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Advancement of an OpenFOAM PEMFC toolbox and its validation on an automotive cell design

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Motivation

- Computational Fluid Dynamics (CFD) methods are commonly applied within the development process of fuel cell stacks
- Advanced models (including the relevant physico-chemical processes) can contribute to a deeper understanding of fundamental mechanism within PEM fuel cells
- Commercial CFD tool like ANSYS® Fluent offer such special PEMFC modules [1]
- PEMFC toolboxes for Open source CFD software OpenFOAM are also available, e.g. the openFuelCell project [2]
- Advantages of OpenFOAM:
  - ➢ Free availability based on the GNU General Public License
  - ➢ Unrestricted implementation of user defined code

Introduction

- OpenFOAM PEMFC toolbox of Kone et al. [3] is analyzed, modified and further developed (OpenFOAM v7)
- Validation of modified toolbox is done by experimental results
- Simulation results are compared to the PEMFC module of commercial CFD Software ANSYS® Fluent (2023R1)

OpenFOAM PEMFC Toolbox

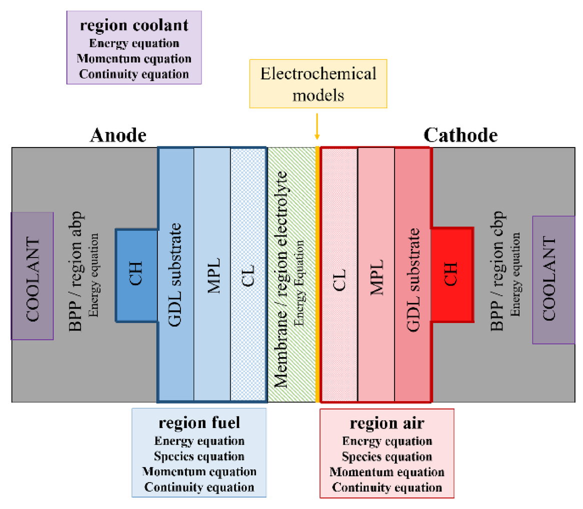

Figure 1: Schematic description of ZSW OpenFOAM toolbox

Assumptions of the electrochemical model

- Steady-state operating condition
- Gas flow: laminar and incompressible, ideal gas
- Fuel cell components: isotropic and homogeneous
- Electrochemical reaction is only modelled at cathode CL membrane interface (2D)

Modifications compared to initial Kone toolbox

- Code corrections, e.g. porous model
- Implementation of coolant channels and MPL properties
- More realistic membrane humidity: average of anode and cathode relative humidity instead fully humidified approach
- Implementation of anode activation overpotential
- Simplified Butler-Vollmer equation ($sinh$ approach, assumption: $\alpha_A = \alpha_C$) for modelling of activation overpotential
- Implementation of hydrogen crossover
- Implementation of additional standard OpenFOAM tools (e.g. fvOptions)

Comparison to ANSYS® FLUENT PEMFC Module

	ANSYS Fluent	OpenFAOM Kone et al.	OpenFOAM ZSW
Transport equation electric and protonic potential	3D	2D Simplified due to η_{ohm}	2D Simplified due to η_{ohm}
Membrane model Transport equation	3D (e-Drag, Diffusion)	Fully humidified	2D Simplified
Liquid phase model	x (simplified)	-	-
Electrochemical modelling	Butler-Volmer	Only Cathode, Tafel	Butler-Volmer (simplified)
Hydrogen Crossover	x	-	x
Multicomponent diffusion	x	x	x
Anisotropic material parameter	x	-	-
Coolant channel	x	-	x

Experimental and Simulation setup

- 300 cm² automotive design developed at ZSW, 5-cell short stack
- Spatially resolved current density measurement board included
- **Simulation**: Repeating unit of active area channels (1/50); symmetry boundary condition

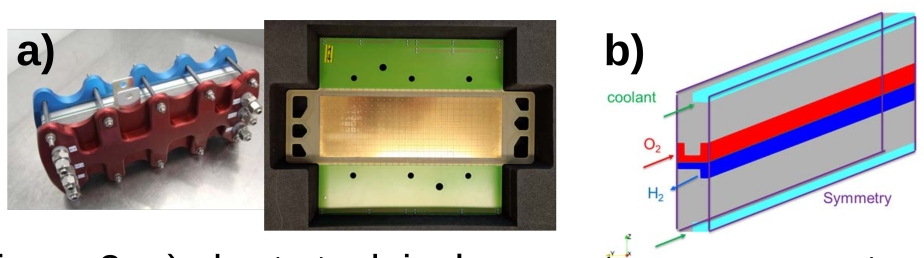

Figure 2: a) short stack incl. current measurement board and b) simulation model

- Automotive operating condition

	Cathode	Anode
Pressure Stack Outlet (bar_a)	2.0	2.2
Temperature Stack Inlet (°C)	73.0	73.0
Stoichiometry	1.6	1.6
Dew point temperature (°)	48.5	53.0
Gas composition	100% Air	30% N_2 / 70% H_2
Coolant Temperature Stack Inlet (°C)		68

