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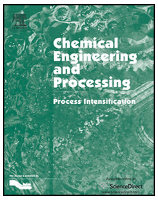

Mathematical modeling of aroma compound recovery from natural sources using hollow fiber membrane contactors with small packing fraction

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ABSTRACT

A numerical simulation was carried out in order to investigate aroma compounds recovery from aqueous phase using an organic solvent. A hollow-fiber membrane contactor with small packing fraction was selected to be used in the study. Momentum, continuity and mass transfer equations were solved simultaneously utilizing finite element method. The simulation results showed that solving the Navier–Stokes equations has significantly diminished average deviation about 55% compared to Happle's velocity model. Simulation results revealed that mass transfer resistance increases along the contactor length in both tube and shell sides. It seems that it is due to the increasing thickness of the boundary layer. Enhancement of the solvent velocity could result in increasing mass transfer rate through the membrane. However, it reduced the extraction efficiency of aroma compounds. Moreover, recovery of 2-hexanal was higher than benzaldehyde due to its higher partition coefficient. Furthermore, n-hexane has higher extraction efficiency than miglyol because of lower Schmidt number.

1. Introduction

Liquid–liquid extraction is one of the important processes in chemical industries [1]. Aroma compounds are widely used as additives for flavoring food and medicines. The quality of the products and the consumer's satisfaction are very important factors in food and medicine industries. These aroma compounds can be recovered from wide varieties of natural sources such as vegetables, fruits and plants [2]. Recently, environmental restrictions related to generating odorous effluents in the food industries have received particular attention. Since some of molecules present in these odorous effluents are used as flavoring food products, it would be interesting to apply methods for recovering of the valuable aroma compounds with eliminating the unpleasant odor of aqueous effluent. This procedure should be considered to compensate for the cost of deodorization process [3–6].

Different types of tower, column and mixer settler are used conventionally as liquid–liquid extraction unit [2,7,8]. Hollow-fiber membrane contactors (HFMCs) are types of new technologies which offer advantages such as high interfacial area and non-dispersive contact of two phases in comparison with conventional contactors. Additionally, modular design allows a membrane unit to operate over a wide range of capacities and also scale up or down in a more straightforward manner [7,9,10]. HFMCs can also be used suitably for the separation of heat-sensitive components like aroma compounds. Due to such advantages, great deals of studies have been investigated hollow-fiber membrane contactors [11–15]. In the case of extraction by liquid solvent, there are some studies for separation of metal ions and proteins [16–18], extraction of organic acids produced by fermentation [19], and pharmaceutical applications [20]. At first, the extraction of aroma compounds from aqueous solutions was performed by Souchon [21] in 1994. Meanwhile, Fabre et al. [22] investigated the recovery and separation of 2-phenylethylalcohol.

Resistance-in-series model has been used by a number of researchers for evaluation of mass transfer through HFMCs [5,18,23–26]. According to this model, the resistances in the aqueous phase, the solvent phase and the membrane are considered in series. Younas et al. developed a kinetic relationship by applying analogy to baffled shell and tube heat exchangers. They presented overall mass transfer coefficient based on the output concentrations. The model was developed on the concept of plug

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Abbreviations: exp, experimental; FEM, finite element method; HFMC, hollow-fiber membrane contactors; 2D, two dimensional.

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Nomenclature

C [mol m^{-3}]	Concentration
d [m]	Diameter
D [m^2 s^{-1}]	Diffusion coefficient
L [m]	Length of the fiber
m [–]	Partition coefficient
M [kg mol^{-1}]	Molecular weight
p [kPa]	Pressure
r_{sh} [m]	Inner shell radius
r_e [m]	Equivalent shell radius
r_{in} [m]	Inner tube radius
r_{out} [m]	Outer tube radius
T [K]	temperature
u [m s^{-1}]	Average velocity
V [m s^{-1}]	Velocity
N [–]	Number of fibers
k [m s^{-1}]	Mass transfer coefficient
Re [$\rho V d \eta^{-1}$]	Reynolds number

Greek symbols

ϕ [–]	Packing fraction
θ [π radian]	Angular coordinate
δ [–]	Membrane thickness
ε [–]	Membrane porosity
τ [–]	Pore tortuosity
κ [m^2]	Permeability of porous media
η [kg m^{-1} s^{-1}]	Viscosity
ρ [kg m^{-3}]	Density

Subscript

A	Component A
i	Component i
fd	Fully developed
r	Radial coordinate
z	Axial coordinate
m	Membrane side
sh	Shell side
t	Tube side
in	Inlet
out	Outlet

Table 2
Membrane module and fiber characteristics [41].

