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# Simulation of convective-diffusional processes in hollow fiber membrane contactors



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#### ABSTRACT

A model for the simulation of the shell-side convective diffusion of a solute in the hollow-fiber contactor with a regular arrangement of fibers is advanced. The model takes into account the impact of the fiber packing density on the shell-side constrained flow and solute transport. A system of periodic rows of parallel monodisperse fibers arranged normally to the laminar flow direction is considered as a model contactor. Flow and solute concentration fields are calculated from the numerical solution of the Navier-Stokes and convective diffusion equations over a broad range of the inter-fiber distances, Reynolds (*Re*) and diffusion Peclet (*Pe*) numbers. For the calculated fiber drag force and for the fiber Sherwood number (*Sh*) for high and intermediate Peclet numbers  $Pe \gg 1$  and at  $Re \leq 50$ , the best-fit regression formulas are found. The fiber Sherwood number governs the contactor retention efficiency via  $E = 1 - \exp(-4\alpha H Sh/a)$ , where *a* is the fiber radius, *H* is the thickness of the layer of fibers,  $\alpha$  is the packing density is demonstrated. Fiber retention efficiency is shown to follow the fiber drag force, which makes it possible to estimate the solute retention efficiency of a contactor from its hydrodynamic resistance to the shell-side flow. A convective-diffusional transport of a solute in the hollow fiber contactor for with a radial Stokes flow is also considered.

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### 1. Introduction

Membrane contactor is a device for separation of species or chemical conversion, when a selective or non-selective (porous) membrane serves as a partition between two phases. In practice, membrane contactors are widely used for gas-liquid absorptiondesorption processes such as water deoxygenation in the semiconductor industry, carbon dioxide removal from various gas mixtures, ozonation of wastewater, beverage carbonation, removal of ammonia from wastewaters and waste gases, air humidity control (dehumidification or humidification) and energy recovery, etc. [1,2]. As basic elements, porous membranes [3–5] and membranes with dense selective layers preventing penetration of a liquid phase into a gaseous phase [6–11] are commonly used. The main limitations of membrane systems based on nondispersive absorption using porous membranes are discussed in [12], where the problems to be solved to achieve an industrially attractive process for CO<sub>2</sub> recovery are outlined.

A contactor with hollow-fiber membranes [8] (Fig. 1) is the most common option which provides high specific surface area. The vast majority of commercial hollow-fiber contactors and heat exchangers are designed for the liquid supply into the inter-fiber (shell-side) space because, in this case, the hydraulic resistance is lower than that in the module where the flux is supplied into the inner fiber space. Contactors with two-dimensional (2D) parallel or transverse flows (Fig. 1a), with predominantly transverse radial flow (Liqui-Cel contactors), and with a three-dimensional parallel-transverse flow (Fig. 1b) are used. Volume fraction occupied by fibers is rather high (reaching 0.45), providing thus high specific membrane surface area up to 30,000 m<sup>2</sup>/m<sup>3</sup>. The highest retention efficiency is attained when the transverse (cross) flow is used. Commercial and experimental contactors were reviewed in [13].

The contactor solute retention efficiency *E* is governed by the fiber retention efficiency due to convection diffusion  $\eta$ :

$$E = 1 - C/C_0 = 1 - \exp(-2aL\eta),$$
 (1)

where  $C_0$  is the inlet solute concentration in the stream, *C* is the outlet solute concentration, *a* is the outer fiber radius, L = lH,  $l = \alpha/\pi a^2$  is the fiber length per unit volume, *H* is the thickness of the layer of