Results

Polarization curve

- Simulation results show comparable results to measured curve
- Mass transport limitation not reflected accurately enough by both PEMFC models

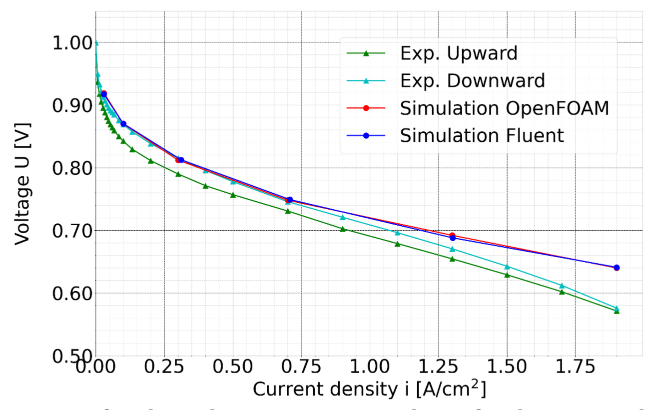

Figure 3: Polarisation curve, simulation and experiment (counter flow, sim. w.o. contact resistance)

Current density distribution

- Good reproduction of current density distribution at 1.9 A/cm² in simulation
- At 0.7 A/cm² increase of current density at cathode inlet not reproduced in simulation
  → Both models do not cover all relevant effects

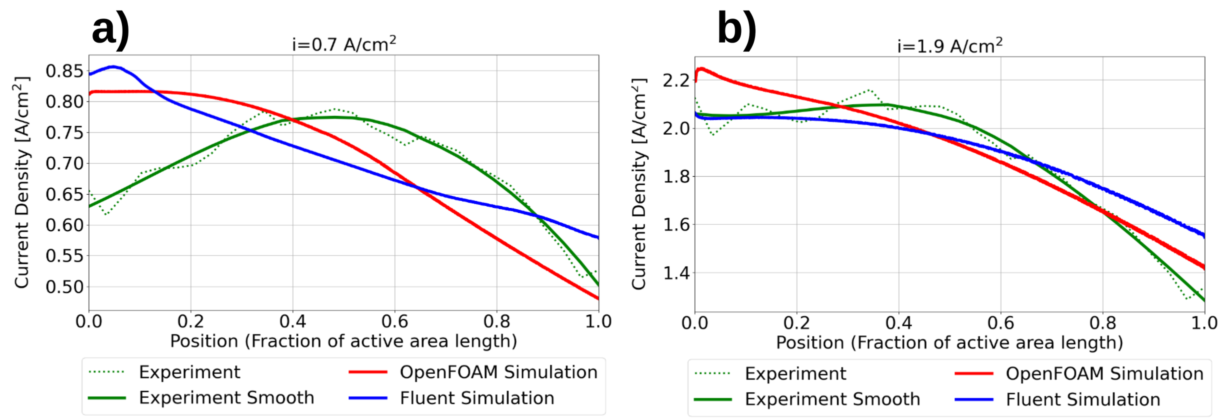

Figure 4: Current density curve along channel (average) at a) 0.7 A/cm² and b)1.9 A/cm²

Conclusion

- Compared to Kone toolbox ZSW toolbox shows improved current density calculation and usability; considering of coolant flowfield is possible
- Comparable results with regard to commercial PEMFC module of Fluent
- Good agreement of simulation data to experimental measured polarization curve
- Differences to experimental current density distribution visible in both PEMFC models
- Further improvements are planned in the future.

References

[1] ANSYS Fluent Theory Guide, www.ansys.com (2023)

[2] https://openfuelcell.sourceforge.io/project

[3] Kone, Jean-Paul ; Zhang, Xinyu ; Yan, Yuying ; Adegbite, Stephen: An Open-Source Toolbox for PEM Fuel Cell Simulation. In: Computation Bd. 6, MDPI AG (2018), Nr. 2, S. 3

Acknowledgements

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