www.sccer-mobility.ch

PAUL SCHERRER INSTITUT

In cooperation with the CTI

Energy
Swiss Competence Centers for Energy Research

Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

Swiss Confederation

Commission for Technology and Innovation CTI

Microscopic Modeling of evaporative heat and mass transfer in the diffusion layer of PEFCs

N. I. Prasianakis[a], R. Sui[a], J. Mantzaras[a], F. N. Büchi[b]

e-mail: nikolaos.prasianakis@psi.ch, ran.sui@psi.ch, ioannis.mantzaras@psi.ch, felix.buechi@psi.ch

[a] Paul Scherrer Institute, Combustion Research Laboratory, CH-5232, Villigen PSI, Switzerland

[b] Paul Scherrer Institute, Electrochemistry Laboratory, CH-5232, Villigen PSI, Switzerland

1. Motivation

During the normal operation of a polymer electrolyte fuel cell (PEFC), liquid water is produced electrochemically in the porous gas diffusion layer (GDL), at the cathode side. Water management is strategic for the cell optimization and efficient operation.

The numerical simulation of transport phenomena at the microscopic level can provide better understanding of the underlying processes e.g. as reported in Refs. [1,2]. Therein, the relative permeability and the effective diffusivity of GDLs, have been obtained as a function of water saturation at in-situ conditions. In this study we focus on the understanding of the phase change processes for the evaporative fuel cell cooling. The modeling framework that we chose to work is the lattice Boltzmann method.

2. Polymer Electrolyte Fuel Cells

The gas diffusion layer is the porous structure located between the fluid distributor and the catalyst layer of the Polymer Electrolyte Fuel Cell (Fig. 1). Saturated water, which is produced electrochemically, limits the access of the gases to the membrane, thus controlling the efficiency of the cell. At the same time, it can potentially be used for the thermal management of the cell (leading to a "thermal-neutral" operation).

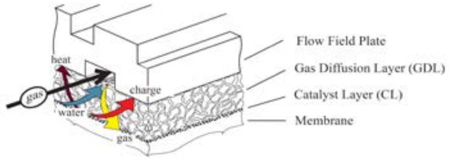

Figure 1. GDL, the inter-connect between the fluid distributor (bipolar plate) and the catalyst layer is the only component through which gases, liquid water, heat and charge need to pass in relevant flux densities

The GDL structures have been visualized using Synchrotron Radiation X-Ray Tomographic Microscopy (SR-XTM), which allows phase discrimination (contrast for carbon, water and void). An example is depicted in Fig. 2.

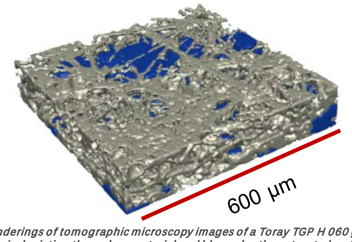

Figure 2. Surface renderings of tomographic microscopy images of a Toray TGP H 060 gas diffusion layer. Gray color is depicting the carbon material and blue color the saturated water. [3,4]

3. Modeling of involved processes

Currently, the following physics have been included:
Gas-phase: Binary mixture flow and diffusion, heat transfer.
Liquid-phase: Heat transfer, mass transfer, no volume change.
Solid-phase: Treated as adiabatic wall boundary.
Interface between gas/liquid-phase: Evaporation processes.
Evaporation rate = f(Xs-X),
Xs: humidity ratio at saturated conditions (Kg_{water}/Kg_{air}) (Fig. 3),
X : humidity ratio of gas mixture (Kg_{water}/Kg_{air}) at the gas/liquid interface.

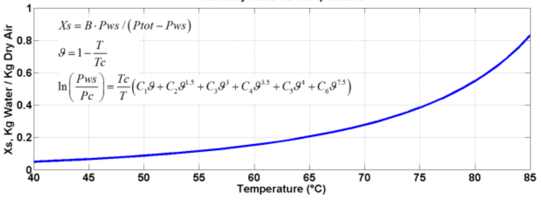

Figure 3. Humidity ratio for different values of the gas mixture temperature.

