Advanced Simulation Technologies

A3-FALCON: Advanced FC Analysis, Diagnostics and its Application

CFD Simulation

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Contents

Introduction

- **Working principle of a PEM fuel cell**
- Why detailed electrochemical 3D simulation?

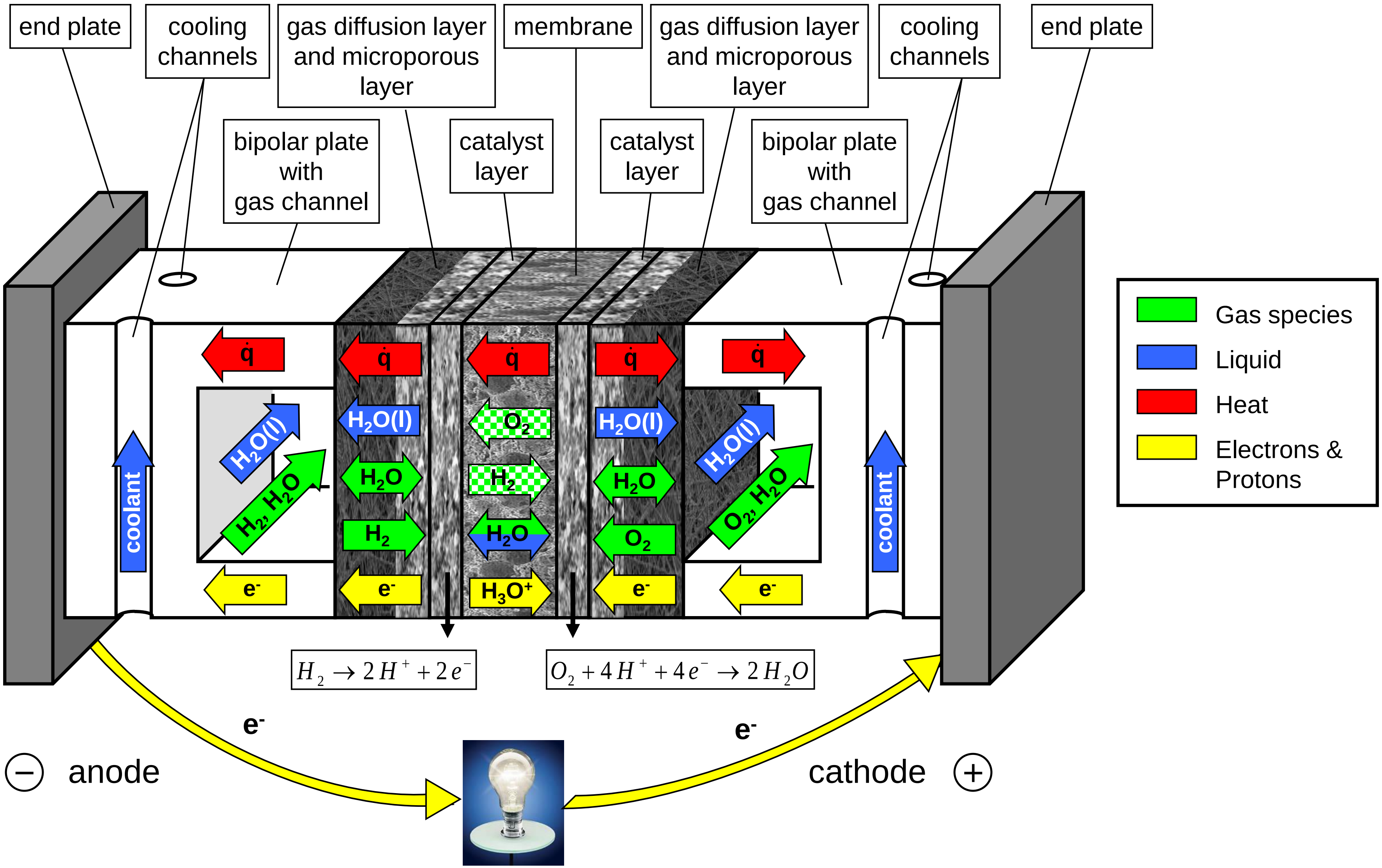
Overview of AVL FIRE Fuel Cell Module

Simulation of AC64-5 stack by IE and comparison to experimental data

- Healthy (new) stack
- Degraded (used) stack

Conclusions and outlook

Introduction – Working principle of a PEM fuel cell



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Introduction – Why detailed electrochemical 3D simulation?

