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A novel Monte Carlo scheme for liquid water distribution in gas diffusion layers of PEFCs

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Abstract

We present a Monte Carlo-based technique to calculate the liquid water distribution in the porous media of polymer electrolyte membrane fuel cells. Here, we focus on the 2D simulation of the gas diffusion layer (GDL). At the pore scale level, intermolecular and surface forces, pore structure and pressure results in a complex interplay of liquid, solid and gas phases [2]. The ensemble Monte Carlo approach allows to capture the fundamental physical interactions in complex geometries. The simulation is carried out using tomographic data of the fiber structure of commercially available gas diffusion media and would serve as input for calculating macroscopic transport properties of the wet GDL.

Introduction

Macro-homogenous models of proton exchange membrane fuel cells enable the study of the complex interplay between operating conditions, materials response and cell performance, which is needed for the cell and stack optimization. However, input parameters to the macrohomogeneous models are needed to account for the micro-scale properties of the single components and interfaces. The water distribution in the GDL determines the transport properties of the gas components and heat, so micro-scale properties must be considered both under dry and wet conditions. Our aim is to calculate these effective transport properties based on the water distribution which we obtain with the Monte Carlo method

Workflow

- Cuts from 2D X-ray tomography data of a SGL25BA sample are used as porous domain.
- Voxel labelling involves graphite and PTFE (solid phase), air (gas phase) and water (liquid phase). The material properties parameters are set accordingly.
- During a Monte Carlo sweep, each water-occupied voxel is considered. For each water-occupied voxel its probability to move to a randomly chosen voxel is evaluated considering the surface energy difference between the voxels involved.
- The algorithm is constructed to minimize the contact surface free energy at the equilibrium and follow the mass conservation (canonical ensemble).

Model

- To model the wet GDL, a statistical mechanics-based model has been developed, with the aim to simulate the interaction of the liquid water with the porous structure at the voxel scale.
- The probability P^{acc} that a state with energy E_i is turned into one with energy E_j is given by:

$$P_{ij}^{acc} = \min\left\{1, \exp(-\beta(E_j - E_i))\right\}$$

where $\beta = \frac{1}{k_B T}$ is a temperature-dependent parameter.

- For each water voxel, the algorithm implemented proceeds as follows [1]:

1. Choose a direction to move to
2. Calculate $\Delta E = E_f - E_i$

- $\Delta E \le 0 \rightarrow$ state accepted
- $\Delta E > 0 \rightarrow$ generate a random number **u** in [0,1] and accept the state only if

$$u < \exp(-\Delta E / k_B T)$$

Results

- The overall energy of the system is a monotonically decreasing function of the iterations, converging to a stable configuration in about 3000 sweeps (Fig.1)

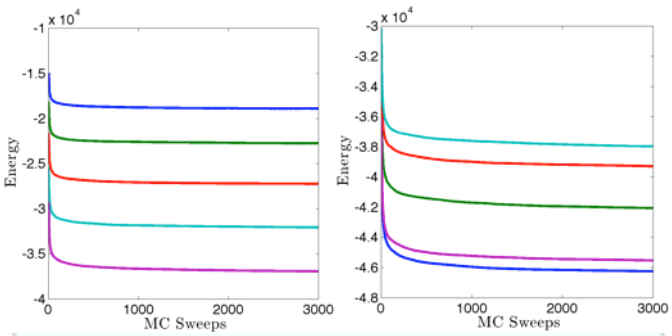

Fig. 1: Interfacial energy of the system as function of different sample size (left) and random cut sections (right) of the GDL. System sizes (in voxels) used in the left figure are: 120 (magenta), 140 (cyan), 160 (red), 180 (green), 200 (blue)

- Starting from a randomized water distribution, the algorithm evolves towards the minimal interfacial energy distribution, showing the typical water clustering patterns and menisci over the solid surfaces (Fig.2).

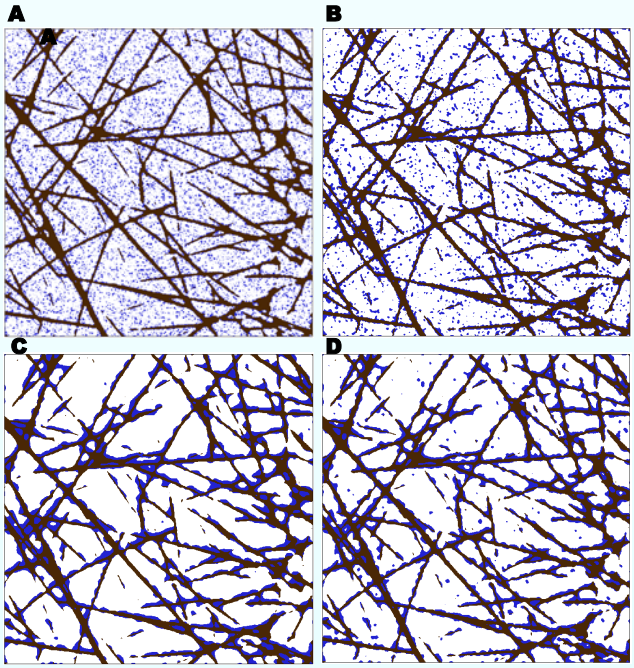

Fig. 2: Water distribution (blue) in a porous medium (brown is solid, white is air) after different simulation sweeps. The figure shows the distribution after 10 (A), 100,(B), 2000 (C) and 3000(D) sweeps respectively

Conclusion and outlooks

The simulation method presented is numerically efficient in determining the water distribution at equilibrium. Preliminary comparisons with experimental datasets of the water distribution are being carried out.
Further improvements of the model are ongoing: this includes the ability to capture evaporation and condensation phenomena, and the 3D (full and stacked) extension, switching to a full grand canonical statistical ensemble.

Acknowledgements

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References

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