



Simulation of supercritical fluid extraction of essential oil from natural products



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ABSTRACT

A transport phenomena based model has been used and solved to predict the extraction of essential oils from three different natural materials. This study discusses the extraction of essential oils and the parameters which control the process of mass transfer. The model presented here considers both intra-particle resistance and external film resistance to mass transfer and partial differential equations for unsteady-state mass balance for solute in both solid & supercritical phases are developed based on the concept proposed by Melreles et al. (2009) and solved numerically based on a linear equilibrium relationship. The intra-particle diffusion coefficient and equilibrium constant are used as adjustable parameters for Basil & Rosemary leaves and Vetiver roots respectively. The adjustable parameter is optimized by Golden Section Method and the remaining variables such as density and viscosity are computed using available empirical correlations. The solute concentration in the supercritical carbon dioxide leaving the packed beds of natural products was predicted as a function of extraction time, bed height, solvent flow rate and particle diameter. This model predicts a cumulative yield within an error limit of +6.22% to -0.42% for Rosemary leaves, +3.68% to -3.29% for Basil leaves and +5.93% to -4.73% for Vetiver roots. The our model shows better results as compare to those obtained in the literature.

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1. Introduction

The essential oils of Rosemary leaves, Basil leaves and Vetiver roots are mostly used in the cosmetic, food, fragrance and pharmaceutical industries due to its antibacterial, antifungal, antioxidant and anti-inflammatory properties (Bozin et al., 2007; Sacchetti et al., 2004; Martinez et al., 2004). The essential oils are traditionally extracted by conventional methods, such as organic solvent extraction and steam distillation, which leads to degradation of thermo labile compounds, partial hydrolysis of water sensible compounds and problems related to waste and toxic formation and disposal (Goto and Sato, 1993). To overcome these issues's supercritical fluid extraction (SFE) has emerged as an alternative extraction technology in the field of natural solid products (Munshi and Bhaduri, 2009). Supercritical fluids have got several beneficial properties in between liquid and gas, such as density, viscosity, diffusivity & high mass-transfer characteristics. Also, their behavior above the critical point is very sensitive to pressure and temperature, which leads to

selective separation (Mukhopadhyay, 2000; McHugh and Krukoniš, 1994). However, the high investment cost of a supercritical fluid extraction plant is a matter of concern for a process engineer. An in-depth understanding of physics of the process along with the development of superior mathematical models for the simulation of extraction yield of natural components from plant materials as a function of operating parameters can help to lower down the production cost of running the process effectively (Sovova 1994, 2005). The extraction of solute from natural products, such as leaves, roots, seeds and other materials, takes place by a series of mass transfer step which all together form a mechanism. Firstly, the molecules of supercritical solvent are transported from bulk solvent to particle surface through the boundary layer adjacent to particle surface. Subsequently, the solvent molecules penetrate into pores of the particle and solute molecules, which are attached to the solid matrix by Van der Waals forces and/or chemical forces, are transferred to the solvent phase by dissolution or desorption. Then the solute molecules diffuse to the solid surface and moves across the stagnant film around the particle into the bulk fluid phase.

Many models for SFE have been proposed in the literature, such as the empirical model (Bozin et al., 2007), the broken and intact cell model (Sovova 1994, 2005), the differential mass balance model (Melreles et al., 2009), the simple single plate model (Gaspar et al.,

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Nomenclature

Bi	Biot number (Bi)
c	Solute concentration in the pore of particle (kmol/m^3)
d_p	Particle diameter (m)
D_e	Effective diffusivity in the particle (m^2/s)
D_{ext}	Extractor diameter (m)
D_m	Molecular diffusion coefficient (m^2/s)
D_l	Axial dispersion coefficient (m^2/s)
F	Cumulative extraction yield
h	Axial coordinate increment number
k	Equilibrium constant between solid and fluid phase
k_f	Mass transfer coefficient (m/s)
L	Extractor length(m)
m	Radial coordinate increment number
m_{feed}	Feed mass (kg)
n_0	Initial mole of solute in the bed (kmol)
P	Pressure (bar)
Pe_b	Peclet number for the bed
Pe_p	Peclet number for the vetiver particle
q	Solute concentration in the solid part of particle (kmol/m^3)
Q	Flow rate of supercritical fluid, (kg/s)
r	Axial coordinate in vetiver root (m)
r_p	Particle radius (m)
Re	Reynolds number
Sc	Schmidt number
Sh	Sherwood number
t	Time (s)
T	Temperature (K)
T_c	Critical temperature (K)
T_r	Reduced temperature
v	Interstitial fluid velocity (m/s)
V	Volume of extractor (m^3)
X_0	Initial mass fraction of solute in solid phase
y	Extraction yield (–), solid and fluid concentration (kmol/m^3)
z	Distance of a point in bed from place of input (m)
Z	Dimensionless axial coordinate along the bed

