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Numerical simulation of droplet merging and chemical reaction in a porous medium

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ABSTRACT

The chemical reaction between droplets merging in a porous medium is numerically investigated by solving the conservation equations of mass, momentum and chemical concentration in the internal and external regions of the porous medium. A level-set formulation for two-phase flows is extended to include the effects of porosity and mass transfer with chemical reaction. The numerical result for one-dimensional mass transfer with chemical reaction shows good agreement with the exact solution. The numerical method is applied to investigate the effects of droplet size, impact velocity and porosity on the droplet merging and the associated chemical reaction in a porous medium.

1. Introduction

The chemical reaction in a liquid film or droplet absorbed in a porous medium is of significant interest in removal or decontamination of hazardous chemicals in the sand, concrete, asphalt and soil regions. However, its general predictive model including the interfacial motion and chemical reaction coupled to mass transfer in the porous medium has not yet been developed.

Extensive numerical models were proposed for chemical reactions in single-phase flows [1–4] and two-phase flows [5–9], but they were not extended to the chemical reaction in a porous medium. Computational studies were also conducted for droplet penetration or evaporation in the porous medium using a marker-and-cell (MAC) method [10,11], a pore network method [12,13], the volume-of-fluid (VOF) method [14] and a level-set (LS) method [15,16]. The pore network method was based on the mass and momentum balances for individual gas and liquid pores whereas the MAC, VOF and LS methods were based on the local volume averaged conservation equations of mass and momentum including the effects of porosity and drag force due to the solid matrix [17–19]. However, only a few computations were made for the chemical reaction in the porous medium.

Recently, Atkinson et al. [20] presented a moving-grid method for computation of the chemical reaction of droplet in a porous substrate. They solved the species mass and momentum conservation equations including the effect of chemical reaction and showed the degradation processes of various chemical agents. However, their numerical method was based on the Lagrangian method, which is not straightforward for implementation of the interface with topology change, such as droplet–droplet merging, as well as relatively simple first-order chemical reaction cases.

In this work, we extend the LS formulation to computation of droplet merging and chemical reaction in a porous medium by solving the concentration equations with irreversible second-order chemical reaction as well as the mass and momentum equations. The effects of droplet size, impact velocity and porosity on the droplet merging and the associated chemical reaction are quantified.

2. Numerical analysis

The present numerical approach is based on the LS formulation developed by Lee and Son [21–23] for particle motion in an evaporating droplet or liquid film and Choi et al. [15,16] for droplet impact and evaporation on a porous surface. The LS method is extended for the droplet merging and chemical reaction in a porous medium. The droplet surface is tracked by the LS function ϕ, which is defined as a signed distance from the liquid–gas interface. The positive sign is chosen for the liquid phase and the negative sign for the gas phase. The interface between the porous and external fluid regions is described by another distance function ψ. The positive sign is chosen for the external fluid region and the negative sign for the porous region. In this work, the following assumptions are made: (1) the flow is axisymmetric, isothermal, incompressible and laminar; (2) the chemical reaction occurs only in the liquid phase which is a mixture of water and reacting chemical components; (3) the porous medium consists of spherical solid

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Nomenclature

B	drag coefficient of a porous solid matrix
d_p	particle diameter
d_{pore}	pore diameter
F	fraction function
h	grid spacing
H_s	height of a porous medium
M	molecular mass
$\mathbf{n}$	unit normal vector
p	pressure
r, y	cylindrical coordinates
R	droplet radius
t	time
$\mathbf{u}$	flow velocity vector, (u,v)
v_0	droplet impact velocity
Y	mass fraction

Greek symbols

α	step function
ϵ	porosity
θ	contact angle
κ	interface curvature
μ	dynamic viscosity
ρ	density
σ	surface tension coefficient
τ	artificial time
ϕ	distance function from the liquid–gas interface
ψ	distance function from the porous–fluid interface

Subscripts

0	initial
A, B	component A, B
i	component i
g, l	gas, liquid
p	particle
s	solid or porous medium

particles with the same diameter, which are uniformly distributed in the porous region; (4) the liquid, gas and solid properties are constant in each phase. We do not include the effect of phase change in the present analysis.

