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Numerical simulation of coalescence phenomena of oil-in-water emulsions permeating through straight membrane pore

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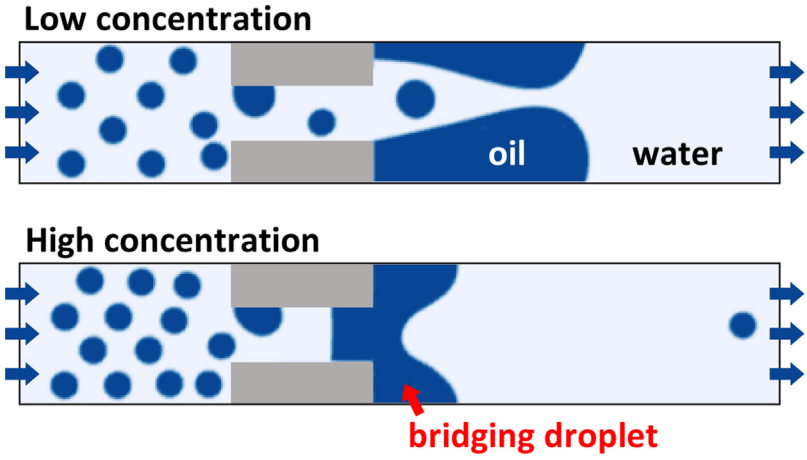
HIGHLIGHTS

- We numerically investigated the demulsification phenomena of oil-in-water emulsions.
- We used the coupled level set and volume-of-fluid (CLSVOF) method.
- Coalescence of droplets captured on the membrane surface provides large droplets.
- Oil droplets blocking the membrane pore is forced away by the permeating flow.

GRAPHICAL ABSTRACT



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ABSTRACT

We numerically investigated the demulsification phenomena of oil-in-water (O/W) emulsions using a membrane coalescence process. We simulated the permeation of O/W emulsions through a membrane with a single straight pore using our numerical framework based on the coupled level set and volume-of-fluid (CLSVOF) method. With a low droplet volume fraction, small droplets, and a large pore size, the oil droplets frequently passed through the membrane without attaching to its surface. After the steady coalescence of the droplets on the membrane surface at the permeation side, large oil droplets could be obtained. With a higher droplet volume fraction, larger oil droplets, and smaller membrane pores, the oil droplets easily blocked the membrane pores and were thus forced away by the permeating flow, which yielded relatively small oil droplets. Our numerical work revealed the fundamental dynamics of the coalescence of oil droplets in an O/W emulsion using a simple membrane model.

1. Introduction

The separation of oil–water mixtures is essential in various industries, including the petrochemical, metallurgical, and food

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processing. Currently, the separation of produced water is a serious problem in the shale gas and oil industries [1,2]. Numerous oil–water separation techniques, including gravity flotation, centrifuge, air flotation, and membrane filtration, have been intensively explored to efficiently and cost-effectively separate oil and water. However, most conventional techniques cannot be applied for separating emulsions, in which droplets of one liquid are stably dispersed in another liquid. The separation of oil-in-water (O/W) emulsions employs preprocessing to convert the emulsion to free oil and water (demulsification). Among the numerous demulsification techniques, membrane-based coalescers have attracted considerable attention because they are energy-efficient, cost-effective, and applicable to finely dispersed emulsions [3,4]. In membrane-based coalescence, a porous membrane acts as a coalescence-accelerating medium, whereas in most membrane separation processes, the oil droplets are rejected, and only the water permeates the membrane. When an O/W emulsion is fed through a membrane, the oil droplets attach to the membrane surface and then coalesce during the permeation through the membrane pores. Because the oil droplets on the permeation-side surface of the membrane are far larger than those in the feed mixture, they can be easily separated from the water phase by an external force, e.g., a buoyancy force, as a result of the density difference between the oil and water.

Previous experimental studies have investigated the effects of the membrane and processing factors – such as the membrane wettability and pore size, superficial velocity, and transmembrane pressure – on the demulsification behavior of oil droplets [3–9]. Although this intensive research has improved the demulsification efficiency, the underlying dynamics of the demulsification behavior through a membrane are not yet fully understood. Numerical simulations are another potential approach to elucidate the membrane demulsification phenomena, as these simulations can independently evaluate the effects of each factor and reveal even the fluid motion inside a membrane.

In the field of membrane engineering, various separation processes have recently been investigated using numerical approaches. Ando et al. [10] and Ishigami et al. [11] studied the dynamics of the particulate flow in dead-end microfiltration using a direct numerical simulation technique based on the discrete element method (DEM) [12] and computational fluid dynamics (CFD) for the particle motions and solvent flow, respectively. Darvishzadeh et al. [13,14] performed numerical simulations based on the volume-of-fluid (VOF) method [15,16] to study the oil-droplet behavior at a pore entrance in the cross-flow microfiltration of oil–water dispersions.