Greek letters

μ	Viscosity (kg/ms)
Δr	Radial coordinate increment (m)
ρ	Density (kg/m^3)
ε	Void fraction of packed bed
ε_p	Particle porosity
ξ	Dimensionless radial coordinate
ξ^*	Parameter in Eqs. (3.2) & (3.3)
$\Delta\xi$	Dimensionless length increment of radial coordinate
τ	Dimensionless time
Δz	Length of axial coordinate increment (m)
ΔZ	Dimensionless length of axial coordinate increment

Subscripts

f	Fluid phase
fs	Surface of particle, in fluid phase
p	Particle
r	Reduced form

2003) and the diffusion model (Crank, 1980; Subra et al., 1998; Reverchon, 1997). The solutions of these models were obtained using various analytical (Sovova, 1994), numerical (Goodarznia and

Eikani, 1998) and evolutionary algorithms (Martínez and Martínez, 2008). In the present investigation, a differential mass balance model has been used with some modification in boundary condition to examine the extraction of Basil leaves, Rosemary leaves and Vetiver roots. To get better results, the model presented here considers an intra-particle diffusion coefficient and equilibrium constant as adjustable parameters for Basil leaves, Rosemary leaves and Vetiver roots respectively. The model equations are solved using the explicit method of lines. After validating from experimental data, the model is also used for parameter study and for evaluating the effects of different operating conditions on the extraction process. An important enhancement in the model developed by authors as compared to the other models (Goodarznia and Eikani, 1998; Reverchon et al., 1993) available in literatures is that the solute concentration in the pore of the solid is considered instead of the solute concentration in the solid itself. Further, the present work is based on an explicit Method whereas the models of other investigators are based on implicit Methods (Melreles et al., 2009; Gaspar et al., 2003; Reverchon and Osseo, 1994).

2. Model description

The key assumptions for the our model are: (1) Axial dispersion is predominating, (2) Radial concentration gradients in fluid phase do not exist, (3) The system is isothermal and isobaric, (4) The physical properties of the supercritical fluid remain constant, (5) Local equilibrium relationship is valid at the fluid-solid interface, (6) Constant bed void fraction and particle porosity during extraction, (7) For small particles, it has been assumed that particle solute concentration is independent of radius and is a function of time only (lumped system) and (8) Solute concentration in particles is symmetrical around the center. Based on the above assumptions, the solute conservation equations were written for both fluid and solid phase:

2.1. Fluid phase mass balance

The concentration 'C' of solute in the fluid phase at height 'z' in a bed of particulate material depends on the rate of mass transfer from particles at height 'z', the fluid flow rate and extent of mixing. Eq. (2.1) is obtained by taking a mass balance around height element Δz of the bed as shown in Fig. 1.

$$\frac{\partial C}{\partial \tau} = \frac{1}{Pe_b} \frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z} - \frac{(1-\varepsilon)3L}{\varepsilon} \frac{Bi}{r_p Pe_p} (C - C_{fs}) \quad (2.1)$$

$$C = 0 \text{ at } \tau = 0, 0 \leq Z \leq 1 \quad (2.2a)$$

$$\frac{\partial C}{\partial Z} = Pe_b (C - 0) \text{ at } \tau > 0, Z = 0 \quad (2.2b)$$

$$\frac{\partial C}{\partial Z} = 0 \text{ at } \tau > 0, Z = 1 \quad (2.2c)$$

where, $\tau = tv/L$, $Pe_p = (r_p v) / D_e$, $Bi = (k_f r_p) / D_e$, $Pe_b = (Lv) / D_l$, $Z = z/L$, $\xi = r / (r_p)$ are dimensionless variables

2.2. General solid phase mass balance

To develop the mass balance equation, a differential element is considered to be inside the particle in case of large sized particles whereas, it is considered at the particle surface for small sized particles. The fluid-solute mass balance for a large porous spherical particle (shown in Fig. 2a) can be written as shown in Eq. (2.3).

$$\frac{1}{Pe_p} \frac{L}{r_p} \frac{1}{\xi^2} \frac{\partial}{\partial \xi} \left(\xi^2 \frac{\partial c}{\partial \xi} \right) = \left[\varepsilon_p + (1 - \varepsilon_p) \frac{\partial q}{\partial c} \right] \left(\frac{\partial c}{\partial \tau} \right) \quad (2.3)$$

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