Parameter	Values
Material type	Polypropylene
Inner fiber diameter, d_{in}	0.22 mm
Outer fiber diameter, d_{out}	0.3 mm
Inner shell diameter, d_{shell}	2.2 mm
Pore dimensions	0.04 × 0.10 μm
Number of fibers N	5
Fiber length L	28 cm
Porosity ε	0.4
Tortuosity τ	2.25

and countercurrent flow pattern [10]. The latter equation was applied by many researchers to model the extraction process for various modules [5,10,25,26]. Due to the bulk concentration in the tube and shell sides using these approaches, determination of concentration profile in the radial direction and consequently thickness of boundary layer is impossible.

Computational fluid dynamics (CFD) provides a favorable method to simulate membrane processes. In this method, the process variables are calculated in a very small zone of module so it is possible to analyze the transport phenomena occurring in the membrane contactor in a better way. This method is based on solving conservation equations including momentum; continuity and energy equations. Most of the researchers have studied modeling of gas–liquid membrane contactors to capture CO_2 using CFD method. Some other studies modeled the membrane modules with baffle which generates a cross flow regime [27–40].

In this study, a HFMC module with parallel flow and small fiber packing fraction ($\phi = 0.093$) was modeled using CFD technique. The extraction of aroma compounds such as benzaldehyde and 2-hexanal from aqueous solution by three different solvents (*n*-hexane, miglyol and sunflower oil) was investigated. Axial and radial diffusions were considered in the equations of mass transfer within the tube, the membrane, and the shell side of a hollow-fiber membrane contactor. In this regard, the aim of this research is to predict distribution of solute concentration, molar flux and liquid velocity in the module.

2. Mathematical modeling

2.1. Theory

The membrane module comprised of 5 parallel microporous polypropylene hollow fibers (X50, Membrana-Charlotte, USA). The bundle of membrane was placed carefully in a glass tube of inner diameter 2.2 mm. Detailed description of the experimental set-up is presented in reference [41]. An aqueous feed contains 100 μl/l of solute flowed in the shell compartment while the organic solvent flowed co-currently in the tube side. Duo to hydrophobicity of membrane, the organic solvents wet the membrane pores. Therefore, an interface of two liquids is produced at outer membrane surface. High partition coefficient of aroma compounds between water and solvents can remove the solute from its aqueous solution completely. The aqueous feed and organic solvents were fed at various flow rates. The resulting Reynolds and Schmidt numbers are listed in Table 1. The characteristics of the membrane contactor module are also presented in Table 2.

Happel's free surface model can be used to estimate the equivalent radius of shell side in order to simplify and reduce the calculation time. Based on this model, only a portion of fluid surrounding the fiber is considered and may be approximated as a circular cross section [41].

$$r_e = \frac{r_{sh}}{\sqrt{N}} \tag{1}$$

Due to axial symmetries in the tube and shell sides, only half of the tube and shell zones in radial direction along with module length are modeled. Although the model is built for a hydrophobic membrane and parallel and co-current flow, the results are simply

Table 1
Range of dimensionless numbers.

	Shell side		Tube side			
	Water, benzaldehyde	Water, 2-hexanal	*n*-Hexane, benzaldehyde	*n*-Hexane, 2-hexanal	Miglyol, 2-hexanal	Sun flower Oil, 2-hexanal
Reynolds number	16–78	27–76	50–248	4–216	0.061–0.49	0.042–0.337
Schmidt number	1229	1193	150	146	426742	457516