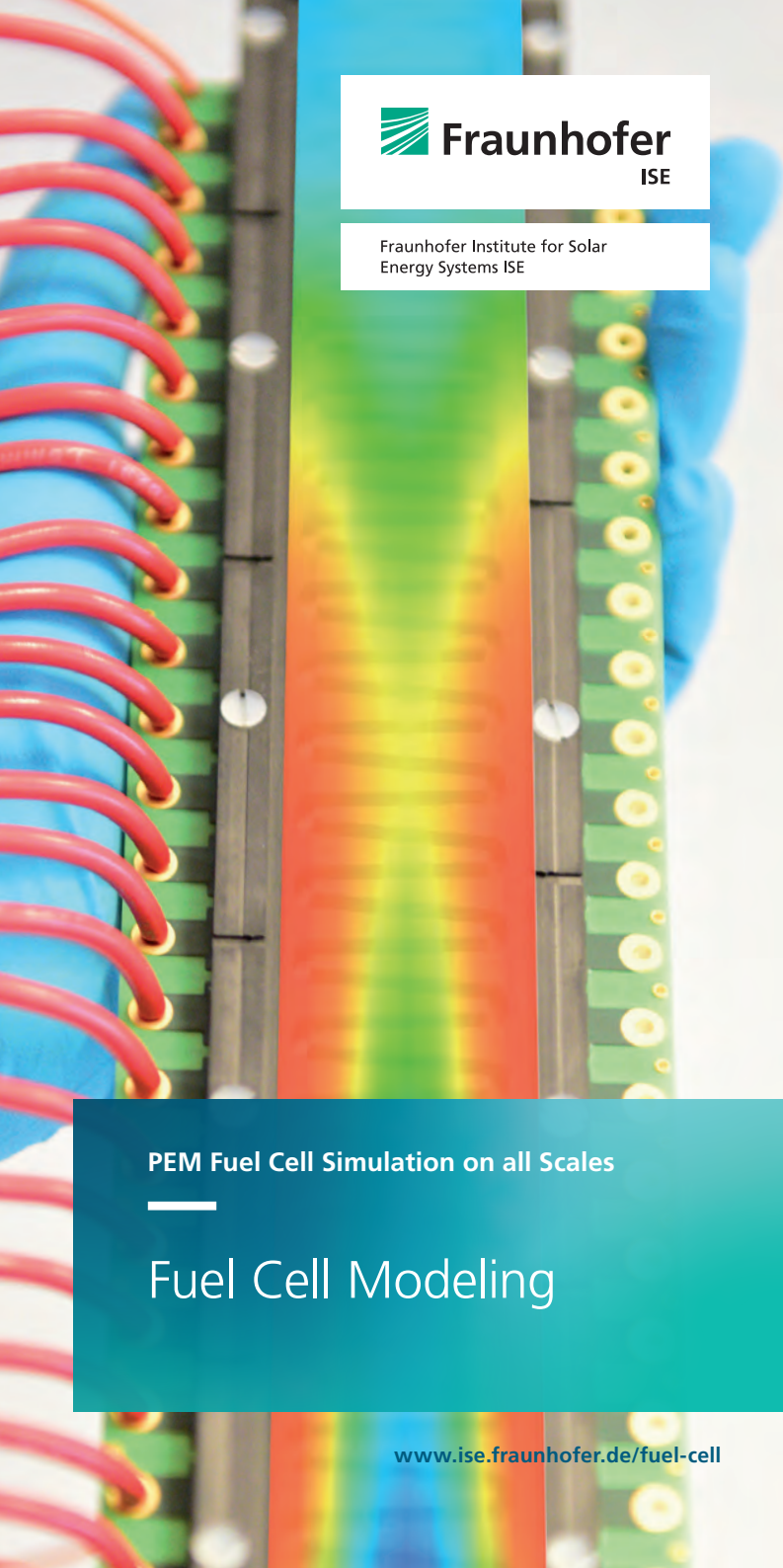


Fraunhofer ISE

Fraunhofer Institute for Solar Energy Systems ISE

PEM Fuel Cell Simulation on all Scales

Fuel Cell Modeling

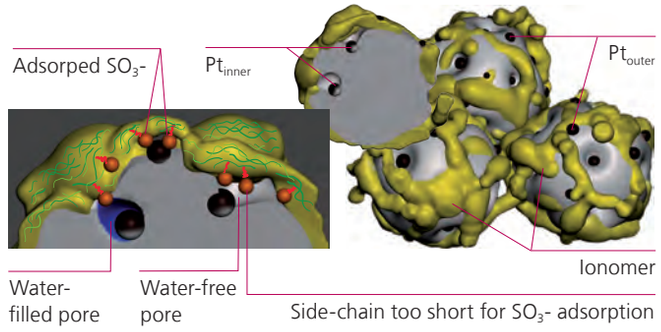
www.ise.fraunhofer.de/fuel-cell

Fuel Cell Modeling

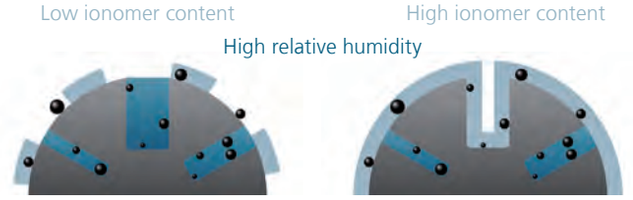
We model PEM fuel cells on all scales with commercial and self-developed codes from electrode structure to system level, from flow field design with CFD to address scientific questions. We place particular emphasis on the experimental validation of our models, which provide you with detailed insights into the physical effects during fuel cell operation, with regard to cell perfomance and aging behavior.