Identification of critical locations

- E.g. hot spots, local water flooding, local fuel starvation

⇒ Optimization of geometry, e.g. layer thicknesses or channel dimensions and structure

Identification of critical operating conditions

- E.g. performance decrease if inlet gases too dry (membrane dries out) but also if they are too humid (water flooding)

⇒ Optimization of operating conditions, e.g. temperature, pressure, mass flow rates, relative humidity

Investigation of material parameters

- E.g. effect of the electrode‘s pore size on performance

⇒ Finding optimum compromise between material costs and performance

Conclusions to cell degradation and lifetime

Exploitation of 3D results for further analysis

- E.g. 3D temperature field calculated with FIRE used as input for stress analysis

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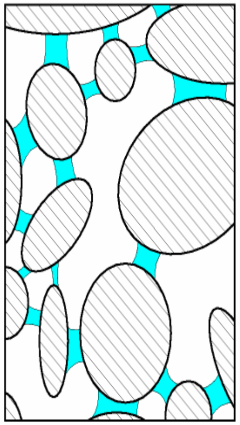
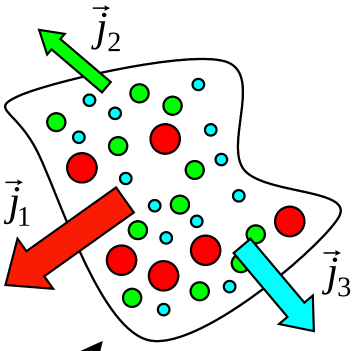
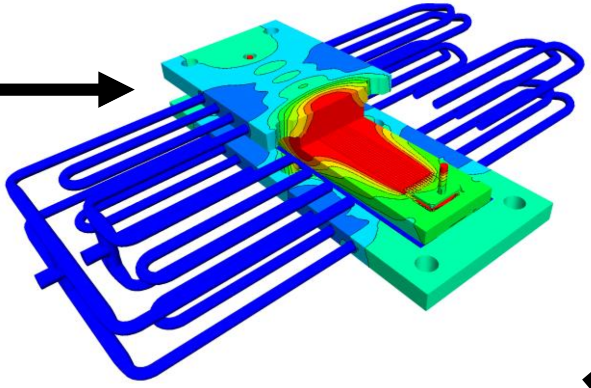
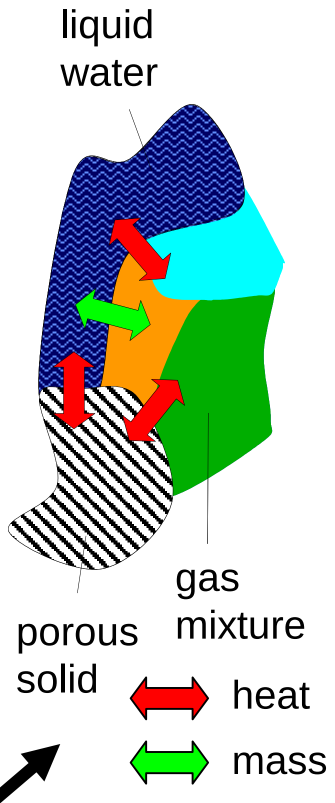
3D distributions of the following physical quantities are calculated

- Electronic potential in all electron conducting solids
- Ionic potential in all ion conducting solids / liquids (electrolyte)
- Velocity, pressure, and volume fraction of all liquids / gases
- Species mass fractions in all multicomponent gases
- Temperature in all thermally conducting solids / liquids / gases
- Water concentration in electrolyte
- Parasitic gas species concentrations in electrolyte









Underlying transport equations coupled via mass, heat, and charge source terms

Overview of AVL FIRE Fuel Cell Module

Degradation model developed in A3-FALCON by TU Graz

- Degradation of membrane, catalyst layer and GDL based on empirical and semi-empirical relations
- Following material and geometry parameters are modified dependent on temperature, pressure, humidity, voltage and operating time
  - Membrane thickness
  - Ionic conductivity
  - Sulfonic acid group concentration
  - Gas species diffusion coefficients in membrane
  - GDL thickness
  - Contact angle in GDL
  - Exchange current density in cathode catalyst layer
- Parameters adapted automatically during simulation; only user input: operating time & membrane type

