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Research Article

Modeling Investigation of Concurrent-Flow Chemical Extraction Process

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ABSTRACT

In this study, modeling investigation of mass transfer in concurrent-flow chemical extraction process is carried out. Continuum Model is used to describe mass transfer process. Concentration curves in organic droplet and aqueous liquid film are firstly calculated and rate limiting step is determined to be mass transfer of solute in aqueous phase. Mass transfer performance in aqueous phase is further calculated. Volumetric mass transfer coefficient and volumetric mass transfer coefficient during mass transfer time before solute concentration decreases to 5%, are calculated for evaluating mass transfer characteristics. The effect of organic droplet size is studied. The result demonstrates that increase in aqueous/organic volume ratio significantly decreases mass transfer performance; decrease in droplet size enhances mass transfer process through both reducing mass transfer resistance and increasing contacting area.

Keywords: Concurrent-flow; Chemical extraction

INTRODUCTION

Solvent extraction (liquid-liquid extraction) is known as a process for separating compounds based on the solubility difference between two immiscible liquids (usually a water phase and an organic solvent phase). Solvent extraction can be divided into physical extraction and chemical extraction. Physical extraction only contains physical process, such as polarity difference between two solvents while chemical extraction contains chemical reactions, which might provide more significant distribution of solute [1]. Due to high separation efficiency, extraction process containing reversible chemical reactions is catching more and more attention from researchers and is applied in wastewater treatment, pharmaceutical industry and nuclear fuel treatment. In extraction process with chemical reactions, there is usually an extractant (E) contained in organic solvent, which coordinates with the solute (S) in aqueous phase [2]. When the organic solvent and aqueous solution contacts, a hydrophobic compounds generates.

$[S]_{aq.} + [E]_{org.} = [A.E]_{org.}$

In extraction process with chemical reactions, the rate-limiting step is usually the mass transfer, because fast or even instant reactions are usually selected. On the other hand, in extraction process with chemical reactions, distribution coefficient is usually higher than 10 or even higher than 50 due to the presence of chemical reactions [3]. Therefore, the water/organic phase ratio is also usually higher 10:1 or even 50:1. High water/organic phase ratio leads to slow mass transfer of solutes in aqueous phase, which is caused by decreased interface area and increased mass transfer resistance in aqueous phase. Understanding of mass transfer mechanism is helpful for process intensification of extraction process with chemical reactions [4].

Since the last decades, microsized liquid-liquid systems were applied in solvent extraction processes and have caught much attention from researchers. In microsized liquid-liquid systems, microsized droplets were generated by dispersion medium, such as microchannel devices and microfiltration membrane [5]. Experimental results demonstrate that solvent extraction process is significantly intensified when microsized liquid-liquid systems were generated. The mechanism that how the decrease in droplets affects liquid-liquid mass transfer process still needs further understanding. Better understanding of mass transfer mechanism as well as prediction of mass transfer characteristics of liquid-liquid systems with different droplet size are important for designing extraction processes with chemical reactions [6].

In this study, a physical model is presented for understanding mass transfer mechanism in extraction process with chemical

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reactions. The effect of droplet size on mass transfer coefficients is then calculated [7].

METHODOLOGY

Figure 1(a) shows a schematic diagram of organic-droplet-in-water system. After the organic phase was dispersed into droplets, the liquid-liquid system flows along the flowing channel concurrently. The relative velocity of organic droplets to continuous water phase is low and therefore, the organic droplet-in-water system can be divided into a large number of mass transfer units. As shown in Figure 1(b), in each mass transfer unit, an organic droplet and a liquid film (aqueous phase) are contained. In each mass transfer unit, mass transfer of solute (S) in aqueous phase and extractant (E) in organic phase take place independently, which could be calculated according to Continuum Model, based on mass balance [8].

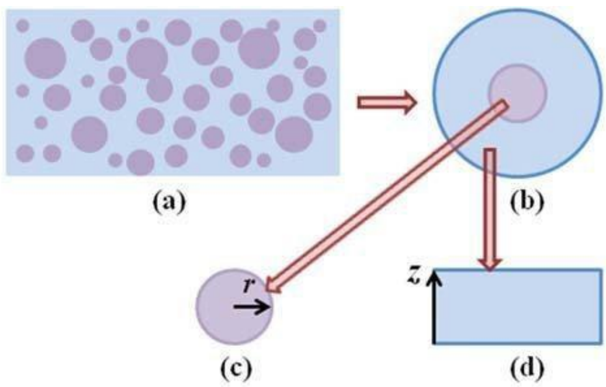

Figure 1: Schematic diagram of (a) flowing system in concurrent extraction process; (b) mass transfer unit; (c) mass transfer in organic droplets; (d) mass transfer in aqueous liquid film [9].

