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Hydrodynamic Simulation of Liquid-Liquid Extraction Drops and the Effect of Mass Transfer on the Hydrodynamics

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Hydrodynamic and mass transfer simulations of toluene rising drops have been investigated. The VOF-PLIC method with the surface tension model of CSS was applied. Drops have been simulated in the three regimes of spherical, circulating, and oscillating regimes. Simulation results agreed well with existing experimental data with the average relative error of 3.63 percent. The current hydrodynamic model predicted the oscillating regime for the drop diameter of 4.4 mm and 3.5 mm drops were identified as the drops with maximum velocity. These findings agreed well with existing experimental data. In the next step of simulations, mass transfer equation was supplemented into the simulations investigating mass transfer effect on the velocity of 2 mm toluene drops. All of the properties of drops were assumed constant except surface tension coefficient. Simulation results showed that, with the assumption of concentration dependent surface tension coefficient, terminal velocity relative error was about 2 percent, while without considering of that, relative error increased to 83 percent. Streamlines, drop shapes, axial velocity, and terminal velocity were also reported.

Keywords: Numerical Simulation, VOF Model, Liquid-Liquid Extraction, Mass Transfer, Hydrodynamics.

Introduction

Simulation of hydrodynamics has greater importance in the liquid-liquid extraction (LLE) systems in order to evaluate the drop sizes, interfacial area, residence time, transient and terminal velocities. These parameters are the most influencing parameter in the mass transfer studies and stage efficiencies of large LLE columns[1-3], as they have been the subject of many studies through recent years [1, 4].

In the current study, the VOF method has been used in order to simulate the hydrodynamics of the LLE system which has not been considered previously. The continuum surface stress model (CSS) has been applied in order to model the effects of interfacial tension force being considered as the source term of momentum equation. For the first time, the effect of mass transfer on the hydrodynamics of LLE single drop system has been considered using the VOF-CSS model with the concentration dependent surface tension coefficient. Terminal velocity, axial velocity, and streamlines have been reported covering three LLE regimes. The effect of mass transfer in the hydrodynamics has been investigated for the 2mm toluene drops containing an initial concentration of 7.5 g/L from acetone.

Methodology

Hydrodynamics

The VOF method proposed by Hirt and Nichols has been used for capturing the interface [5]. The averaged continuity and momentum equations of two immiscible incompressible fluids are respectively:

$$\frac{\partial \rho}{\partial t} + \nabla.\rho\vec{U} = 0 \tag{1}$$

$$\frac{\partial\left(\rho\vec{U}\right)}{\partial t} + \nabla.\rho\vec{U}\vec{U} = -\nabla P + \nabla.\mu\left(\nabla\vec{U} + \nabla\vec{U}^{T}\right) + \rho\vec{g} + \vec{F}_{SF} \tag{2}$$

Mixture density and dynamic viscosity are defined by the volume fraction averaging:

$$\rho = \alpha\rho_d + \left(1-\alpha\right)\rho_c \tag{3}$$

$$\mu = \alpha\mu_d + \left(1-\alpha\right)\mu_c \tag{4}$$

By solving a transport equation, the motion of the interface can be traced as:

$$\frac{\partial(\alpha)}{\partial t} + \left(\vec{U}.\nabla\alpha\right) = 0 \tag{5}$$

The CSS model proposed by Lafaurie has been used for the surface tension force calculation in the interface (Eq.6) [6]. The source term of Eq.7 has been added to the momentum equation from the CSS formulation (Eq. 2).

$$T = \sigma\left(\left|\nabla\alpha\right| I - \frac{\nabla\alpha\otimes\nabla\alpha}{\left|\nabla\alpha\right|}\right) \tag{6}$$

$$\vec{F}_{SF} = \nabla.T = \nabla.\left(\sigma\left(\left|\nabla\alpha\right| I - \frac{\nabla\alpha\otimes\nabla\alpha}{\left|\nabla\alpha\right|}\right)\right) \tag{7}$$

Which is tangential to the surface.

