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Pore-level modelling of phase-change induced flow and mass transfer in porous media:

Evaporative cooling of polymer electrolyte fuel cells (PEFC)

Water management is a critical issue in the operation of a polymer electrolyte fuel cell (PEFC). The liquid water generated by the electrochemical reaction invades the porous gas diffusion layer (GDL) and can greatly affect efficiency of the PEFC. Numerical studies at the microscopic level can eventually help optimizing the fuel cell [1, 2]. Based on the lattice Boltzmann (LB) methodology for flow and mass diffusion, a modelling framework is designed so as to understand the phase change processes of water in the GDL. The porous geometry is obtained from X-ray tomographic microscopy at the Swiss Light Source (SLS) facility of Paul Scherrer Institut. Validations against available experimental data for the exact same porous GDL and at a reference temperature are carried out, which pave the way to better understand the phase change process in fuel cells.

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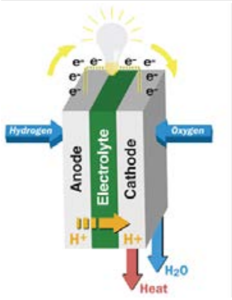
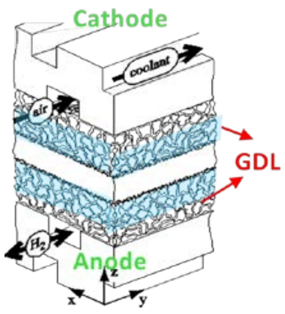
Evaporative Cooling in Feul Cells



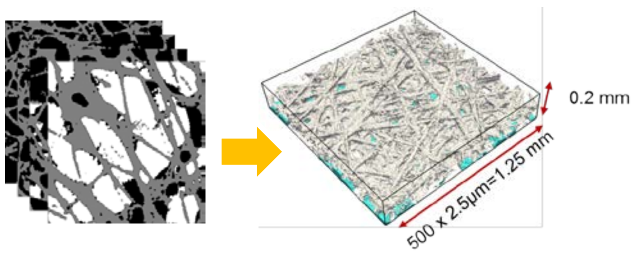
Evaporative cooling:
In modern fuel cells the system produces power, heat and water. In order to maintain the efficiency, evaporative cooling is used to remove water and dissipate heat in the gas diffusion layers (GDL).

Problem:
Current understanding of the evaporation process at the pore scale is very poor, while carrying out experiments are probe the porous structure are either very difficult or impossible.



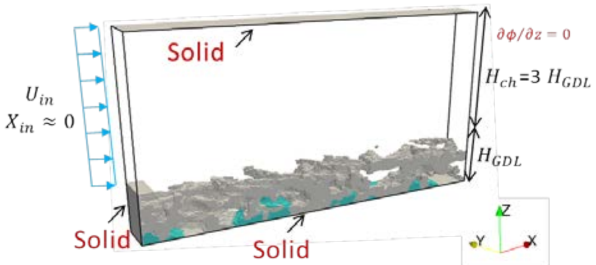
Constructing Simulation Setup

In order to study the evaporation phenomena, a numerical simulation setup is constructed based on the X-ray tomographic imaging of the GDL



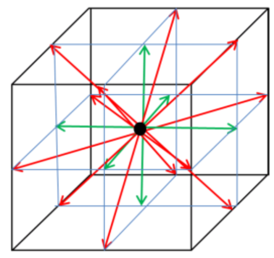
X-ray imaging   Ternary data for LB code

Final 3D simulation setup



Lattice Boltzmann Framework

A passive scalar LB model is used for the binary flow



D3Q19 LB stencil

Parallel computations on modern Tesla K80 GPUs

MRT LBE for bulk flow:

$$f_\alpha(x + c_\alpha \Delta t, t + \Delta t) = f_\alpha(x,t) + \frac{1}{\tau_b}\left(f_\alpha(x,t) - f_\alpha^{eq}(x,t)\right)$$

SRT LBE for binary gas diffusion (Air-Vapor):

$$h_{\alpha,j}(x + c_\alpha \Delta t, t + \Delta t) = h_{\alpha,j}(x,t) + \frac{1}{\tau_c}\left(h_{\alpha,j}(x,t) - h_{\alpha,j}^{eq}(x,t)\right)$$

Diffusive boundary condition at water /gas interface:

$$f_\alpha = f_\alpha^{eq}(\rho, v_{evp}) \quad , \quad v_{evp} = g_s/\rho_0$$

g_s = Evaporation rate in kg/(m²s)

