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Lattice-Boltzmann flow simulation of an oil-in-water emulsion through a coalescing filter: Effects of filter structure

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HIGHLIGHTS

- The permeation of O/W emulsion through a coalescing filter was numerically studied.
- A simulation model was developed based on the free-energy lattice Boltzmann method.
- The effects of filter properties on the coalescing behaviors were investigated.
- Our simulations demonstrated the effectiveness of the bilayer structure of filters.

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ABSTRACT

The permeation of an oil-in-water (O/W) emulsion through a coalescing filter was numerically studied using the lattice Boltzmann method (LBM). A numerical simulation model for the coalescing phenomena was developed based on the free-energy LBM. We investigated the effects of the wettability of fibers, filter porosity, and fiber diameter on the coalescing behaviors by performing two-dimensional permeation simulations for the O/W emulsions through modeled fibrous filters. We mainly focused on hydrophilic filters because they did not generate small secondary droplets during oil droplet detachment from the filter, and this is preferred for precise separation of oil and water. Our simulations demonstrated that filters with larger pore spacings enable formation of larger droplets but allow more droplets to pass without coalescing. To solve this problem, we designed bi-layered filters composed of a small-pore filter to accurately catch the droplets and a large-pore filter to enlarge the droplets; we demonstrated the effectiveness of the bilayer structure for membrane coalescence.

1. Introduction

Liquid wastes consisting of oil-water mixtures are generated in various industrial processes, such as the petrochemical industry, food industry, and shale gas and oil industries (Khatib and Verbeek, 2003; Shaffer et al., 2013; Vidic et al., 2013). These mixtures often take the form of an emulsion, in which droplets of one liquid are finely dispersed in another liquid, and it is generally difficult to separate the dispersed liquid from the continuous liquid. Among numerous oil-water separation techniques, membrane coalescence (Agarwal et al., 2013; Hlavacek, 1995; Kocherginsky et al., 2003; Kukizaki and Goto, 2008) is an energy-efficient, cost-effective, and small-footprint separation technique that is applicable to emulsions. In normal membrane separation processes (Choong et al., 2015), because membranes having larger contact angle for the droplet and smaller size of pores are used, dispersed droplets cannot enter the membrane pore. Thus, the droplets are rejected by the membrane surface, and only the solvent permeates the membrane. On the other hand, in the coalescence process (the target in this study), both dispersed and continuous liquids permeate a membrane filter. During the separation of an oil-in-water (O/W) emulsion, the oil droplets coalesce with each other as they pass through the membrane filter. When the oil droplets that have passed through the membrane are large enough, they can be easily separated from the water phase based on the different densities of the two liquids.

Understanding the coalescing dynamics of droplets that pass through the filter is essential to design and prepare a coalescing

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filter with a high performance. One approach to directly explore the coalescing dynamics is *in situ* observations of the permeation process using an optical microscope (Akamatsu et al., 2015; Kawakatsu et al., 1999). Although this experimental approach has successfully clarified the effects of porous media and processing factors on the coalescence, the observable situations and conditions are limited by realizable experimental setups such as the performance of optical microscope and processing accuracy to prepare the microfluidic systems.

Numerical simulation is another approach that can solve this difficulty and provide a deeper understanding of the coalescing dynamics. When designing an appropriate simulation model for the target system, we can consider a wide range of situations and conditions, and quantitatively and visually evaluate the coalescing phenomena. In our previous studies, we constructed simulation models based on a direct numerical simulation, where the numerical methods describing the two-phase flow were the coupled level set and volume-of-fluid (CLSVOF) method (Sussman and Puckett, 2000; Yokoi et al., 2009) and phase-field method (Anderson et al., 1998; Jacqmin, 1999). We performed coalescing simulations of droplets passing through a single membrane pore (straight-type pore (Kagawa et al., 2014; Mino et al., 2016a) and fibrous filter-type pore (Mino et al., 2016b)). The oil droplets captured by the fibers coalesced with other droplets to grow larger. When the droplets blocked the flow path, they were forced away immediately, yielding relatively small droplets. However, droplet pore blockage seriously affects the droplet dynamics in a single-pore system. Consequently, the coalescing behavior of O/W emulsions in a multi-pore system requires further investigation using a larger computational area.

Here, we develop a new simulation model for the coalescence of O/W emulsions based on the lattice Boltzmann method (LBM) (Chen and Doolen, 1998; Succi, 2001). The LBM is a computational fluid dynamics technique and is applied to calculations of viscous fluid flows in the Cartesian grid without solving the Poisson equation for the pressure field. Because of its simple formulation, the LBM calculation can be straightforwardly implemented on parallel computer architectures, allowing us to consider membrane coalescence for a multi-pore system. Among the three major models for two-phase flow calculations (color-fluid LBM (Grunau et al., 1993; Gunstensen et al., 1991), interparticle-potential LBM (Shan and Chen, 1993, 1994), and free-energy LBM (Swift et al., 1995, 1996)), we employ the free-energy LBM. The free-energy LBM can naturally describe the complicated motions of liquid-liquid interfaces induced by droplet coalescence and wetting of a droplet on a solid surface based on the thermodynamic theory. Recently, the free-energy based LBM was developed significantly (Antonini et al., 2016; Mazloomi et al., 2015a, 2015b, 2016, 2017; Semprebon et al., 2016). In this study, we use the free-energy LBM that was developed by Inamuro et al. (2003) because it is simple and easily applied to the wetting phenomena of droplets on a solid surface of complicated geometry.

