathematically. Several parameters influencing extraction model basing on mass transfer balance for solid and supercritical fluid phases have been identified and studied such as: pressure (15.2-36.4 MPa), temperature (37-61 ^{o}C), solvent flow rate (0.5-1.5 ml/min) and particle size (2.5-19$\times 10^{-4}$ m) at the fixed static extraction time (20 min) in order to state the process behavior mathematically.

Mathematical modeling of complex phenomena, such as extraction of natural materials, is an activity of increasing importance because of the economic potentials. It is important to develop models for the extraction process when the extraction operations are optimized for commercial applications. However, such predictions require the establishment of model predicting the phase behavior, equilibrium, solubility, adsorption, desorption etc. [1].

The extracts of underground parts (roots and rhizomes) form valerian (*Valeriana Officinalis* L.) have been used for medicinal purposes for over a century [2]. Certain valerian extracts, including aqueous extracts, were known to have sedative and anxiolytic effects.

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Valerenic acid along with its derivatives are the most well known compound in the medicinal researches worldwide. The preparation of modern phytomedical products, mild traditional sedatives, antianxiety and digestive formulations [3,4] for nervous tension, insomnia and stress [5,6], available in the market in the form of teas or tinctures, tablets and capsules as either powdered root or root extracts [7] have been made valerian to be one of the most selling medicinal herbs in the world [8-10].

Effective diffusivity (D_{eff}), axial dispersion coefficient (D_L), film mass transfer coefficient (k_i) and equilibrium coefficients were the model parameters. Linear, Langmuir, Freundlich-Langmuir and Toth adsorption isotherm were used to describe the equilibrium state of solid to fluid phase. Using method of line, the proposed model was numerically solved and using Nelder-Mead method, the parameters of the model was estimated.

The main objective of this study was to model the extraction process and determine the effect of extraction parameters on the yield of oil and valerenic acid obtained from valerian roots.

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