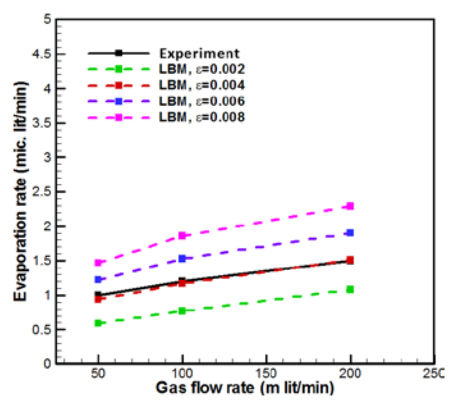
Validation Against Experiments

Evaporation rates obtained by LBM are then validated against experimental ones, thus regulating the evaporation coefficient ε, in the kinetic model:

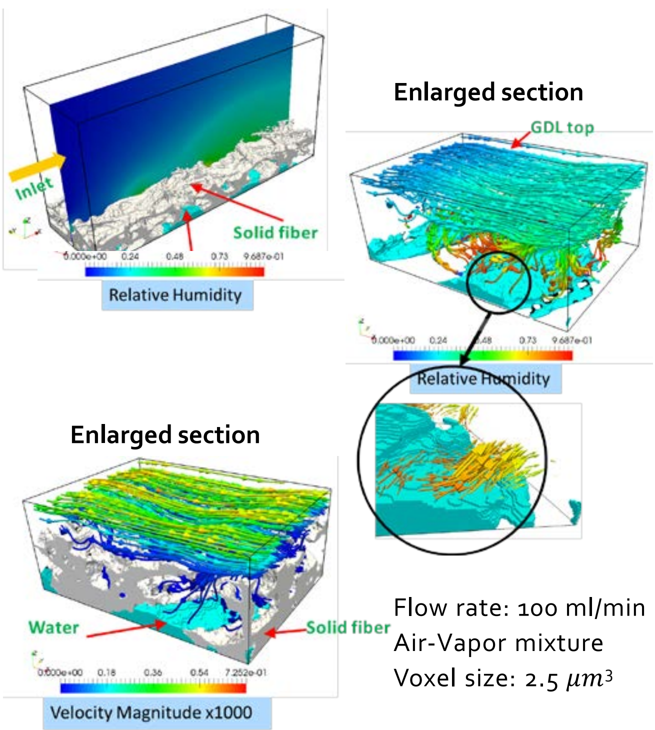
$$g_s = \frac{\varepsilon}{1 - 0.5\varepsilon}\left(\frac{m_v}{2\pi k}\right)^{1/2}\left[\frac{P_{w,sat}}{\sqrt{T_w}} - \frac{P_v}{\sqrt{T_v}}\right]$$

Operating conditions:

- Isothermal condition (not limited to) T_w=T_v=30°C
- Vanishing inlet humidity X_{in}≈0

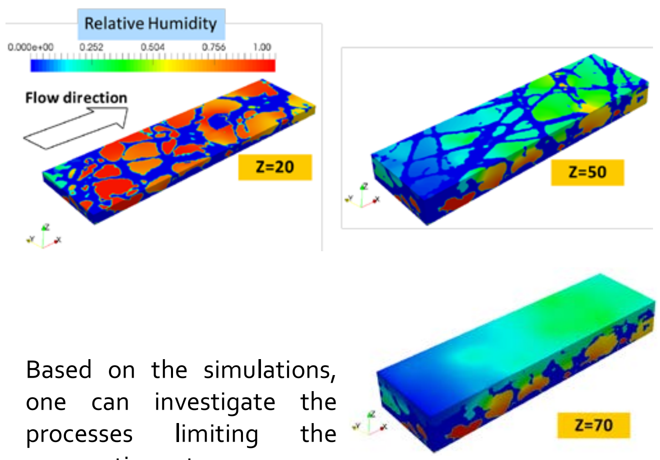


3D Numerical Results



Flow rate: 100 ml/min
Air-Vapor mixture
Voxel size: 2.5 μm^3

Summary of Results



Based on the simulations, one can investigate the processes limiting the evaporation rate:

→ Inside the GDL, flow is mostly governed by the upward velocities induced by evaporation.

→ Humidity is carried by evaporation-induced currents and then by the bulk flow outside GDL.

→ ***A mixed kinetic and transport*** controlled regime is thus observed.

References

[1] T. Rosen, J. Eller, J. Kang, N. Prasianakis, J. Mantzaras, F. N. Büchi, Saturation dependent effective transport properties of PEFC gas diffusion layers. J. Electrochem. Soc. 159, 9 F536 (2012).

[2] N.I. Prasianakis, T. Rosen, J. Kang, J. Eller, J. Mantzaras, F.N. Büchi, Simulation of 3D porous media flows with application to polymer electrolyte fuel cells, Commun. Comput. Phys. 13, 851-866, (2013).