Assumptions

Before calculation, the following assumptions are made:

a) The dispersed organic droplets are in the middle of mass transfer unit and uniform. Averaged droplet-diameter, d_{org}, is used in modeling.

b) The thickness of aqueous liquid films are uniform and averaged-liquid-film-thickness, Laq, is used in modeling, which is calculated according to dorg and organic/aqueous flow rate ratio, F_{org}/F_{aq}.

c) d_{org} and L_{aq} are both constant during contacting period, where average values before and after contacting period are applied and therefore coalescence of organic droplets can be ignored.

d) During contacting period, both organic droplets and aqueous liquid films are stagnant, and therefore, only effects of diffusion of solute in aqueous phase and extractant in organic phase are considered, respectively [10].

e) Reaction as Equation (1) takes place between solute in aqueous phase and extractant in organic phase, intrinsic dynamics of which is fast enough for consuming solute (S) as soon as it reaches droplet-liquid-film interface.

f) In each mass transfer unit, only process of mass transfer though interface between organic droplet and aqueous liquid film around it is considered, while process of mass transfer though outer surface of aqueous liquid film to adjacent mass transfer units is not taken into account, by considering uniformity of mass transfer units [11].

Based on Assumption a-f, in each isolated mass transfer unit, mass transfer of solute in aqueous phase and extractant in organic phase can be calculated, respectively.

Firstly, mass transfer performance in organic droplet and aqueous liquid film are calculated, respectively, for determining the rate-limiting step in concurrent-flow chemical extraction. The decrease in concentration of extractant in organic droplet and solute in aqueous liquid film are determined respectively by assuming all substrate is consumed instantaneously as it reaches liquidliquid interface. When chemical extraction is carried out, F org/F aq is usually higher than 10 because of high distribution coefficient. Thus, results under operating conditions of F_{org}/F_{aq} = 10, 20, 40, 80 and 160 are calculated. Also, droplets size affects mass transfer characteristics significantly, thus, situation with droplet radius of 100 μm and 1 mm are calculated. During the calculation in this section, DE_{org} and DS_{aq} are both set as 1 * 10-9 m^2/s, considering the similarity of solute and extractant in liquids [12].

As shown in Figure 2, at the same droplet size, the curve of $C\ E_{org}$ / CE_{org}, 0 is significantly steeper than curves of CS_{aq} / CS_{aq}, 0. For instant, contacting time for CS_{aq} / CS_{aq},0 to reach 5% in aqueous phase when F_{org}/F_{aq}=10:1 is about 50 times longer than contacting time for CE_{org} / $C\ E_{org}$,0 to reach 5% in organic phase and even longer at higher F_{org}/F_{aq} value. This result indicates concurrent flow chemical extraction process is limited by mass transfer of solute in aqueous phase. Comparison among curves with different F_{org}/F_{aq} values at the same droplet size demonstrate that CS_{aq} / CS_{aq}, 0 curves become flatter as the increase in F_{org}/F_{aq} value, indicating weakening in mass transfer characteristics. Comparison among curves with different droplet size at the same F_{org}/F_{aq} value indicates significant intensification in mass transfer performance caused by the decrease in droplet size, which is in coincidence with experimental results in litre [13].

MODELING RESULTS AND DISCUSSION

Comparison of mass transfer performance in organic droplet and aqueous liquid film

Firstly, mass transfer performance in organic droplet and aqueous liquid film are calculated, respectively, for determining the rate-limiting step in concurrent-flow chemical extraction. The decrease in concentration of extractant in organic droplet and solute in aqueous liquid film are determined respectively by assuming all substrate is consumed instantaneously as it reaches liquid-liquid interface. When chemical extraction is carried out, F org/F aq is usually higher than 10 because of high distribution coefficient. Thus, results under operating conditions of F org/F aq =10, 20, 40, 80 and 160 are calculated. Also, droplets size affects mass transfer characteristics significantly, thus, situation with droplet radius of 100 μm and 1 mm are calculated [14].

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Comparison among curves with different F org/F aq values at the same droplet size demonstrates that CS aq / CS aq, curves become flatter as the increase in F org/F aq value, indicating weakening in mass transfer characteristics. Comparison among curves with different droplet size at the same F org/F aq value indicates significant intensification in mass transfer performance caused by the decrease in droplet size, which is in coincidence with experimental results in literatures [15].

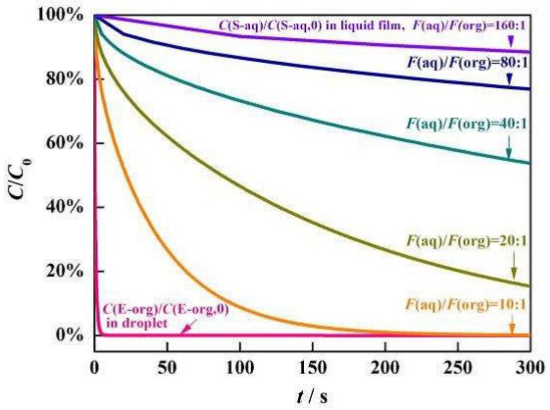

Figure 2: Comparison of concentration curve in organic droplet and aqueous liquid film with droplet radium 100 μm.

CONCLUSION

In this study, modeling investigation of mass transfer in concurrent-flow chemical extraction process is conducted using the Continuum Model. The rate-limiting step is firstly determined by calculating concentration curves in organic droplet and aqueous liquid film, respectively. Mass transfer characteristics in aqueous liquid film is calculated further, which is evaluated by volumetric mass transfer coefficient and mass transfer coefficient during mass transfer time before solute concentration decreases to 5% of initial concentration. Influence of organic droplet size is studied. The result demonstrates the increase in aqueous/organic volume ratio significantly decreases mass transfer performance; the decrease in droplet size enhances mass transfer process through both reducing mass transfer resistance and increasing contacting area.

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