A new open-source PEMFC simulation tool for easy assessment of material parameterizations

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Introduction

After almost three decades of PEM fuel cell modeling, there are only two open-source codes capable of simulating the state of the art in PEMFC modeling at the scale of single cells or MEAs:

- OpenFCST [1], a rather heavy FEM package consisting of more than 120 000 lines of C++ code (not counting library dependencies)
- FAST-FC [2], a finite volume tool built on top of OpenFOAM, consisting of about 12 000 lines of code (not counting the required OpenFOAM)

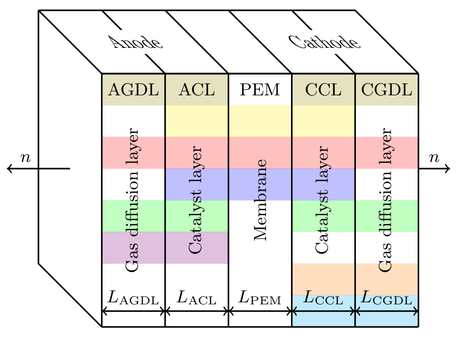
Albeit highly capable, these tools require significant effort and programming know-how to be set up and modified, and they are not well suited for quick substitution of material parameterizations.

We have recently developed the first open standalone implementation of a steady-state, non-isothermal two-phase MEA model for PEM fuel cells [3] to overcome these limitations. It implements the through-plane transport of charge, energy, gas species and water.

Here, we demonstrate how this new simulation tool may be used for easy assessment of experimental material parameterizations.

MEA Model

Overview of the 1D MEA model and governing equations (layer thicknesses not to scale):



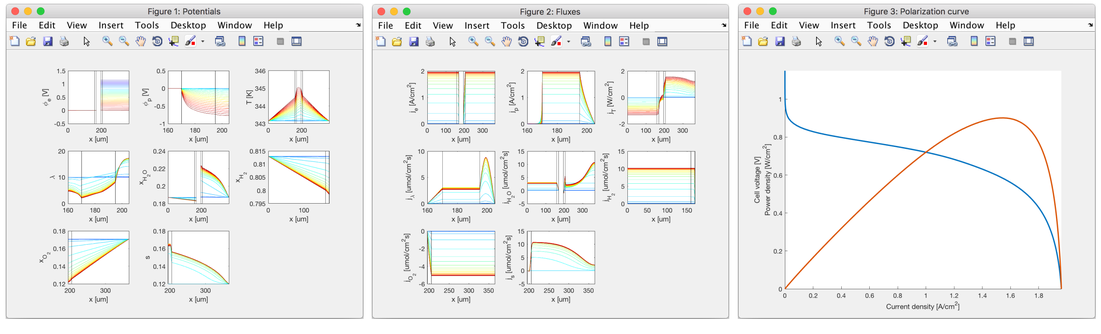
8 coupled PDEs:

- Electron transport
- Proton transport
- Heat conduction
- Dissolved water transport
- Water vapor diffusion
- Hydrogen diffusion
- Oxygen diffusion
- Liquid water transport

MATLAB Implementation: MMM1D

- Free open-source standalone MATLAB function
- Commented and easily readable code with less than 400 lines
- One-click PEMFC simulation with no programming know-how required
- All plots are generated automatically
- Material parameterizations can be substituted with a single line of code
- BSD 3-clause license for free commercial and non-commercial use
- Complete documentation submitted as paper to *Comput. Phys. Commun.* [3]
- Web app, free download and more info soon at `https://isomorph.ch`

Example simulation output at $T = 80\,°\mathrm{C}$, $P = 1.5\,\mathrm{bar}$, $\mathrm{RH} = 90\%$:



- Membrane: Nafion NR-211 (25 µm)
- Catalyst layer: Pt/C with 30 vol% Nafion (10 µm)
- GDL: Toray TGP-H-060 (190 µm)

Example 1: Electro-osmotic drag

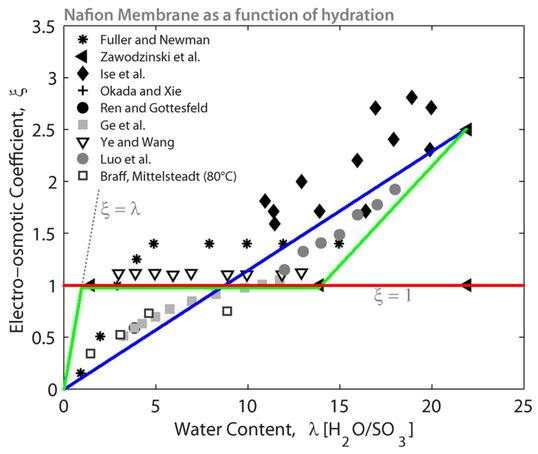


Fig. 1: Electro-osmotic drag coefficient in Nafion [4].