The objective of this study is to conduct two-dimensional (2D) simulations of permeation of O/W emulsions through a modeled fibrous filter and to investigate the effects of fundamental factors involved in the fibrous filter design, i.e. fiber wettability, fiber diameter, and fiber filling fraction, on the coalescing behaviors. Based on the simulation results, we propose a bi-layered structure as a more optimal configuration for a coalescing filter. Generally, it is difficult to evaluate the real effects of porosity and tortuosity of porous media and also interfacial tension of droplets in the 2D systems. However, the simulation model with 2D geometry enables to explain the coalescing behavior well qualitatively and theoretically. For more detailed evaluations of the factors, three-dimensional calculations are preferred.

2. Numerical method

2.1. Free-energy lattice Boltzmann method

We used the free-energy LBM that was developed by Inamuro et al. (2003) to describe the two-phase flows with the same density. The non-dimensional variables used in this section are defined by a characteristic length, L, flow speed, U, particle speed, c, time scale (the diffusive time scale), $t_0 = L/U$, and reference density, ρ_0. A 2D lattice with nine velocity vectors (D2Q9) model was used in this study. The D2Q9 model has the velocity vectors $\mathbf{c}_i = (0, 0)$, $(0, \pm1)$, $(\pm1, 0)$, $(\pm1, \pm1)$ for $i = 1, 2, \ldots, 9$.

The two-phase LBM by Inamuro et al. (2003) uses two particle velocity distribution functions, f_i and g_i. The function f_i is used to calculate an order parameter, ϕ, which distinguishes the two phases, and the function g_i is used to calculate the velocity, $\mathbf{u}$, and the pressure, p, of the two-phase fluid. The two phases (phases I and II) are defined as the regions of $\phi = \phi_\mathrm{I}$ and $\phi = \phi_\mathrm{II}$, whereas the intermediate region, $\phi_\mathrm{I} < \phi < \phi_\mathrm{II}$, represents the diffusive interface between the two phases. The evolutions of the particle distribution functions, $f_i(\mathbf{x}, t)$ and $g_i(\mathbf{x}, t)$, with velocity $\mathbf{c}_i$ at point $\mathbf{x}$ and time t are computed by the following equations:

$$f_i(\mathbf{x} + \mathbf{c}_i\Delta x, t + \Delta t) - f_i(\mathbf{x}, t) = -\frac{1}{\tau_f}\left[f_i(\mathbf{x}, t) - f_i^{\mathrm{eq}}(\mathbf{x}, t)\right] \tag{1}$$

$$g_i(\mathbf{x} + \mathbf{c}_i\Delta x, t + \Delta t) - g_i(\mathbf{x}, t) = -\frac{1}{\tau_g}\left[g_i(\mathbf{x}, t) - g_i^{\mathrm{eq}}(\mathbf{x}, t)\right] \tag{2}$$

where f_i^{eq} and g_i^{eq} are equilibrium distribution functions, τ_f and τ_g are dimensionless single relaxation times, Δx is the spacing of the square lattice, and Δt is the time step during which the particles travel the lattice spacing. The effect of gravity was neglected for simplicity.

The order parameter, ϕ, distinguishing the two phases, the flow velocity, $\mathbf{u}$, and the pressure, p, are calculated as

$$\phi(\mathbf{x}, t) = \sum_{i=1}^{9} f_i(\mathbf{x}, t) \tag{3}$$

$$\mathbf{u}(\mathbf{x}, t) = \sum_{i=1}^{9} \mathbf{c}_i g_i(\mathbf{x}, t) \tag{4}$$

$$p(\mathbf{x}, t) = \frac{1}{3}\sum_{i=1}^{9} g_i(\mathbf{x}, t) \tag{5}$$

The two equilibrium distribution functions are described as

$$f_i^{\mathrm{eq}} = H_i\phi + F_i\left[p_0 - \kappa_f\phi\nabla^2\phi - \frac{\kappa_f}{6}|\nabla\phi|^2\right] + 3E_i\phi c_{i\alpha}u_\alpha + E_i\kappa_f G^{\phi}_{\alpha\beta}c_{i\alpha}c_{i\beta} \tag{6}$$

$$g_i^{\mathrm{eq}} = E_i\left[3p + 3c_{i\alpha}u_\alpha - \frac{3}{2}u_\alpha u_\alpha + \frac{9}{2}c_{i\alpha}c_{i\beta}u_\alpha u_\beta\right] + E_i\kappa_g G^{\phi}_{\alpha\beta}c_{i\alpha}c_{i\beta} \tag{7}$$

The appropriate coefficients are given as follows:

$$\begin{gathered} E_1 = 4/9, E_2 = \cdots = E_5 = 1/9,\ E_6 = \cdots = E_9 = 1/36, \\ H_1 = 1,\ H_2 = H_3 = \cdots = H_9 = 0, \\ F_1 = -5/3,\ F_i = 3E_i\ (i = 2, 3, \ldots, 9) \end{gathered} \tag{8}$$

$$G^{\phi}_{\alpha\beta} = \frac{9}{2}\frac{\partial\phi}{\partial x_\alpha}\frac{\partial\phi}{\partial x_\beta} - \frac{9}{4}\frac{\partial\phi}{\partial x_\gamma}\frac{\partial\phi}{\partial x_\gamma}\delta_{\alpha\beta} \tag{9}$$

with $\alpha, \beta, \gamma = x, y, z$, respectively (subscripts α, β, and γ represent the Cartesian coordinates, and the summation convention is used). In