2.1. Governing equations in the external fluid region ($\psi > 0$)

The conservation equations of mass and momentum in the liquid and gas phases and the mass fraction (Y_i) of component i in the liquid phase can be expressed as

$$\nabla\cdot\mathbf{u} = 0 \tag{1}$$

$$\hat{\rho}\frac{\partial \mathbf{u}}{\partial t} = -(\nabla p + \sigma\kappa\nabla\alpha_\phi) + \nabla\cdot\hat{\mu}\nabla\mathbf{u} + \mathbf{f} \tag{2}$$

$$\frac{\partial Y_i}{\partial t} = -\mathbf{u}\cdot\nabla Y_i + \nabla\cdot D_i\nabla Y_i + s_i \quad \text{if } \phi > 0 \tag{3}$$

$$\mathbf{n}\cdot\nabla Y_i = 0 \quad \text{if } \phi = 0 \tag{4}$$

where

$$\alpha_\phi = 1 \quad \text{if } \phi > 0 \tag{5}$$

$$\alpha_\phi = 0 \quad \text{if } \phi \le 0 \tag{6}$$

$$\mathbf{n} = \nabla\phi/|\nabla\phi| \tag{7}$$

$$\kappa = \nabla\cdot\mathbf{n} \tag{8}$$

$$\mathbf{f} = -\hat{\rho}\mathbf{u}\cdot\nabla\mathbf{u} + \hat{\rho}\mathbf{g} + \nabla\cdot\hat{\mu}(\nabla\mathbf{u})^T \tag{9}$$

$$\hat{\rho} = \rho_l F_\phi + \rho_g(1 - F_\phi) \tag{10}$$

$$\hat{\mu}^{-1} = \mu_l^{-1}F_\phi + \mu_g^{-1}(1 - F_\phi). \tag{11}$$

Here, the discontinuous step function α_ϕ, the interface normal $\mathbf{n}$, and the interface curvature κ are evaluated from the LS function. The effective density $\hat{\rho}$ and viscosity $\hat{\mu}$ are interpolated by using a fraction function F_ϕ, which is defined as

$$\begin{aligned} F_\phi &= 1 && \text{if } \alpha(\phi_A) = \alpha(\phi_B) = 1 \\ &= 0 && \text{if } \alpha(\phi_A) = \alpha(\phi_B) = 0 \\ &= \frac{\max(\phi_A, \phi_B)}{\max(\phi_A, \phi_B) - \min(\phi_A, \phi_B)} && \text{otherwise} \end{aligned}$$

where the subscripts A and B denote the grid points adjacent to the location where F_ϕ is evaluated.

The LS function ϕ is advanced and reinitialized as

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = 0 \tag{12}$$

$$\frac{\partial\phi}{\partial\tau} = \frac{\phi}{\sqrt{\phi^2 + h^2}}(1 - |\nabla\phi|) \quad \text{if } |\phi| \ge h/2 \tag{13}$$

where h is a grid spacing.

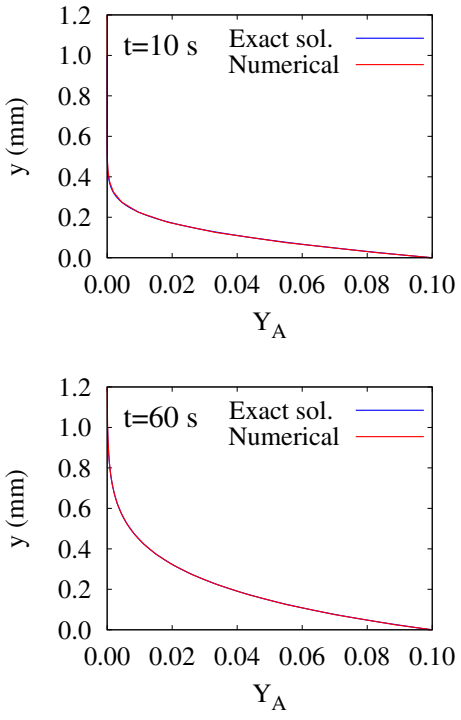

Fig. 1. Concentration profiles at different times for the 1-D mass transfer with chemical reaction.