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Application of CFD Techniques for Prediction of NH_3 Transport Through Porous Membranes

AZAM MARJANI* and SAEED SHIRAZIAN

Islamic Azad University, Arak Branch, Department of Chemistry, Arak (Iran).
*Corresponding author: a-marjani@iau-arak.ac.ir

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ABSTRACT

This paper presents application of CFD techniques for simulation of wastewater treatment using membrane technology. Finite element method (FEM) was used as numerical solver. A comprehensive model is developed to predict the system. The model considers equations of momentum and mass transfers. The influence of process parameters on the system efficiency was evaluated. The results showed that concentration boundary layer (CBL) is formed near the membrane surface. The modeling predictions also confirmed that the developed model is capable to evaluate the effective parameters which involve in the ammonia removal by means of membranes.

Key words: Mass transfer, Modeling, CFD, Wastewater treatment, Membrane.

INTRODUCTION

Wastewater treatment is the most important issue in the field of environment. It can be carried out by various separation processes. Designing new processes for wastewater treatment is a subject of research for the scientists worldwide. At the moment, attempts are done to find new solutions to remove all contaminants from water and wastewater. Among the water contaminants, ammonia (NH_3) is a major contaminant which can cause adverse effects. Ammonia is present in municipal and industrial wastewater. Dissolved ammonia in solutions is produced from industrial activities such as petroleum refining, coking, chemical fertilizer, coal gasification, pharmaceutical and catalyst factories[1-7]. From environmental perspective, a complete separation of ammonia from wastewater is desirable. The concentration of ammonia in industrial wastewaters varies from 5 to 1000 mg/L[8]. The removal of dissolved ammonia from wastewaters is thus mandatory to protect the environment and human health.

Currently, conventional separation processes including selective ion exchange, air stripping, break-point chlorination, denitrification, and biological nitrification are applied to remove ammonia from water and wastewater[1, 9-11]. Recently, porous membranes have attracted large attentions as contactors for ammonia separation. A major part of the interest towards membrane contactors is due to their capability in providing a dispersion free contact between 2 phases. In addition, the velocities of both phases can vary independently, while neither flooding nor unloading problems may happen[12]. Membrane contactors can be considered as a promising technology for separation of ammonia from wastewater.

The main aim of this work is to develop a 2D model for the simulation of ammonia transport through porous membranes. The type of membrane contactor is assumed to be polymeric hollow-fiber. The equations of the model are solved by CFD techniques. An algorithm is developed for the numerical simulation. Mass transfer and Navier-Stokes equations are solved simultaneously for the ammonia in the membrane contactor to obtain the concentration distribution[13].

Mass transfer model

Equations of the model

A 2D mass transfer model is developed and solved in this study to determine the concentration distribution of NH_3 in a porous membrane considered as the membrane contactor. Fig. 1 shows basic of separation using a membrane contactor.

The feed solution containing dissolved ammonia (NH_3) flows with a laminar velocity inside the hollow fibers. Since the diameters of hollow fibers are very low, flow regime is assumed to be laminar in the calculations. The feed solution is flown to the lumen side, while the stripping solution is passed through the shell side. Ammonia is removed from the feed phase by subsequent diffusion through the bulk of liquid and membrane, and becomes absorbed into the solvent.