Mass transfer

Concentration equation is considered separately for the toluene (dispersed phase) and water (continuous phase) phases as:

$$\frac{\partial C_d}{\partial t} + \nabla.\left(C_d\vec{U}\right) = \nabla.\left(D_d\left(\nabla C_d\right)\right) \tag{8}$$

$$\frac{\partial C_C}{\partial t} + \nabla.\left(C_C\vec{U}\right) = \nabla.\left(D_C\left(\nabla C_C\right)\right) \tag{9}$$

At the liquid-liquid interface, continuity of solute flux exists as:

$$D_d\frac{\partial C_d}{\partial n} = D_C\frac{\partial C_C}{\partial n} \tag{10}$$

The species concentration on both sides of the interface is discontinuous in the thermodynamic equilibrium condition and causes a concentration jump in the interface:

$$\frac{C_d}{C_C} = K \tag{11}$$

Where K is distribution coefficient and equals 0.63 for toluene/acetone/water system [7]. In order to solve simultaneous equations (Eqs. 8-11), the new concentration field is defined as:

$$\frac{\partial \hat{C}}{\partial t} + \nabla.\left(\vec{U}\hat{C}\right) = \nabla.\left(D\left(\nabla \hat{C}\right)\right) \quad (12)$$

Where

$$\hat{C} = C_d \quad , \alpha = 1$$

$$\hat{C} = C_c \quad , \alpha = 0$$

Similar formulation has also been used with the level set method by the previous authors [2, 8].

Geometry, boundary conditions and solution method

The schematic diagram of the computational domain has been displayed in Fig. 1. The wall boundary conditions have been considered in the right and bottom sides and pressure boundary was assumed at the upper side of the computational domain. The displayed pressure on the figure is the modified pressure to simplify the specification of boundary conditions [9]. In the simulations, material properties except surface tension were supposed independent of acetone concentration due to small concentrations. The surface tension coefficient was considered as [7]:

$$\sigma = 0.0025 + 0.03285\exp(-0.0145C_D) \quad (13)$$

In order to discretize the governing equations, the finite volume method was used, and explicit time discretization was applied in order to solve volume fraction equation (Eq. 5). PLIC method was used to solve the convective fluxes of Eq. 5. Convective terms of velocity component were solved using Quick method and unsteady terms in Eqs. 1 and 2 were discretized using implicit method. The Pressure-Implicit with Splitting of Operators algorithm (PISO), was used in order to relate the pressure and velocity corrections.

Discussion and results

The terminal velocity of drops in the case of no mass transfer has been presented in Fig. 2 in the three regimes of spherical, circulating and oscillating. It can be seen that the VOF-CSS model has successfully predicted the terminal velocity values of all drop types. Streamlines of drops in the three regimes have been shown in Fig. 3 representing the drop shape change from spherical to oblate in the oscillating regime. Streamlines of drops in the case of mass transfer have also been reported in Fig.4 in the different times. It can be observed that concentration dependent surface tension causes multi circulation zones inside of droplet which have not appeared in the no mass transfer case. Comparison of axial velocity values in the two cases of with/without mass transfer has been given in Fig.5. It can be seen that the appearance of multi circulation zones inside of the drop and destruction of regular flow pattern (as it can be seen in Fig. 3), causes the increase of drag coefficient consequently decrease of axial velocity and terminal velocity values. The transient/terminal velocity values of 2mm toluene drop have been displayed in Fig. 6 demonstrating an excellent agreement between the current simulation results and experimental data in the two cases of with/without mass transfer [10, 11]. Concentration profiles of the toluene drop has been given in Fig. 7 in the two states of constant surface tension coefficient and concentration-dependent surface tension (Marangoni effects). It can be seen that in the case of Marangoni effect, regular patterns have been replaced by multi circulation zones which are also apparent in the concentration profiles similar to streamlines of Fig. 4.