In our previous study [17], we constructed a numerical simulation framework based on the coupled level set and volume-of-fluid (CLSVOF) method [18,19], which combines the level set (LS) method [20,21] and volume-of-fluid (VOF) method [15,16], and investigated the permeation of concentrated O/W emulsions through a membrane pore. In the CLSVOF method, the interface is captured by the VOF function, and the interfacial tension is evaluated using the LS function which is constructed according to the VOF function. The CLSVOF-based simulation, which can accurately evaluate the interfacial tension force and ensure volume conservation, enabled us to describe the large deformation of the interfaces accompanying the coalescence of dispersed droplets and wetting on a pore surface. We examined the effects of the membrane wettability, pore size, and filtration flux on the permeation behavior of the O/W emulsions and demonstrated that high wettability on the membrane surface and low fluid velocity inside the pore increased the demulsification efficiency.

To further understand the membrane demulsification phenomena, we simulated the permeation of O/W emulsions through a membrane with a single straight pore using a two-dimensional (2D) numerical simulation framework based on the CLSVOF method. The present study mainly focused on the effects of the basic physical factors of O/W emulsions on the demulsification behavior because the motion of a droplet held on a membrane surface is restricted, and thus greatly affected by the physical factors. We investigated the droplet size and volume fraction, which especially affect the demulsification performance. Furthermore, as one of the simplest operation factors to increase the coalescing performance of an O/W emulsion that is difficult to demulsify, the effect of the membrane pore size was explored. Note that physical–chemical factors, such as the interactions of the droplets and droplet-membrane (e.g., van der Waals forces [22] and electric forces) and the adsorption of surfactants on the interfaces [23], are also important factors and will be investigated in a future study.

2. Numerical method

Numerical simulations were performed using the numerical framework constructed in our previous work [17]. The numerical formulation is briefly explained in the following paragraphs.

Our numerical framework is based on the CLSVOF method proposed by Yokoi et al. [19]. This CLSVOF method consists of the tangent of the hyperbola for the interface-capturing/weighted-line-interface-calculation (THINC/WLIC) method [24,25] and the LS method with the CSF model for evaluating the interfacial tension. Yokoi applied this framework to some free-interfacial flow problems, including dynamic wetting [19] and splashing on a solid substrate [26,27] and droplet impact to a liquid [25], which are related to the attachment of droplets to a surface, interfacial motion, and the coalescence of liquid interfaces in membrane demulsification. The numerical simulation results presented in those papers were in good agreement with experimental results. We also checked the validity of the simulation program in our previous paper [17], where the 2D droplet motion under a simple shear flow calculated by our program was in good agreement with the results reported by Chinyoka et al. [28]. Consequently, the numerical framework employed gives accurate solutions in the simulation.

The VOF function is advected by

$$\frac{\partial \chi}{\partial t} + \nabla \cdot (\boldsymbol{u}\chi) - \chi \nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

where $\mathbf{u}$ is the fluid velocity, t is the time, and χ is the characteristic function. In the 2D case, the VOF function $C_{i,j}$ is the cell average of χ,

$$C_{i,j} = \frac{1}{\Omega_{i,j}} \iint \chi dx dy, \tag{2}$$

where $\Omega_{i,j}$ is the cell area. The $C_{i,j}$ is evolved by an approximation using a dimensional splitting algorithm as follows:

$$C^{*}_{i,j} = C^{n}_{i,j} - \frac{F^{n}_{x,i+1/2,j} - F^{n}_{x,i-1/2,j}}{\Delta x} + C^{n}_{i,j} \frac{\boldsymbol{u}_{i+1/2,j} - \boldsymbol{u}_{i-1/2,j}}{\Delta x} \Delta t, \tag{3}$$

$$C^{n+1}_{i,j} = C^{*}_{i,j} - \frac{F^{*}_{y,i,j+1/2} - F^{*}_{y,i,j-1/2}}{\Delta y} + C^{n}_{i,j} \frac{\boldsymbol{u}_{i,j+1/2} - \boldsymbol{u}_{i,j-1/2}}{\Delta y} \Delta t. \tag{4}$$

Here $F_{x,i+1/2,j}$ and $F_{y,i,j+1/2}$ are the advection fluxes for the x and y directions, respectively.

$$F_{x,i+1/2,j} = -\int_{x_{i+1/2,j}}^{x_{i+1/2,j}-u_{i+1/2,j}\Delta t} \chi_{is,j}(x,y)\,dx, \tag{5}$$

$$F_{y,i,j+1/2} = -\int_{y_{i,j+1/2}}^{y_{i,j+1/2}-v_{i,j+1/2}\Delta t} \chi_{i,js}(x,y)\,dy, \tag{6}$$