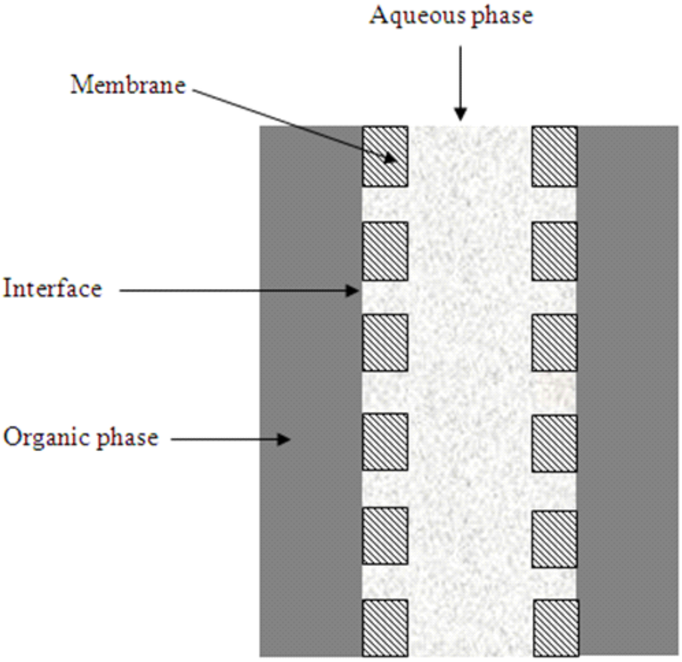

Fig. 1: Basic principle of separation in membrane contactors

The model is built considering the following assumptions:

- Steady state and isothermal conditions.
- Laminar flow in the membrane contactor.
- Henry's law is applied for feed-membrane interface.
- Non-wetted mode for the membrane is assumed; in which the feed aqueous solution do not fills the membrane pores.
- There is no reaction zone.
- Velocity of both ammonia solution and sulfuric acid are constant.

The steady state continuity equation for ammonia transport in the membrane contactor in cylindrical coordinate is obtained using Fick's law of diffusion. Diffusive flux is estimated from Fick's law. The continuity equation may be written as [14]:

$$\frac{\partial C_{NH_3}}{\partial t} + D_{NH_3}\left[\frac{\partial^2 C_{NH_3}}{\partial r^2} + \frac{1}{r}\frac{\partial C_{NH_3}}{\partial r} + \frac{\partial^2 C_{NH_3}}{\partial z^2}\right] = V_z \frac{\partial C_{NH_3}}{\partial z} \quad ...(1)$$

The term V_z is z-velocity in the membrane contactor. To solve Eq. 1, an equation for velocity distribution is required. Velocity distribution in the feed phase is calculated by solving the momentum equation. The most appropriate momentum equation here is Navier-Stokes equations. Therefore, the momentum and the continuity equations should be coupled and solved simultaneously to calculate the concentration distribution of ammonia in the feed side. The Navier-Stokes equations are defined as follows [14]:

$$\begin{aligned} &-\nabla \cdot \eta(\nabla V_{z-lumen} + (\nabla V_{z-lumen})^T) + \rho(V_{z-lumen}.\nabla)V_{z-lumen} + \nabla p = F \\ &\nabla . V_{z-lumen} = 0 \end{aligned} \quad ...(2)$$

where η , , and ρ denote fluid dynamic viscosity (kg/m.s), velocity vector (m/s), and density (kg/m^3), respectively; is pressure (Pa) and is a body force term (N).

Numerical solution of the equations

The main objective of the present study is to simulate a membrane contactor using CFD techniques based on finite element method (FEM). The equations of ammonia transport in the contactor with the boundary conditions were solved using COMSOL Multiphysics. The latter utilizes finite element method for numerical solution of the partial differential equations. The finite element method is combined with adaptive meshing and error control using numerical solver of UMFPACK. The applicability, robustness and accuracy of this numerical method for the membrane contactors have been proved by some researches [12, 15]. It should be pointed out that the COMSOL creates triangular meshes that are isotropic in size. A large number of elements are then created. A scaling factor was employed for the membrane contactor in the z direction due to a large difference between *r* and *z*. Adaptive mesh refinement in COMSOL, which generates the best and minimal meshes, was applied to mesh the whole geometry of membrane contactor. An IBM-PC-Pentium 4 (CPU speed is 2800 MHz) was used to solve the sets of equations. Parameters used for numerical simulations are taken from literature [10-15].