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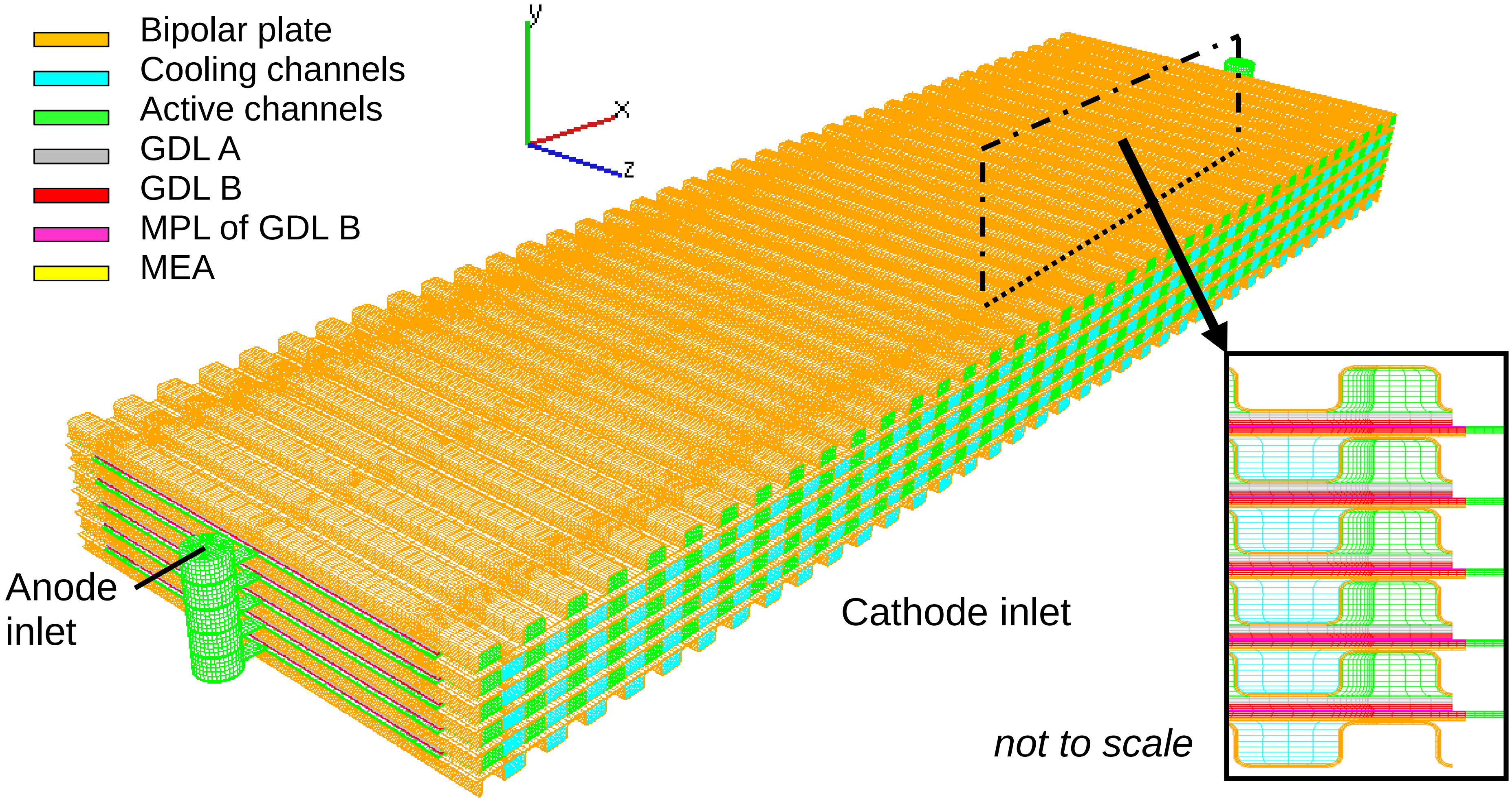
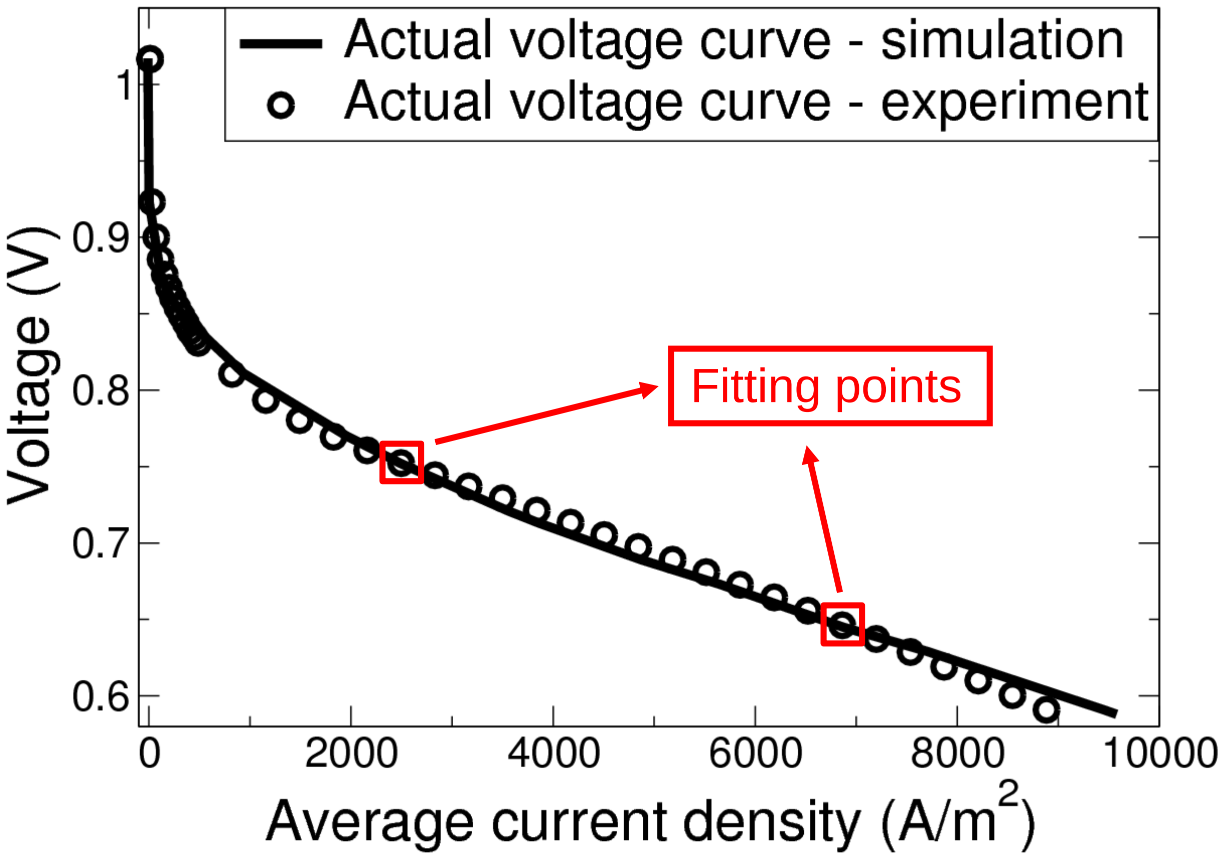
Simulation of AC64-5 stack – healthy (new) stack

