Commun. Comput. Phys.
doi: 10.4208/cicp.341011.310112s

Vol. **13**, No. 3, pp. 851-866
March 2013

Simulation of 3D Porous Media Flows with Application to Polymer Electrolyte Fuel Cells

N. I. Prasianakis[1,*], T. Rosén[1,2,†], J. Kang[1], J. Eller[2], J. Mantzaras[1] and F. N. Büchi[2]

[1] *Combustion Research Laboratory, Paul Scherrer Institute, Villigen PSI 5232, Switzerland.*
[2] *Electrochemistry Laboratory, Paul Scherrer Institute, Villigen PSI 5232, Switzerland.*

Received 31 October 2011; Accepted (in revised version) 31 January 2012

Available online 29 August 2012

Abstract. A 3D lattice Boltzmann (LB) model with twenty-seven discrete velocities is presented and used for the simulation of three-dimensional porous media flows. Its accuracy in combination with the half-way bounce back boundary condition is assessed. Characteristic properties of the gas diffusion layers that are used in polymer electrolyte fuel cells can be determined with this model. Simulation in samples that have been obtained via X-ray tomographic microscopy, allows to estimate the values of permeability and relative effective diffusivity. Furthermore, the computational LB results are compared with the results of other numerical tools, as well as with experimental values.

AMS subject classifications: 65D18, 76G25, 76M28, 76S05

Key words: Porous media, GDLs, lattice Boltzmann, fuel cells, fluid dynamics.

1 Introduction

The simulation of porous media flows has recently attracted a lot of attention. The engineering applications related to porous media flows, are of interest in many industrial sectors that span from the chemical and oil industry to the fuel cell development. Polymer electrolyte fuel cells (PEFCs) have been considered in the last decades as a promising solution for future mobile and stationary energy conversion systems. Although the overall fuel cell performance has been substantially improved the last years, a significant

*Corresponding author. *Email addresses:* nikolaos.prasianakis@psi.ch (N. I. Prasianakis), rosen@mech.kth.se (T. Rosén), jinfen.kang@psi.ch (J. Kang), jens.eller@psi.ch (J. Eller), ioannis.mantzaras@psi.ch (J. Mantzaras), felix.buechi@psi.ch (F. N. Büchi)
†Current address: Linné FLOW Centre, KTH Mechanics, SE-100 44 Stockholm, Sweden.

limitation still persists related to the mass transport losses in the so-called gas diffusion layers (GDLs). The GDL's main purpose is to collect current over the flow channels and to provide uniform access of the fuel and oxidant gases to the electrocatalyst. This requires not only high permeability and relative diffusivity in the pore space, but also high conductivity in the solid. Permeability and diffusivity in the pore space are crucial to PEFC performance, as they determine the flux of reactants to the MEA (membrane-electrode-assembly). Testing various designs in a computer model using flow solvers is simpler and more efficient than carrying out the actual experiments. The GDL has a porosity of around 80% and is typically composed of carbon fibers with diameters typically of the order of 6-10μm. The pore size distribution shows a maximum in the range of 20-40μm [1]. The internal structure of the GDL and the nature of the surfaces can play a significant role for the transport of gases inside the GDL. The transport properties of the material can change due to compression [2], or due to the presence of water under normal operating conditions of the fuel cell [3]. The use of computational methods along with structures obtained via X-ray tomographic microscopy (XTM), can provide the insight needed to optimize the design and the working efficiency of such devices [4–7]. Using a flow solver, apart from optimizing the flux of reactants to the MEA, it can also determine if water accumulation can be correlated to high/low velocity regions of the GDL (or other flow properties). As a result, regions where water accumulates can be reduced by optimizing the design.

Lately, the lattice Boltzmann method has received a lot of attention due to its strong kinetic-based theoretical background and its computational efficiency [8]. A domain of application of the method, usually considered as its strong asset, is the flows in porous media. For three dimensional complex geometry simulations, there exists a multitude of candidate lattice Boltzmann models. The usual 3D standard lattices are extensions of the two-dimensional with nine discrete velocities, the D2Q9, in three dimensions. Depending on the number of discrete velocities there exist: the D3Q13, the D3Q15, the D3Q19 and the D3Q27 [8–11] models. One of the characteristic features of these lattices is that communication and exchange of information occurs only within the next neighboring nodes. This results in: a) a simple implementation of complex geometry boundary conditions, and b) efficient parallelization of the algorithm. For the aforementioned lattices, the larger the number of discrete velocities, the better the accuracy and the correspondence to the continuous kinetic theory. At this point, accuracy refers to the ability of recovering the correct value of the relevant equilibrium higher order moments needed for establishing the Navier-Stokes at the continuum limit. It should be noted that this is not strictly true for extended lattices (beyond next-neighbor communication) and specific rules need to be applied in order to guarantee increase in accuracy when constructing such lattices [12–16]. All aforementioned next-neighbor lattices are lacking Galilean invariance, rotational isotropy, and reference temperature independence [12, 17]. For small magnitude of velocity, (Mach number $\ll 1$), these deficiencies are negligible, while for larger values they become more pronounced, manifesting unphysical behavior. Among these models, the most accurate velocity set for isothermal flows, is the D3Q27 guided equi-