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NOTE

Computational Fluid Dynamics Simulation of Ammonia Removal from Wastewaters by Membrane

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Ammonia removal from wastewaters was studied theoretically by means of hollow-fiber membrane contactors. An unsteady state and 2D mathematical model was developed to study ammonia removal in hollow-fiber membrane contactors. The model predicts the unsteady state concentrations of ammonia in the contactor and feed tank. Two sets of equations were solved for membrane contactor and feed tank using computational fluid dynamics techniques. Modeling predictions were then validated with the experimental data obtained from literature and were found to be in good agreement. Simulations showed that the developed model can be used to evaluate the parameters that affect ammonia removal in the contactor and feed tank.

Key Words: Ammonia, Wastewater, Numerical simulation, Membrane, Mass transfer.

Ammonia has been recognized as a major pollutant in both municipal and industrial wastewaters. Dissolved ammonia exists in industrial wastewaters such as coking, chemical fertilizer, coal gasification, petroleum refining, pharmaceutical and catalyst factory[1]. From environmental perspective, a complete removal or a very low ammonia concentration is desirable in wastewaters. This obligation is because ammonia is extremely toxic to most fish species and it will be bio-oxidized by nitrifying microorganisms to nitrite and nitrates which are undesirable to humans. High concentrations of ammonia are commonly present in industrial wastewaters[1-5]. The ammonia concentration in wastewaters varies[1] from 5 to 1000 mg/L. The removal of ammonia dissolved in wastewaters is thus mandatory to protect the environment and human health. The main objective of the present study is to develop and solve a mathematical model for simulation of ammonia removal in a hollow-fiber membrane contactors with recycling mode. The model equations are solved by numerical method based on computational fluid dynamics techniques.

In the dissolved state, ammonia exists in two forms. One is toxic ammonia and the other is less harmful ammonium ions. The composition of these components depends on pH and temperature of solution from the following dissociation equilibrium:

$$NH_3 + H_2O \underset{K_a}{\overset{K_b}{\rightleftharpoons}} NH_4^+ + OH^- \quad (1)$$

Equilibrium constants can be defined from following equations:

$$K_a = \frac{[NH_3][H^+]}{[NH_4^+]} \quad (2)$$

$$K_b = \frac{[NH_4^+][OH^-]}{[NH_3]} \quad (3)$$

However, K_a and K_b values are equal to 5.6×10^{-10} and 1.8×10^{-8}, respectively[5]. The total ammonia concentration in the feed solution is the summation of equilibrium concentrations of ammonium and ammonia in the feed solution.

Mass transfer model: The first equation is obtained for ammonia tank using mass balance. The mass balance equation over ammonia tank considering uniform mixing can be written as follows:

$$V\frac{dC_{tank}}{dt} = QC|_{z=L} - QC_{tank} \quad (4)$$

$$@t = 0, \qquad C_{tank} = C_0 \quad (5)$$

where Q is volumetric flow rate, m^3/s, V is volume of feed, m^3, t is time, s and C is ammonia concentration, mol/m^3. $C|_{Z=L}$ is concentration of ammonia at the outlet of contactor which is inlet for the feed tank.

The unsteady state continuity equation for ammonia in the lumen side of the HFMC in cylindrical coordinate is obtained using Fick's law of diffusion for estimation of diffusive flux[6]:

$$-D_{NH_3}\nabla\cdot(\nabla C_{NH_3}) + \nabla\cdot(C_{NH_3}V) = 0 \quad (6)$$

Velocity distribution in the lumen side is determined by solving the momentum equation, *i.e.* Navier-Stokes equations. Therefore, the momentum and the continuity equations should be coupled and solved simultaneously to obtain concentration distribution of the ammonia in the lumen side. The ammonia concentration in the shell side of membrane contactor is assumed to be zero because of instantaneous reaction between ammonia and sulfuric acid (stripper).

The main objective of the present study is to model hollow-fiber membrane contactors with recycling mode using computational fluid dynamics of mass and momentum transfers. The equations of contactor related to lumen side and membrane with the appropriate boundary conditions were solved using COMSOL Multiphysics version 3.2 software, which uses finite element method (FEM) for numerical solutions of the equations.