RESULTS AND DISCUSSION

Concentration distribution of ammonia in the feed side

Numerical solution of the continuity equation results in calculation of concentration distribution of ammonia in the feed side of membrane contactor. Fig. 2 shows the concentration

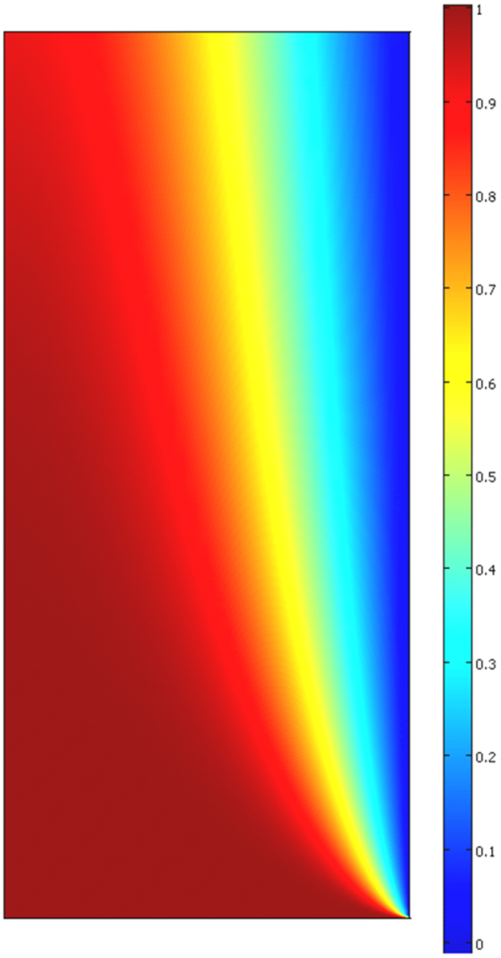

Fig. 2: Concentration distribution of ammonia in the contactor

distribution of NH_3 in the feed side of the contactor. The feed solution flows from the lumen side at $z = 0$. The chemical solvent solution flows from the shell side counter-currently. As the feed solution passes in the lumen side, due to the concentration gradient, ammonia is transferred from the bulk of the feed towards the feed-membrane surface. At the surface of the membrane, only ammonia evaporates into the membrane pores and reaches the shell side. At the shell side of the membrane contactor, an instantaneous chemical reaction occurs between ammonia and acid sulfuric. Fig. 2 also shows that

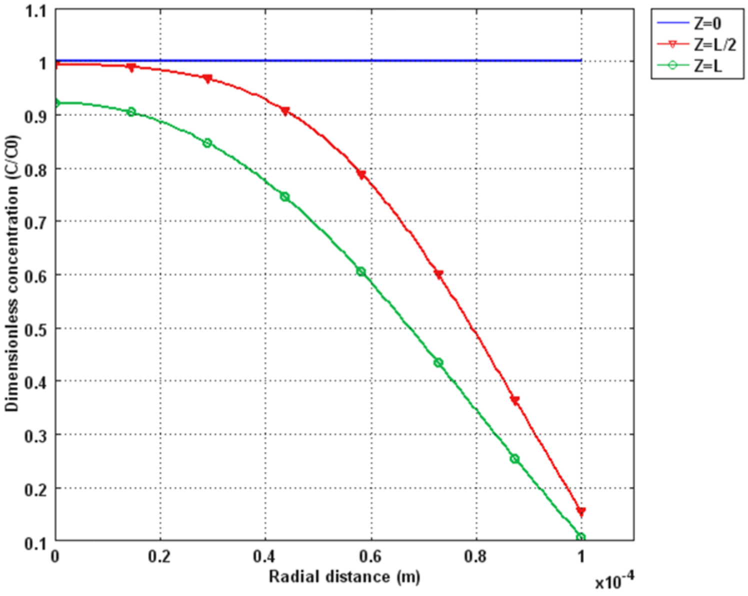

Fig. 3: Radial concentration profile of ammonia in the feed at different axial positions

