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An investigation into fixed-bed microreactors using lattice Boltzmann method simulations

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Abstract

The fixed-bed microreactor is an important component in many biochip, microsensor, and microfluidic devices. The lattice Boltzmann method (LBM) provides a powerful technique for investigating such microfluidic systems. Accordingly, this study performs LBM-based simulations to examine fluid flows through a fixed-bed microreactor comprising a microarray of porous solids. During operation, the fluid and porous solid species are heated to prompt the chemical reaction necessary to generate the required products. Using the LB model, the flow fields and temperature fields in the microreactor are simulated for different Reynolds numbers, heat source locations, the reacting block aspect ratios, and porosity. A simple model is proposed to evaluate the chemical reactive efficiency of the microreactor based on the steady-state temperature field. The results of this model enable the optimal configuration and operating parameters to be established for the microreactor.

Keywords: Microreactor; Porous media; Lattice Boltzmann method (LBM)

1. Introduction

Microreactors play a key role in many biosensor and microfluidic applications and have been the subject of many experimental and theoretical studies. Aoki and Hasebe et al. [1] used a set of dimensionless geometric design factors to examine the microreactors. These geometric design factors were utilized to arrange the fluid segments of reactor inlet and to determine the cross-sectional shape of the fluid segments. These dimensionless factors enable to predict the reactor performance for any given set of geometric design factors. Or inversely, the dimensionless numbers provide the means to determine the geometric design factors of the fluid segments required to obtain the desired reactor performance. Masuda and Suzuki et al. [2] developed numerical solutions for the heat and fluid flows in the T-junction region of a supercritical microreactor. The authors showed that a nonlinear k–ε model with the low Reynolds number effect was the appropriate computational method for their cases. Microreactors effectively enhance the product selectivity of extremely fast exothermic reactions. Furthermore, micromixing enhances the selectivities of competitive parallel reactions and competitive consecutive reactions [3]. Previous studies of microfluidic systems and biosensor devices with a reaction function generally assumed the microreactor to be a fixed-bed type designed in the form of a microarray of porous solids. Investigating the heat and fluid flows in such systems requires a powerful tool capable of performing pore-scale analysis and not restricted by the hydrodynamic continuum condition.

The kinetic-based lattice Boltzmann method (LBM) has emerged as a promising numerical technique for simulating fluid flows and modeling the physics in fluids [4–7]. Many lattice Boltzmann (LB) models have been proposed for analyzing the problem of fluid flow through porous media. Spaid and Phelan [8] proposed a LB model for simulating fluid flow in fibrous porous media. In their approach, the Brinkman equation was recovered by modifying the particle

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Nomenclature

AR	aspect ratio $\mathrm{AR} \equiv H^*/W$, where H^* and W are the height and width of porous block for microreactors
c_i	microscopic particle velocity in each lattice link i
c_s	speed of sound
Da	Darcy number
f	distribution function for the flow field
g	distribution function for the temperature field
H	height of channel
k	permeability of the porous medium
L	length of channel
$\overline{L}$	flow path length of the porous medium
L^*	unit length of computational domain for local pore structure
Nu	Nusselt number
Pr	Prandtl number
PRF	integral porous reacting fraction
Re	Reynolds number for channel
Re_{D}	Darcy Reynolds number inside porous medium
Re_{F}	flux Reynolds number for porous boundary
SR^*	local surface reacting ratio
T	temperature
$\overline{U}$	mean velocity (Darcy flux) within porous medium
T_{att}	temperature of effective activation energy for chemical reaction
t	macroscopic time
u_A	macroscopic flow velocities, where subindex A is the components of Cartesian coordinates
u_{i}	injection velocity normal to porous boundaries
u_{W}	sliding upper wall velocity for Couette flow

Greek symbols

α	thermal diffusivity
Δt	time interval (step) of LBM
ϕ	porosity of porous medium
ν	kinetic viscosity
ρ	fluid density
τ_D	relaxation time for the temperature field
τ_v	relaxation time for the flow field
ω_{OV}	overall reaction rate

equilibrium distribution function to reduce the magnitude of the momentum at specified lattice sites for porous regime while leaving the direction of the momentum unchanged. Alazmi and Vafai [9] conducted a detailed analysis of various fluid flow and heat transfer conditions at the interface between a porous medium and a fluid layer. Martys [10] presented a new approach for generalizing the LBM to ensure fluid flow consistent with those of the Brinkman equation. In this literature, a lattice Boltzmann model is proposed for isothermal incompressible flow in porous media. The key point is to include porosity into equilibrium distribution, and to add a force term to the evolution equation to account for the linear and nonlinear drag forces of the medium [11]. Zeiser and Lammers et al. [12] employed a LB automata to study the behavior of a reacting, viscous flow within the complex geometry of a fixed-bed reactor. Recent study for convection heat transfer in porous media has also been proposed [13].

The present study uses LBM-based simulations to investigate the characteristics of a 2-D porous type microreactor with a microarray structure, as shown in Fig. 1. Specifically, the simulations investigate the heat and fluid flows in the microreactor for different operational and geometric conditions, including the Reynolds number (Re) of the channel flow, the position of the heat source, and the aspect ratio (AR) and porosity (ϕ) of the reacting block. Additionally, a simple model is proposed to evaluate the chemical reactive efficiency of the microreactor based on the steady-state temperature distribution. This model avoids the requirement for time-consuming iterative calculations and provides a straightforward means of identifying the optimal operational and geometric parameters of the microreactor.

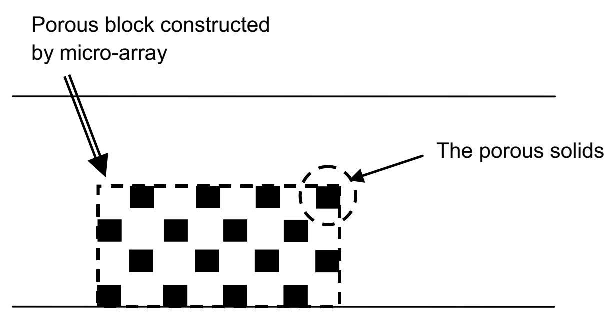

Fig. 1. Fixed-bed microreactor comprising microarray of porous blocks.

2. Numerical method

2.1. Lattice Boltzmann model

In simulating the flow and temperature fields within the microreactor using the LBM, the following assumptions are made:

(1) No external body forces (e.g. buoyancy) are applied to the flow field.
(2) The flow is incompressible in the low Reynolds number regime, and hence the effects of viscous heat dissipation can be neglected.
(3) Radiative heat transfer is ignored.
(4) The flow field is unaffected by the chemical reaction process or by the heat transfer. Hence, the flow field