3. Lattice Boltzmann Method

The lattice Boltzmann method is based upon the solution of the Boltzmann BGK equation:

$$\partial_t f_i + c_{i\alpha}\partial_\alpha f_i = -\frac{1}{\tau}\left[f_i - f_i^{eq}\right].$$

Population f_i is defined as the velocity distribution function, which is the probability density of finding particles at time t, in position x moving with velocity c_i. For the two-dimensional simulations, the most commonly used discrete velocity set is the one with nine discrete velocities, the ***D2Q9***.

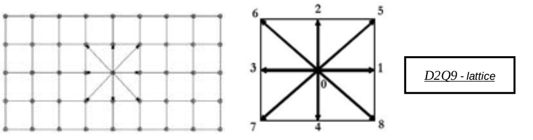

Figure 4. Schematic of the computational grid and the "2-dimensional 9 velocities lattice".

Based on the ***D2Q9*** lattice, Galilean invariant models as well as multi-component models have been recently derived [**5**,**6**].

5. Preliminary simulations

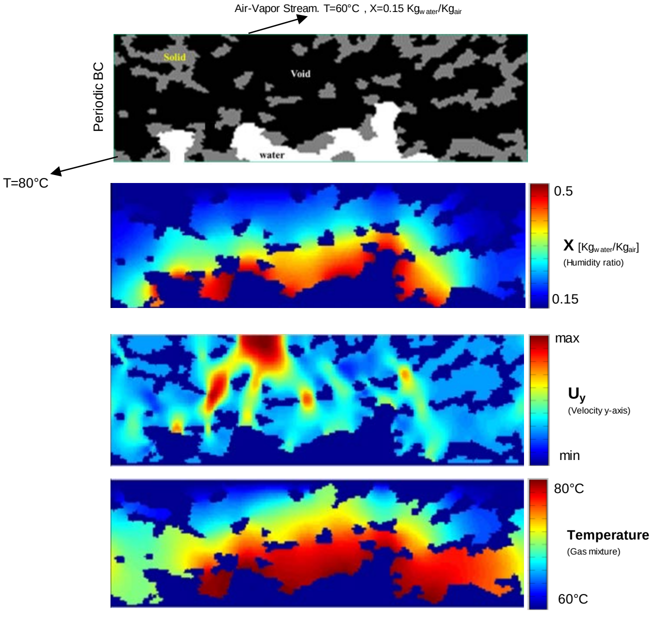

Figure 5. Top: GDL Simulation domain: Gray: Solid material, Black: void, White: saturated water. The catalyst layer is found at the bottom of the domain and is at temperature T=80°C. A stream of water vapor-ait (X=0.15) flows at the top of the channel with Temperature T=60°C . Water evaporates from the liquid water surface and is advecting and diffusing to the channel. Side walls are treated as periodic boundaries. Contours of humidity, velocity in the y-direction and temperature are plotted.

6. References

[1] N.I. Prasianakis, T. Rosen, J. Kang, J. Eller, J. Mantzaras, F.N. Büchi, Comm. Comp. Phys. **13**, 851-866 (2013).
[2] T. Rosén, J. Eller, J. Kang, N.I. Prasianakis, J. Mantzaras, F.N. Büchi, J. of Electrochem. Soc. **159**, 536 (2012).
[3] F.N. Büchi, J. Eller, F. Marone, M. Stampanoni, ECS Trans. **33**, 1397 (2010).
[4] Fig. 2, 3D rendering is provided by Dr. Adrien N. Lamibrac, LEC, PSI (2014).
[5] N.I. Prasianakis, I. Karlin, J. Mantzaras, K. Boulouchos, Phys. Rev. E **79**, 066702 (2009).
[6] J. Kang, N.I. Prasianakis, J. Mantzaras, Phys. Rev. E, **89**, 063310 (2014).