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Multiscale lattice Boltzmann modeling of two-phase flow and retention times in micro-patterned fluidic devices

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ABSTRACT

Recent advances for fabricating micro-featured architectures such as posts or pillars in fluidic devices provide exciting opportunities for multiphase flow management. Here we describe a novel, multiscale modeling approach for two-phase flows in microfeatured architectures developed within the Shan and Chen Lattice Boltzmann method. In our approach a fine scale is used to resolve the true microfeatured architecture, with a coarser scale used to model the gross geometry of the device. We develop the basic features of the approach and demonstrate its applicability to modeling retention times of droplets of a dispersed phase in an array of microposts – an architecture used in microfluidic reactors, bioreactors, and biomedical devises. Additionally we show that it is feasible to model the microfeatured geometry in a piecewise manner which includes extrapolating dispersed phase flow characteristics in the entire system based on simulations in smaller subdomains.

1. Introduction

Microtechnology and process intensification are gaining an increasingly larger role in the engineering design of emerging technologies. A major impetus in introducing microscale-based technologies emerges from fundamental, architectural, economical, and safety/security advantages. As a technical approach a microscale-based engineering design establishes directions for potentially innovative solutions in many aspects of technology design (intensification of mass and heat transfer, intensification of chemical process rates, chemical product distribution and yield, process control, process safety, process scale-up) and applications (organic and inorganic chemical synthesis and processing, unit operations, environmental technologies, energy conversion technologies, renewable energy technologies). A comprehensive review of these topics can be found in Jensen (2001). For more general considerations of microreactors alone we refer to review articles such as Kolb and Hessel (2004), Kiwi-Minsker and Renken (2005) and Hartman and Jensen (2009).

Multiphase flows in microscale structures provide additional complexity and opportunity for the engineering design. Novel designs of multiphase systems in chemical reaction processes (Hessel et al., 2005; Günther and Jensen, 2006), phase separations (Lam et al., 2013; Wiesegger et al., 2013), mixers (Zhao et al., 2006), and analytical devices (Huh et al., 2002), are all evidences for the proliferation of microscale-based technologies. Multiphase flows can also be an undesirable side effect occurring during device operation; a scenario that can be a consequence of normal process performance such as boiling in microscale heat exchangers. Often two-phase flow originates through introduction of the unwanted phase into the system from its surroundings, such as leaks of air bubbles entering the system through equipment gaps or with process feed (Gravesen et al., 1993; Jensen et al., 2004; Sparks et al., 2007). An unaccounted second phase may lead to systems' reduced efficiency, malfunctions and damage. Elimination of undesirable phase in microscale-based devices is often difficult, thus, a large part of research efforts are focused on proper accommodation of unwanted phases and their influence. Doku et al. (2005) provides an outline of different multiphase microreactor designs, whereas Kohnle et al. (2002), Litterst et al. (2004) and Chung et al. (2008) report on microchannel based architectural solutions for improved bubble mobility.

Microscale architectures with features such as microposts or pillars partially or fully replacing classic microchannel arrays, represent a relatively unexplored and advantageous design option. Deployment of microposts in microscale-based devices creates flexible technical solutions. The introduction of microposts has the potential for addressing numerous microscale-based process

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requirements due to conveniently positioned internal surface areas for catalyst deposition and new opportunities for manipulation of two-phase flow. The benefits of chemical processes with solid catalysts is emphasized in Doku et al. (2005) whereas their application in microscale heat exchangers is experimentally and theoretically investigated in Krishnamurthy and Peles (2008).

Theoretical and mathematical models for multiphase flows in microscale-based structures differ substantially from macroscale systems due to the small characteristic dimensions of microscale features, and very large aspect ratios. In immiscible fluid mixtures, interface physics becomes a major contributor to fluid dynamics, and eat and mass transfer. Interfacial and viscous forces often dominate over inertia and buoyancy. In addition, the proximity of walls, the presence of architectural microfeatures, and catalysts coatings create important fluid–solid interactions. The hydrodynamic characteristics of gas–liquid flows in pillared microstructures were experimentally investigated and compared to conventional theoretical models and correlations by Krishnamurthy and Peles (2007) and De Loos et al. (2010). Results varied from established models and furthermore Krishnamurthy and Peles (2007) defined a new two-phase flow pattern regime, bridge flow, observed in micropillar arrays.

