



NOTE

Investigation on Copper Extraction Using Numerical Simulation

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Extraction of Cu^{2+} with a kerosene solution of di(2-ethylhexyl)phosphoric acid (D2EHPA) in membrane contactors was studied in this work. Simulations were performed using computational fluid dynamics (CFD) of mass and momentum transfer in all subdomains of a circular membrane contactor. Conservation equations were derived and solved for Cu^{2+} in the membrane contactor. With solving conservation equations, concentration and pressure distributions were obtained for solute. Simulation results showed an extraction efficiency of 85.8 % for Cu^{2+} .

Key Words: Copper extraction, Numerical simulation, Membrane, Computational fluid dynamics.

Extraction of heavy metals such as Zn^{2+} , Cu^{2+} , Co^{2+} , Ni^{2+} and Cd^{2+} with organophosphorus extractants such as di(2-ethylhexyl)phosphoric acid (D2EHPA) is an important separation process in chemical industries¹. Conventional metal extraction processes are carried out using equipments such as packed towers, mixer-settlers, *etc.* which try to maximize the contact area of two phases for mass transfer operation². Membrane technology can overcome the drawbacks of conventional metal extraction processes^{3,4}. The current study, presents a numerical simulation using Computational fluid dynamics (CFD) of mass and momentum transfer in a membrane contactor for laminar flow conditions. The aim of this simulation is to predict the concentration and pressure distribution in the contactor.

Fig. 1 shows a concentric circular membrane extractor with inserting a hydrophobic microporous permeable barrier (membrane) to divide a circular tube into two subdomains conducting a double-flow operation. The feed phase containing aqueous solution of Cu^{2+} flows inside the inner tube (fiber) while the extractant solution flows counter-currently inside the shell side. Because of hydrophobicity of the membrane, the extractant-containing phase which is organic penetrates the membrane pores and wets them. An interface is established at the pores mouth adjacent to the feed phase. At the interface, chemical reaction occurs between metal ion (Cu^{2+}) and organometallic complex is formed and diffuses through the membrane pores and is transferred to the shell side. Therefore, the driving force in this process is concentration difference of solute.

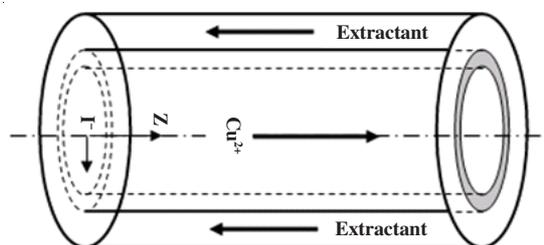


Fig. 1. Concentric membrane contactor for extraction of Cu^{2+}

The main equation that describes the transfer of copper from aqueous phase to organic phase is continuity equation. This equation is derived from mass balance of solute within an element. The differential form of continuity equation for solute may be written as⁵:

$$\frac{\partial C_i}{\partial t} + \nabla \cdot (-D_i \nabla C_i + C_i V) = R_i \quad (1)$$

where C_i denotes the concentration of solute (mol/m^3), D_i denotes its diffusion coefficient (m^2/s), V the velocity vector (m/s) and R_i denotes the reaction term ($\text{mol/m}^3 \text{ s}$). The velocity vector can be expressed analytically or obtained by coupling a momentum balance to the equation system. This equation is also called convection and diffusion equation.

The model equations including continuity and Navier-Stokes equations (momentum) related to shell, membrane and tube side of contactor with the appropriate boundary conditions were solved numerically using COMSOL software.

Concentration distribution of solute along the extractor:

Fig. 2 illustrates the dimensionless concentration distribution (C/C_0) of solute in the tube side of the membrane extractor. The feed phase including aqueous solution of Cu^{2+} flows from one side of the contactor ($z = 0$) where the concentration of solute is the highest (C_0), whereas the organic phase (extractant) flows from the other side ($z = L$) where the concentration of solute is assumed to be zero. As the feed flows through the tube side, copper ion moves towards the membrane due to the concentration difference. At the membrane-aqueous phase interface chemical reaction occurs and metallic complex is formed. The formed complex diffuses through the membrane pores which is filled with the organic phase and reaches at the shell side. Finally, the complex is swept by the moving extractant and leaves the extractor.