Model validation: The results of ammonia stripping (simulated values as predicted from model) are presented in Fig. 1. Fig. 1 indicates the concentration of ammonia in the feed tank at different experimental runs over time. The experimental data were taken from literature[1].

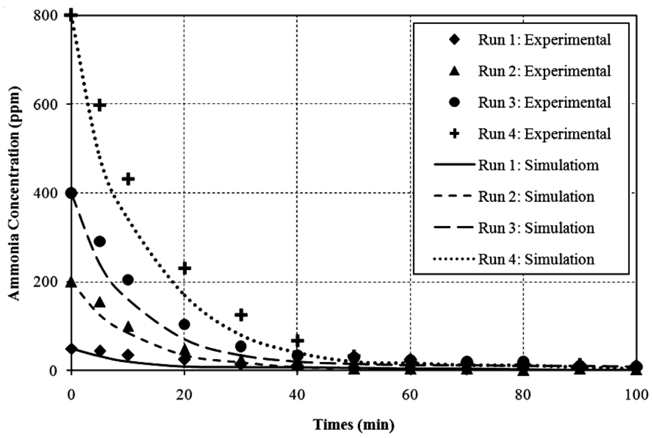

Fig. 1. Variations of ammonia concentration in the feed tank *vs.* time: comparison between experimental results and simulated values

As it can be seen from the figure, ammonia concentrations change exponentially with time. Concentrations of ammonia drop sharply at the initial times and then slightly at final times. This could be attributed to this fact that at the first times of operation, driving force of ammonia between lumen and shell side of contactor is high because of high concentration difference. As ammonia transfers to the shell side, its concentration decreases and results in lower driving force. Fig. 1 also confirms the validation of the simulation results using experimental data. As it is evident, there is good agreement between the simulated and experimental data.

Radial concentration distribution of ammonia in the contactor: Variations of radial concentration of ammonia in the lumen side of membrane contactor were also investigated. In order to obtain the radial concentration profile in the lumen side, a time at which the effect of the ammonia removal is significant, was identified. A time of 1 min contact was chosen. Fig. 2 shows a plot of the radial concentration profile at t = 1 min at different axial positions along the lumen side of membrane contactor. As seen, in the region near the axis of the fiber (r = 0), the bulk-phase concentration of ammonia changes slightly. The maximum concentration of ammonia is located in the center of lumen due to axial symmetry. Radial concentration of ammonia then reduces gradually in the region between center and wall of lumen side. In the region adjacent the membrane surface, concentration decreases sharply.

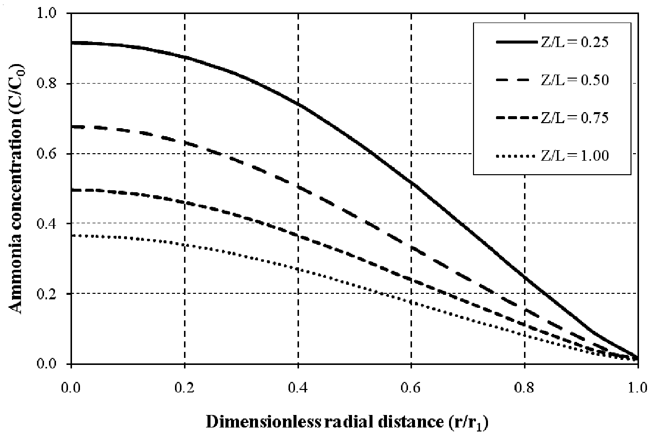

Fig. 2. Radial concentration distribution of ammonia in the contactor at different axial positions, t = 1 min

Conclusion

An unsteady-state, 2D mathematical model was developed to study the removal of ammonia from aqueous solutions by means of a hollow-fiber membrane contactor. The model predicts the unsteady state concentration of the ammonia in the membrane contactor and feed tank by solving the conservation equations including continuity and momentum. The model was developed considering a hydrophobic membrane which is not wetted by the aqueous feed solution. Both axial and radial diffusions within the lumen and membrane of the contactor were considered. The predictions of the mass transfer model were validated by comparing the results of ammonia removal with experimental data.

Nomenclature

C	Concentration (mol/m^3)
D	Diffusion coefficient (m^2/s)
p	Pressure (Pa)
r	Rradial coordinate (m)
t	Time (s)
T	Temperature (K)
V	Velocity in the module (m/s)
z	Axial coordinate (m)

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