Our Offer

- modeling the impact of catalyst layer morphology on local performance and aging as a function of potential or load cycles and the materials used
- 3D computational fluid dynamics (CFD) and electrochemical simulation for the purpose of designing individual flow fields and cells
- machine learning modeling to predict cell performance based on production processes
- system modeling to optimize system efficiency
- investigation of the effects of different operating strategies



Modeling of ionomer poisoning as a function of the platinum position (Pt_{inner}/Pt_{outer}) on the porous carbon support.

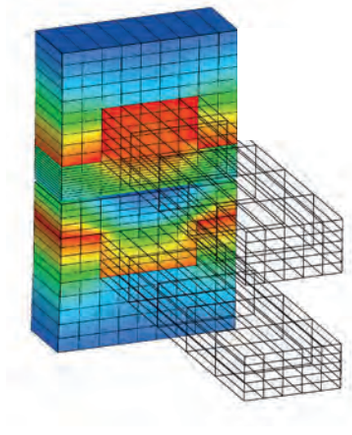


Electrode modeling: impact of platinum-ionomer distribution on a carbon particle on fuel cell performance at high relative humidity.

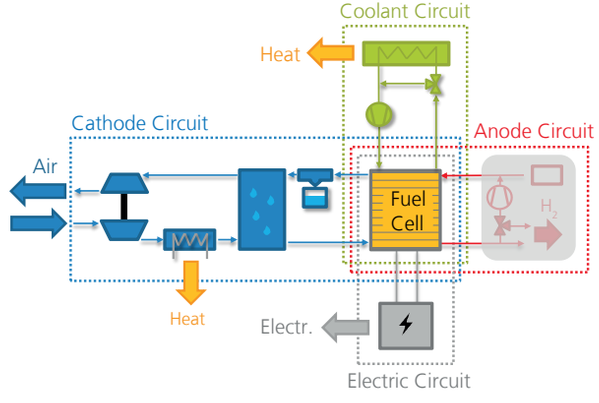
PEM Fuel Cell Simulation on all Scales

When modeling the PEM fuel cell, one must consider not only the dimensional aspect of the technology but also the various phenomena that take place. In our department, we use various modeling methods to shed light onto the various transport properties at the cell, the stack and the system level. We use state-of-the-art CFD models to perform spatially resolved steady-state simulations of the reaction and transport processes in the porous layers, along the channel and in the through-plane and in-plane directions, as well as to investigate the effects of operating conditions on fuel cell behavior. In addition to performance modeling, we simulate flow field variations, to support cell design development. The performance of the fuel cell model is validated with in-house measurement data.

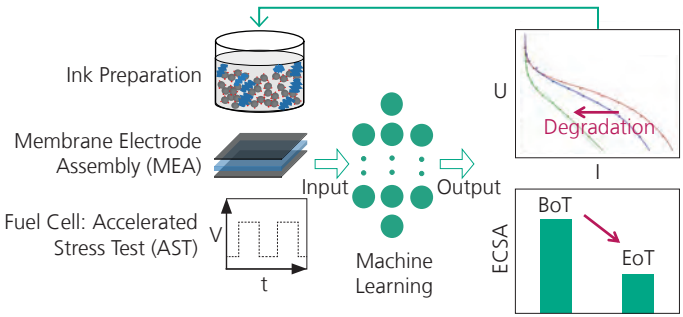
Using sophisticated morphology models, we reconstruct the effects of the catalyst layer structure to analyze the overall performance. The catalyst design begins with tailoring a single carbon particle, whose dimensions, specific surface area and internal meso-structure are meticulously adjustable. Platinum (Pt) particles are subsequently deposited onto this carbon support with careful consideration of the coalescing effect. Moreover, the distribution of Pt within the inner meso-pores can be finely controlled. The next step involves the aggregation of the catalyst, in which the cluster morphology can be modified by altering the inter-particle bonding forces. Upon integrating ionomers to form the catalyst layer, the design is evaluated for performance and transport resistance, as calculated by pore-scale modeling. Such models can be used to explain structural changes in the catalyst layer caused by degradation or variation of production parameters.



Simulated temperature distribution (bipolar plate) and humidity (gas channels) through a PEM fuel cell cross section.



Schematic overview of a PEM fuel cell system model.



A neural network model trained to forecast fuel cell performance over degradation, ink and MEA production properties and prior characterizations.

Our core competence in fuel cells lies in our understanding of the membrane electrode assembly (MEA) – the electrochemical heart of a fuel cell. We emphasize four perspectives in our research and development.

- A strong in-situ characterization with state-of-the-art electrochemical measurement techniques enables us to evaluate MEA behavior in fuel cell operation.
- Together with a broad range of ex-situ analytical equipment we can correlate MEA performance and degradation to its microstructure.
- With our industry-like MEA production processes we are able to design specific MEA architectures and use selected material compositions.
- Our modeling confirms our physical understanding of the MEA and allows for assessment of variations with regard to materials and operation mode.

Our gained knowledge helps our customers – fuel cell developers, integrators and suppliers – to identify and choose optimal fuel cell materials, geometries and operating conditions.

Further Information

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