Computational mesh of AC64-5 stack, 9.114.628 cells



Simulation of AC64-5 stack – healthy (new) stack

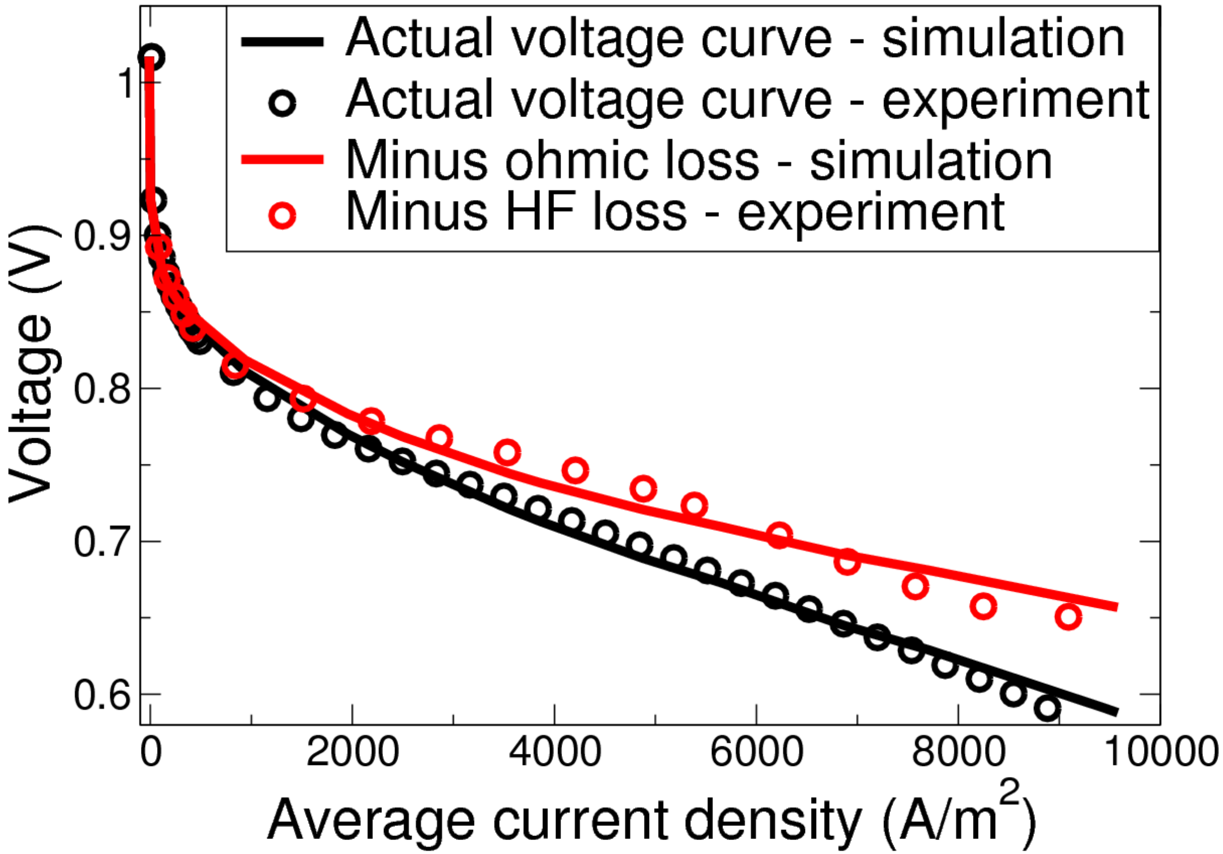
VI curve (simulation: single cell, measurement: 6-cell stack)