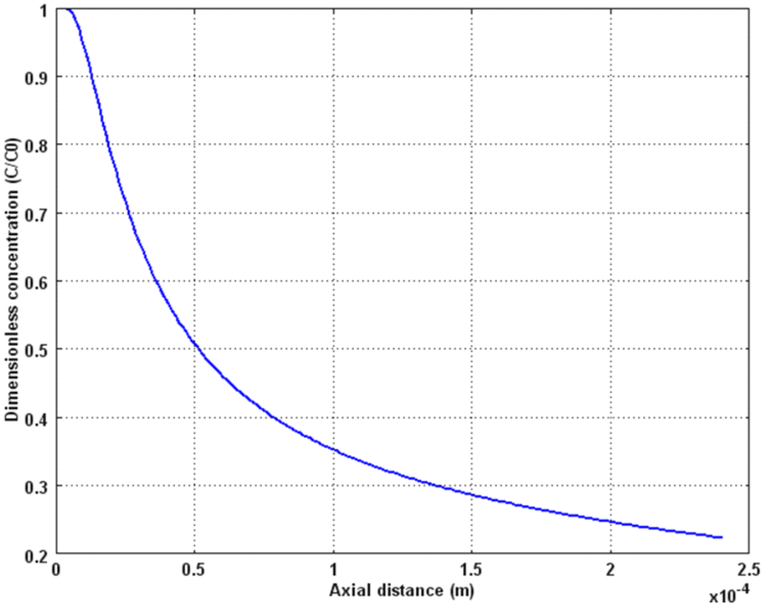

Fig. 4: Axial concentration distribution of ammonia in the lumen side.

concentration gradient is the highest near the membrane, adjacent to the fiber wall.

Radial concentration profile of NH_3

Radial concentration distribution of ammonia in the lumen side of the membrane contactor was also investigated in this work. A plot of the radial concentration profile at different axial positions along the lumen side of the membrane contactor is shown in Fig. 3. It is clearly shown that in the region near the axis of the hollow fiber i.e., $r = 0$ the bulk concentration of ammonia slightly changes. The maximum concentration of ammonia can be observed in the center of the hollow fiber due to axial symmetry assumption. Concentration of ammonia decreases gradually in the region between the center and wall of the fiber side. Eventually, in the region adjacent the membrane-feed interface, concentration sharply decreases. This behavior could be attributed to the formation of the concentration boundary layer near the fiber wall.

Axial concentration profile of NH_3

Investigation of concentration profile of ammonia in axial direction would be valuable. In axial direction, the contribution of convective mass transfer flux is dominant. Therefore, axial concentration profile of ammonia along the lumen side of the membrane contactor is shown in Fig. 4. Obviously, at the inlet of membrane contactor, ammonia concentration is the highest. As the feed solution flows in the lumen side, concentration decreases significantly due to interphase mass transfer between feed and solvent (stripping solution). Fig. 4 also reveals that at the region near the contactor entrance, concentration falls sharply. This could be attributed to this fact that in this region, concentration gradient is high and causes significant decrease in the ammonia concentration.

CONCLUSIONS

A mass transfer model was developed to study the transport of ammonia through porous membranes. The model is based on mass transfer between two phases. The model predicts the steady state concentration of ammonia in the membrane contactor. The model was developed considering a hydrophobic membrane which is not wetted by the aqueous feed solution. FEM analysis was applied for numerical solution of the equations. The simulation results revealed that the developed model can predict the formation of concentration boundary layer (CBL).

Nomenclature

C	concentration, mol/m^3
D	diffusion coefficient, m^2/s
J_i	diffusive flux of species i, mol/m^2s
L	length of the fiber, m
p	pressure, Pa
r	radial coordinate, m
r_{in}	inner radius of fibers, m
r_{out}	outer radius of fibers, m
ρ t	time, s
T	temperature, K
u	average velocity, m/s
V	velocity in the module, m/s
z	axial coordinate, m
Greek symbols	
η	dynamic viscosity (kg/m.s)
	density (kg/m^3)

Abbreviations

FEM	finite element method
HFMC	hollow-fiber membrane contactor
2D	two dimensional
CFD	computational fluid dynamics
CBL	concentration boundary layer

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