# MULTI-SCALE MODELING OF PEM FUEL CELLS: FROM ELEMENTARY KINETICS TO THE SYSTEM

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## Introduction

The polymer electrolyte membrane fuel cell (PEMFC) is an outstanding example for a multi-scale system. This situation is shown schematically in Fig. 1. Electrochemical reactivity takes place on a nanometer scale and strongly depends on nano- and microstructural properties. Mass, charge and heat transport takes place from a micrometer up to meter scale at the system level. Time scales vary from sub-nanoseconds (electrochemical reactions) over seconds (transport) up to days or even months (structural and functional degradation). All process are strongly, and often nonlinearly, coupled over the various scales. Processes on the microscale can therefore dominantly influence macroscopic behavior. In order to understand these processes and their interaction, we apply a detailed multi-scale modeling and simulation approach.

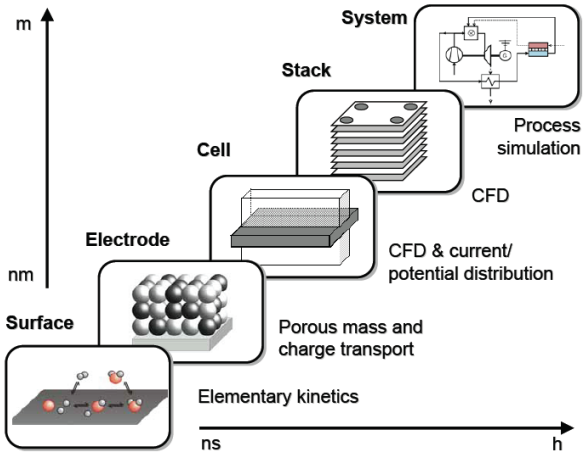


Fig. 1: Multi-scale modeling methodology

## Modeling and simulation methodology

Electrochemical reactivity on the surface scale is described using elementary kinetics within the mean field assumption. Continuum models are used for mass and charge transport in the porous catalyst and gas diffusion layers. The membrane model includes water transport and gas permeation. These models are coupled to a 2D cell-level description with channel gas transport. The cell-level model is included in a system-level description, where the fuel cell is coupled to blowers and humidifiers. All models are formulated in a fully transient way.

The simulation methodology is based on the coupling of the DLR in-house software DENIS [1] with MATLAB/SIMULINK. DENIS is a C code that implements the description of the surface, electrode and cell levels. It can be used as stand-alone code for steady-state polarization curves and transient impedance simulations [2]. For integration into system-level models, a SIMULINK S-function wrapper was developed, making the full functionality of the code available as SIMULINK model block. The simulations are furthermore compared to the CEA MEMEPHYS software package [3].

## Results and Discussion

The multi-scale methodology was applied to a Nafion-based PEMFC operated at 80°C. The surface/ electrode/cell-level model was validated against single-cell measurements of polarization curves and electrochemical impedance spectra (Fig. 2).

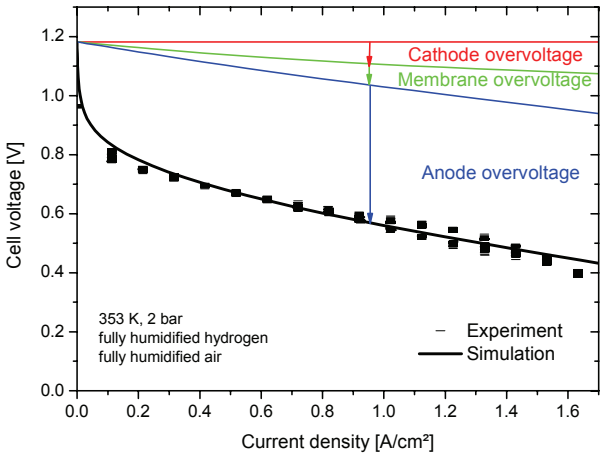


Fig. 2: Experimental and simulated polarization curves

## Conclusions

A multi-scale modeling and simulation methodology covers a full description of the surface, electrode, cell, and system levels. It is used to improve our understanding of the coupling over the various scales.

## References

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