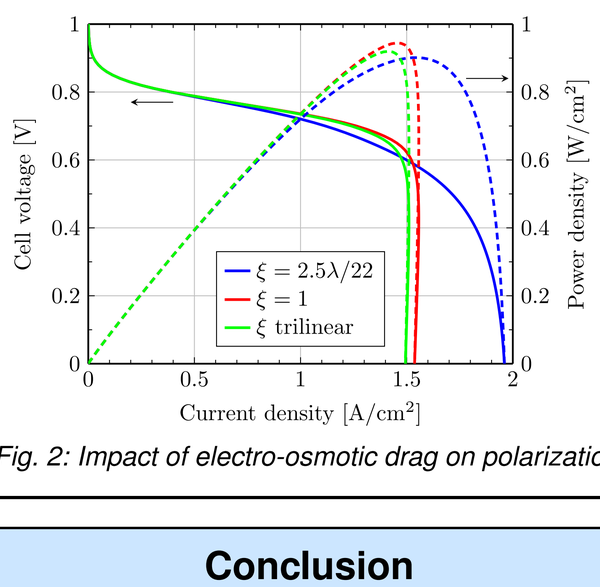


Fig. 2: Impact of electro-osmotic drag on polarization.

Example 2: Vapor sorption kinetics

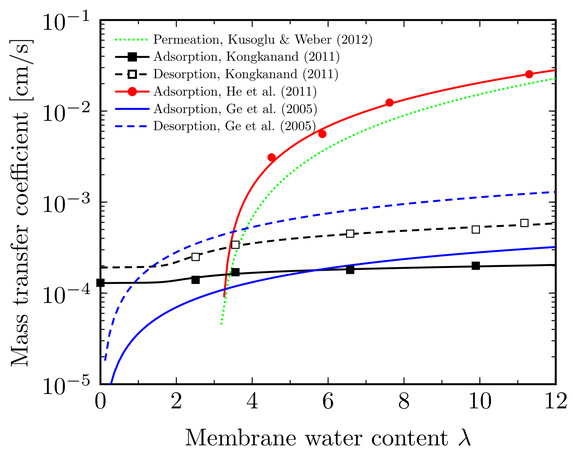


Fig. 3: Vapor sorption mass-transfer coefficients for Nafion.

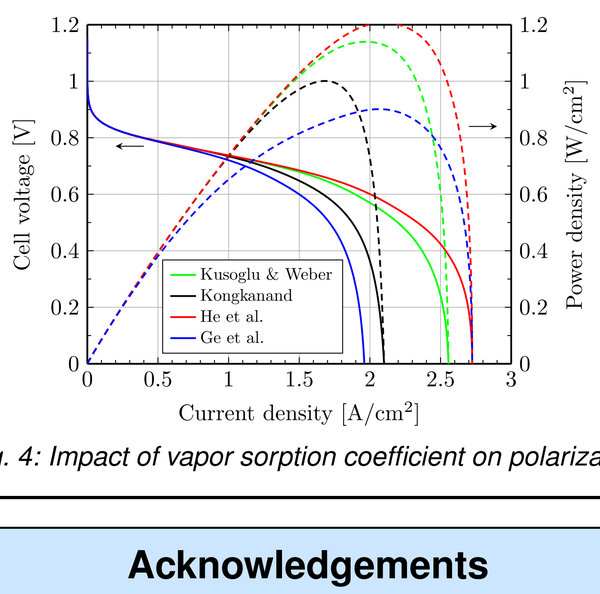


Fig. 4: Impact of vapor sorption coefficient on polarization.

Example 3: Water diffusivity

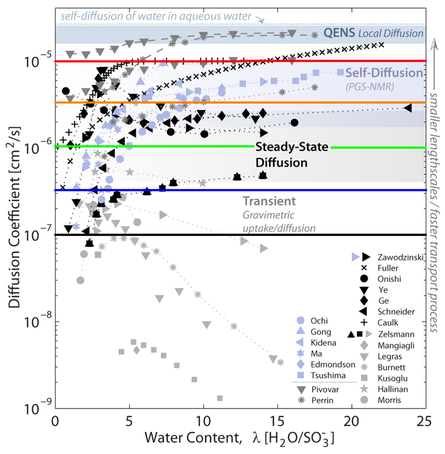


Fig. 5: Water diffusion coefficient in Nafion [4].

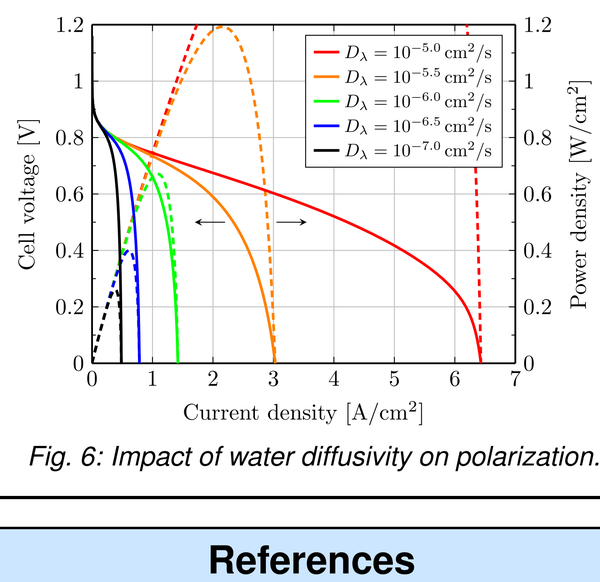


Fig. 6: Impact of water diffusivity on polarization.

Conclusion

With our new open-source tool MMM1D, extensive parameter studies and quick assessment of measurement data and material parameterizations are now possible in a matter of seconds, without requiring deep programming knowledge.

Acknowledgements

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