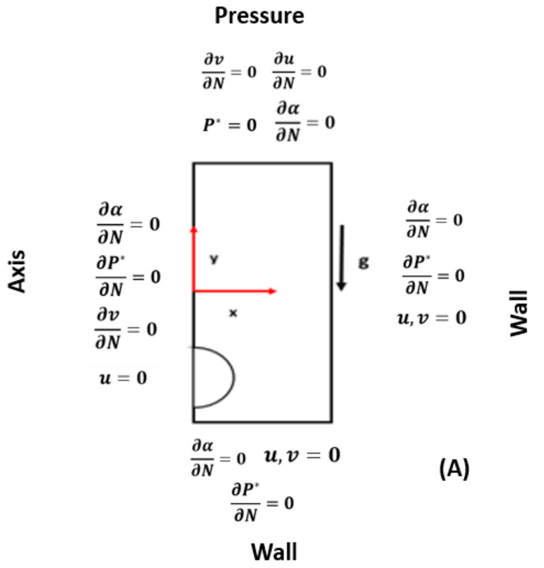

Figure1: The schematic of computational domain with boundary conditions

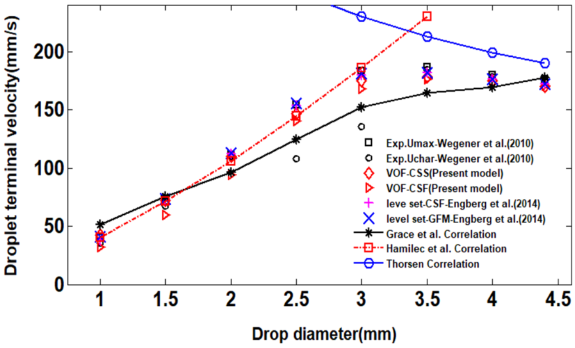

Figure2: Terminal velocity of drops in three LLE regimes

Conclusion

Hydrodynamic and mass transfer simulations of toluene rising drops have been investigated in the three regimes. The VOF-PLIC method with the surface tension model of CSS was applied. The hydrodynamics simulation results agreed well with the existing experimental data with the average relative error of 3.63 percent. The mass transfer equation was supplemented.

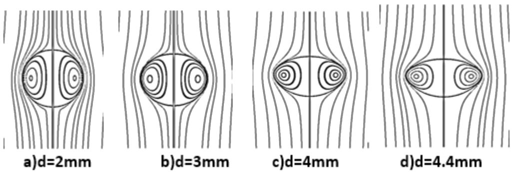

Figure3: Streamlines of drops in three LLE regimes

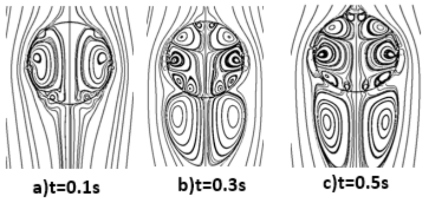

Figure4: Streamlines of 2mm drops containing initial concentration of 7.5 g/L in different times

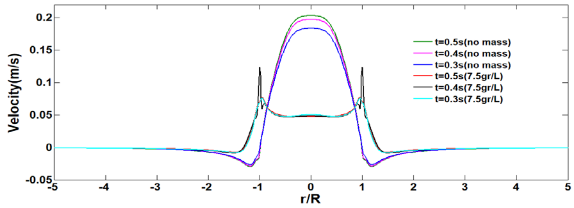

Figure5: Axial velocity of toluene 2mm drops in the two cases of with/without mass transfer

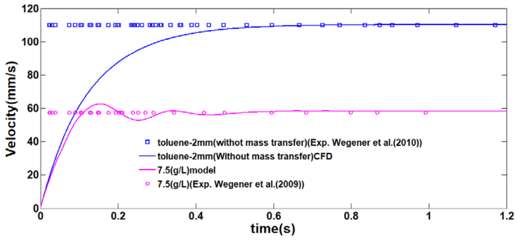

Figure6: Transient velocity of toluene 2 mm drops in the two case of with/without mass transfer

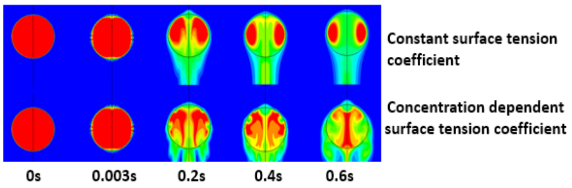

Figure7: concentration profiles in the two cases of constant/variant surface tension coefficient

Into the hydrodynamic equations investigating the mass transfer effect on the velocity of 2mm toluene drops. VOF-CSS model has been used for the mass transfer simulations for the first time. All of the drops properties were assumed constant except surface tension coefficient. Simulation results showed that, with the assumption of concentration dependent surface tension coefficient, terminal velocity relative error was about 2 percent, while without considering of that, relative error increased to 83 percent. Streamlines, drop shapes, axial and terminal velocities were also reported.

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