Bull. Aust. Math. Soc. (First published online 2024), page 1 of 3*
doi:10.1017/S0004972724000418
*Provisional—final page numbers to be inserted when paper edition is published

COMPUTATIONAL FLUID DYNAMICS SIMULATION OF OSCILLATORY FLOW IN PERIODIC MICROPORE STRUCTURES

SAMUEL STEPHEN

(Received 24 April 2024)

2020 *Mathematics subject classification*: primary 76-10.

Keywords and phrases: fluid mechanics, numerical simulation, lattice, Boltzmann method.

Recent experimental studies, in conjunction with numerical simulations, have investigated the possibility of using microporous membranes in microfluidic devices to separate particles within a fluid. The specific design of this class of separation device involves pumping a particle-laden fluid back and forth through a membrane of axisymmetric, periodic micropores. Even though there is no net flow of the carrier fluid in such cases, introducing spatial asymmetry in the periodic pore profile has been shown to lead to directed particle transport; however, it is not currently understood how to control and optimise this transport. Deterministic solutions for the motion of individual particles are not available due to the presence of random thermal fluctuations in these microscale systems. Hence, a comprehensive statistical routine for predicting the magnitude and direction of the bias in suspended particle trajectories would be beneficial in the design of effective particle separation devices. Modelling this two-phase flow problem is commonly divided into two parts: carrier fluid flow field determination and stochastic simulations of travelling suspended particles. This thesis aims to refine existing techniques and establish new methods for approximating solutions to these two sub-problems.

It should be noted that assumptions and simplifications are required to study these flow problems because solving a complete theoretical model of the flow and transport problems is intractable. Existing approximations of oscillatory fluid flow in periodic micropore structures have some undesirable limitations. First, the geometry of the microporous membranes typically makes fluid–solid boundary conditions very difficult to implement. Additionally, inertial terms from the governing hydrodynamic flow equations usually have to be ignored to ensure simulation feasibility.

Thesis submitted to Griffith University in August 2023; degree approved on 17 November 2023; supervisors Peter Johnston and Barbara Johnston.

In this thesis, we propose to use a computational fluid dynamics solver not restricted by the same drawbacks present for standard solvers. An axisymmetric formulation of the lattice Boltzmann method has robust boundary conditions that are readily generalised to any pore shape, and the formulation approximates the Boltzmann equation instead of the Navier–Stokes equations, inherently incorporating inertial effects. For the particle transport aspect of the simulation, we opt for a simplified stochastic model. This particular approach has been used previously on an asymmetric sinusoidal pore profile; however, we can generalise it to any geometry using the lattice Boltzmann method for the flow field determination. Our complete numerical description allows us to investigate the physical factors that impact the resulting oscillatory flow fields and particle transport within the flow.

The axisymmetric lattice Boltzmann method and stochastic implementations used throughout the thesis are independently developed. Accordingly, we verify the implementations with error calculations in preliminary problems that have analytic solutions, while also finding agreement between our results and published numerical approximations for more complex flows. We also qualitatively compare our solutions to experimental observations where possible. We then identify and investigate six factors that have the most influence on particle transport induced by an oscillatory pressure gradient within periodic micropores: the Womersley number, the Reynolds number, the size of the suspended particle, the longitudinal skewness in the pore profile, the pore expansion radius and the length between pore expansions.

The Womersley number relates oscillation frequency to viscous effects. Typically, microscale flow systems are characterised by low Womersley numbers. In this thesis, we formulate a novel low-Womersley-number approximation, based on the analytic solution to Womersley flow in a straight tube, which temporally scales the relevant steady-state flow field. We find that increases in the Womersley number can lead to increases in the magnitude of the particle drift. We also find that increasing the Reynolds number increases the magnitude of the fluid velocities, which can significantly influence the motion of the suspended particles. The size of the particle determines the balance between interactions with the pore wall and the extent of the random thermal fluctuations. This trade-off results in a critical particle radius that reverses the direction of net particle transport for certain parameter sets. The extent of longitudinal asymmetry in the periodic profile affects the magnitude of mean particle current. Changing the maximum expansion radius of the periodic pore profile has a more complicated effect on the average current of the particulate suspension; for example, it determines the occurrence of recirculation zones in the flow field. We also show that the length between pore expansions can alter the bias in the particle drift. Finally, by tracking particle proportions, we show that increasing the axial membrane length, optimising geometric design and using alternating flow phases can each lead to enhanced particle separation efficiency.

Our findings contribute to the understanding of oscillatory flow and particle transport within periodic micropore structures. Advancements in numerical simulations of the aforementioned systems can aid in the design of microfluidic particle separation devices. Furthermore, the various numerical methods described throughout this thesis can be generalised to any fluid flow problem with an axisymmetric and periodic geometry, greatly extending the applicability and usefulness of the research.

SAMUEL STEPHEN, School of Environment and Science,
Griffith University, Nathan, Queensland 4111, Australia
e-mail: samueljacobstephen@gmail.com