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#### Nomenclature

а	hollow-fiber radius, L	r
b	outer radius of the layer of fibers in the radial flow con-	R
	tactor, –	S
С	solute concentration in the stream, –	L
D	solute diffusion coefficient, L <sup>2</sup> T <sup>-1</sup>	u
Ε	contactor solute retention efficiency, –	0
F	the drag force per unit length of the fiber, –	r
Н	thickness of the fiber layer, L	ĸ
2h	distance between the axes of fibers in the row, –	μ
1	the length of the fibers per unit volume of the fibrous	ν
	layer, L <sup>-2</sup>	θ
Ре	diffusion Peclet number, –	
$\Delta p$	pressure drop in the fiber layer, Pa	

fibers,  $\alpha$  is the fiber packing density. Fiber retention efficiency is related to the fiber Sherwood number [14] as follows:

$$\eta = 2\pi \, Sh(Re, Pe, \alpha), \tag{2}$$

where  $Pe = 2aUD^{-1}$  is the diffusion Peclet number,  $Re = 2aUv^{-1}$  is the Reynolds number, v is the liquid kinematic viscosity, D is the solute coefficient of diffusion, U = q/S is the uniform inlet flow velocity, q is the flow-rate, S is the cross-sectional surface. Fiber retention efficiency  $\eta$  depends on the flow regime and on the fiber contactor parameters and can be calculated from the solution of the convective diffusion equation. The  $\eta$  value depends also on the presence of neighboring fibers and can be expressed in terms of the fiber packing density (fiber volume fraction) or the inter-fiber distance (blockage ratio). Contactors with hollow-fiber membranes are used at the pumping velocities corresponding to the laminar flow regime. In the system of fibers, the Reynolds numbers per averaged inlet velocity U = q/S lie within the range Re = 0.1-100.

Mass transport in contactors was studied in detail for the case of a parallel flow in the system of parallel fibers [15]. The existing empirical dependences of the Sherwood number on the Reynolds and Schmidt numbers were reviewed in [16]. For hydrophobic and hydrophilic membranes with the account for the packing density of fibers, the corresponding approximate empirical correlations for *Sh* were presented in [17]. These correlations were derived for given systems and for prescribed conditions.

Over many years, the cell model is being used [18] for the computation of  $\eta$  with the account for neighboring fibers at  $Re \ll 1$ under the assumption that, behind each row of fibers, concentra-



tional mixing is complete. According to this model, each fiber is located at the center of a circular cell with the radius  $b = a/\alpha^{1/2}$ . To account for the effect from neighboring fibers, different boundary conditions at the outer cell radius were suggested by various authors. The cell model (free surface model) was used within the Happel boundary conditions for parallel (longitudinal) [19] and transverse flows [20,21]. Another solution by Kuwabara appeared to be consistent with the experiments for transverse flow in a hexagonal lattice of fibers [22] and later was analytically and numerically confirmed [23,24]. Based on this flowfield, fiber collection efficiencies due to diffusion were also computed, and equations relating  $\eta$  with filter parameters and viscous flow conditions were derived [25].

Detailed studies on the convective diffusion in the fiber systems were performed at  $Re \ll 1$  under the boundary condition of a complete absorption at the fiber surface, C = 0. For the system of parallel fibers arranged normally to the flow direction, the following equation for the fiber retention efficiency was derived [26]

$$\eta = 2.9k^{-1/3}Pe^{-2/3} + 0.624Pe^{-1}.$$
(3)

Eq. (3) was repeatedly confirmed by experiments [27] and simulations [28]. Here,  $k = 4\pi/F$  is the hydrodynamic factor, where  $F = \tilde{F}/U\mu$  is the fiber drag force per unit length,  $\mu$  is the dynamic viscosity of the liquid, ~ denotes the dimensional quantity; note that  $k = -0.5 \ln \alpha - 0.75 + \alpha - 0.25\alpha^2$  in the cell model by Kuwabara. Thus, the retention efficiency is determined by the constrained nature of the flow and is related to the flow resistance



64

Fig. 1. Design of hollow fiber membrane modules with a cross (a) and predominantly longitudinally-cross (b) external flows: 2 – shell-side, 1 – inner flow in the hollow fiber (lumen-side).

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