Design opportunities for micropillared complex architectures therefore include not only geometric considerations, but also variables such as solid affinities towards different phases, surface tension manipulation, surface modification of posts with functional chemical groups, and others. Comprehensive and efficient design requires computational tools though the benefits of numerical simulations are not confined to the design aspects only (Jensen, 2001). The importance of interfaces, geometric complexity, and commonly occurring device high aspect ratios imply high resolution and large computational efforts. Multiscale modeling provides the capacity for sufficiently accurate simulations with reasonable computational costs.

We propose a novel, multiscale modeling approach for numerical simulations of two-phase flow in complex microarchitectures developed within framework of the Lattice Boltzmann method. Due to its capabilities in representing fluid–fluid and fluid–solid interactions. The proposed approach can be extended to multiphase systems but here we present results obtained for two-phase flow only.

We focus on multiscale modeling of dispersed phase retention time. We perform simulations with fully resolved microfeatured geometry based on which we develop a force operator that when applied on the dispersed phase in an empty geometry yields sufficiently similar dispersed phase retention time. The force operator is robust and once developed becomes applicable for a range of dispersed phase sizes and operating conditions. This provides an opportunity for reducing computational effort by replacing part of the simulations in the geometrically resolved domain with computationally less intensive empty domain. Additionally, we demonstrate that it is possible to extrapolate information on the flow based on piecewise simulations instead of the entire domain. This feature is an especially important capability of the proposed approach as it could enable accurate computations of systems previously too large to simulate.

2. Description of multiscale modeling approach

2.1. Scope

The proposed multiscale modeling approach is suitable for the modeling of two-phase flow phenomena in microscale-based structures with features such as posts and pillars (Fig. 1). The repetitive design of these microarchitectures enables identification of representative regions that can provide the bases for estimates of a global behavior similar to representative volumes and unit cells in porous media.

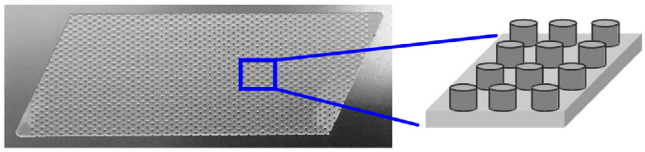

Fig. 1. Microscale device with cylindrical pillars as schematically displayed. Device image courtesy of Microproducts Breakthrough Institute.

The multiscale modeling approach we propose here has the ability to communicate critically needed information from locally highly resolved model or domain into a global, less resolved model/domain. An observed phenomenon could emerge from considerations of mass or heat transfer, chemical kinetics, characteristic process times, specific surface area, presence of energy fields/forces, interfacial forces, or any other observable occurrence which arises from structural, operating or process dynamic characteristics of the microscale-based structure.

Example of variables that can undergo proposed multiscale modeling are dispersed phase retention time, flow direction and chemical reactivity. Here we demonstrate the applicability of our approach on dispersed phase retention time which we define as the time needed for the dispersed phase to cross either the whole system in question or different subsections of the system.

2.2. Components

We distinguish two modeling levels that represent *fine* and *coarse* modeling scales connected through an information carrier, coupling operator.

- Fine scale (lower level)
  The fine scale or lower level is the entire microscale-based structure or its subdomain with fully resolved architecture such as posts and pillars. In general, this level requires implementation of finer computational grids to capture correct inter-fluid and fluid–solid interactions.
- Coarse scale (upper level)
  The coarse scale or upper level is the same structure without the micro-features, an “empty” or geometrically uniform domain. This level retains only gross architectural features such as walls, inlets and outlets. The computational grid on this level can be significantly coarser than in the fine scale simulations.
- Coupling operator
  The coupling operator ensures transfer of information from fine to coarse scales. Here it provides sufficiently close retention time of dispersed phase on the coarse scale as on the fine scale. The coupling operator is a discrete scalar or vector field applied on the interface of the dispersed phase. In the case of retention time it is a vector field with the vector quantities referred to as *forcing terms* or *interfacial forcing terms*.

The forcing terms magnitudes may be constant throughout the system and, in which case the upper level simulations model the dispersed phase behavior as average over the entire device. The magnitudes can also have different values in distinct sections of the device such as in or around inlet or outlet regions, or in the bulk of a post array, leading to separated effective behavior in each section considered. The direction of the coupling operator depends on the influence of system architecture and flow parameters on the dispersed phase. The information passed to the upper level through the coupling operator is reduced. For example, in the case

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