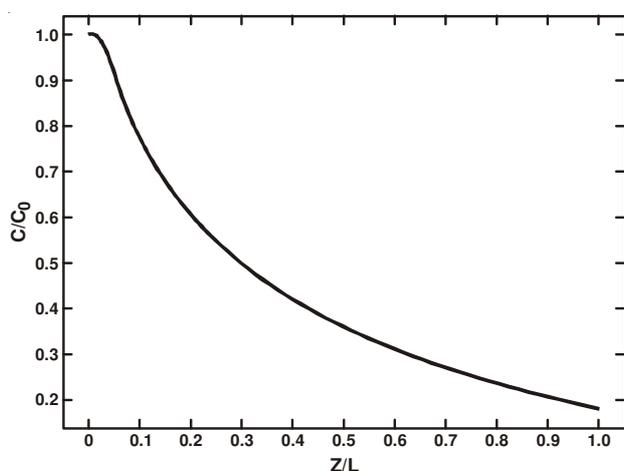


Fig. 2. Concentration distribution of copper along the extractor. Inlet concentration of solute = 8 mol/m^3 , Temperature = 298 K , Pressure = 1 atm

The extraction efficiency of solute is defined as the ratio of the solute transfer from the feed phase to extraction phase to total solute in the initial feed phase was determined using Fig. 2. The extraction efficiency for solute is calculated 85.8% for extraction of Cu^{2+} using membrane extractor. The extraction efficiency could be enhanced with increasing organic phase flow rate and decreasing feed flow rate.

Pressure distribution along the extractor: Pressure distribution in the shell side of extractor is shown in the Fig. 3. As it can be seen from the figure, the pressure drop along the membrane extractor is less than 12 Pascal .

This is one of advantages of membrane contactors for extraction of heavy metals. The pressure drop along the

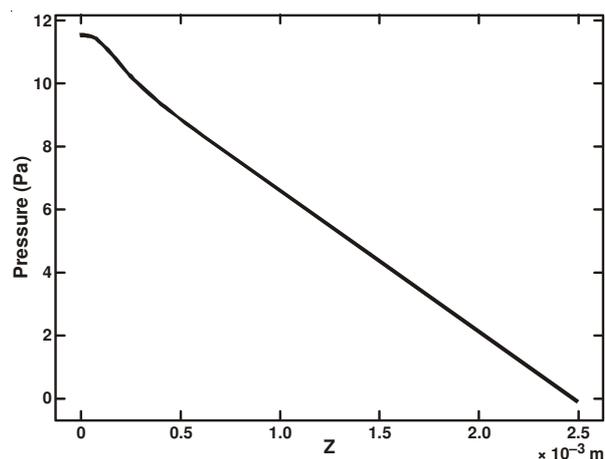


Fig. 3. Pressure distribution in the extractor. Temperature = 298 K , Pressure = 1 atm

membrane extractors is not appreciable. This advantage can reduce the operating costs of process.

Conclusion

Numerical simulation of Cu^{2+} extraction with a kerosene solution of di(2-ethylhexyl)phosphoric acid (D2EHPA) in membrane contactors was studied in this study. Simulations were carried out using computational fluid dynamics of mass and momentum transfer. Concentration and pressure distributions of solute were obtained to investigate the effect of process parameters on the extraction of Cu^{2+} . The simulation results showed that pressure drop is not appreciable in the membrane contactor which can reduce the operating costs.

Nomenclature

C	Concentration (mol/m^3)
D	Diffusion coefficient (m^2/s)
J_i	Diffusive flux of species i ($\text{mol/m}^2 \text{ s}$)
P	Pressure (Pa)
r	Radial coordinate (m)
R_i	Overall reaction rate of any species ($\text{mol/m}^3 \text{ s}$)
T	Temperature (K)
V	Velocity in the module (m/s)
z	Axial coordinate (m)

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