- Excellent fit, current density in low voltage range slightly overestimated

Simulation of AC64-5 stack – healthy (new) stack

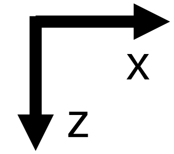
VI curve with ohmic potential loss



- Good agreement also in ohmic overpotential

Simulation of AC64-5 stack – healthy (new) stack

Current density (left) and temperature (right) in experiment and simulation



Experiment:

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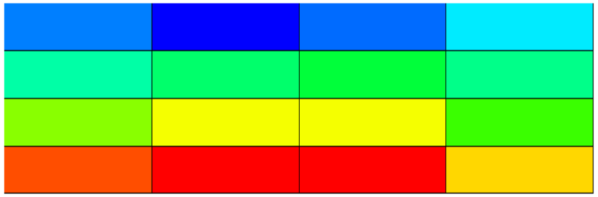

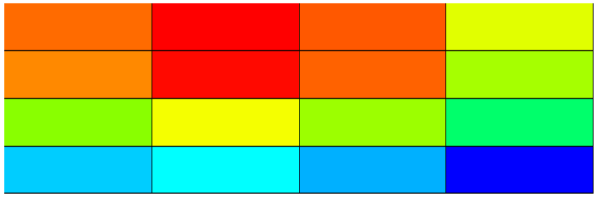

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Simulation (resolution of measurement plate):

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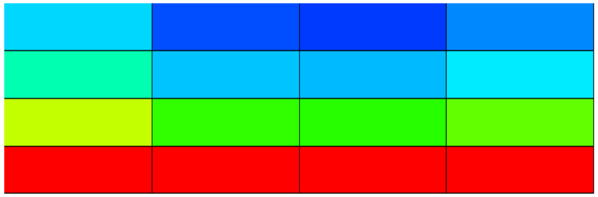

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Simulation (resolution of computational mesh):

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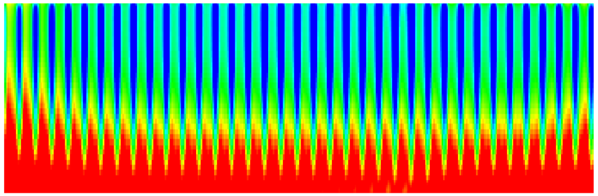

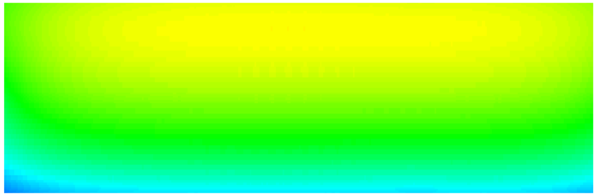

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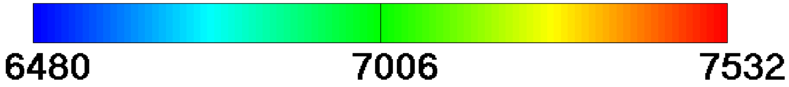
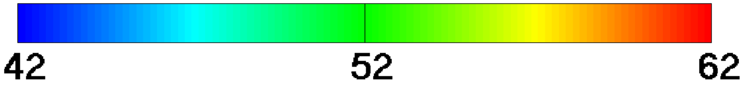
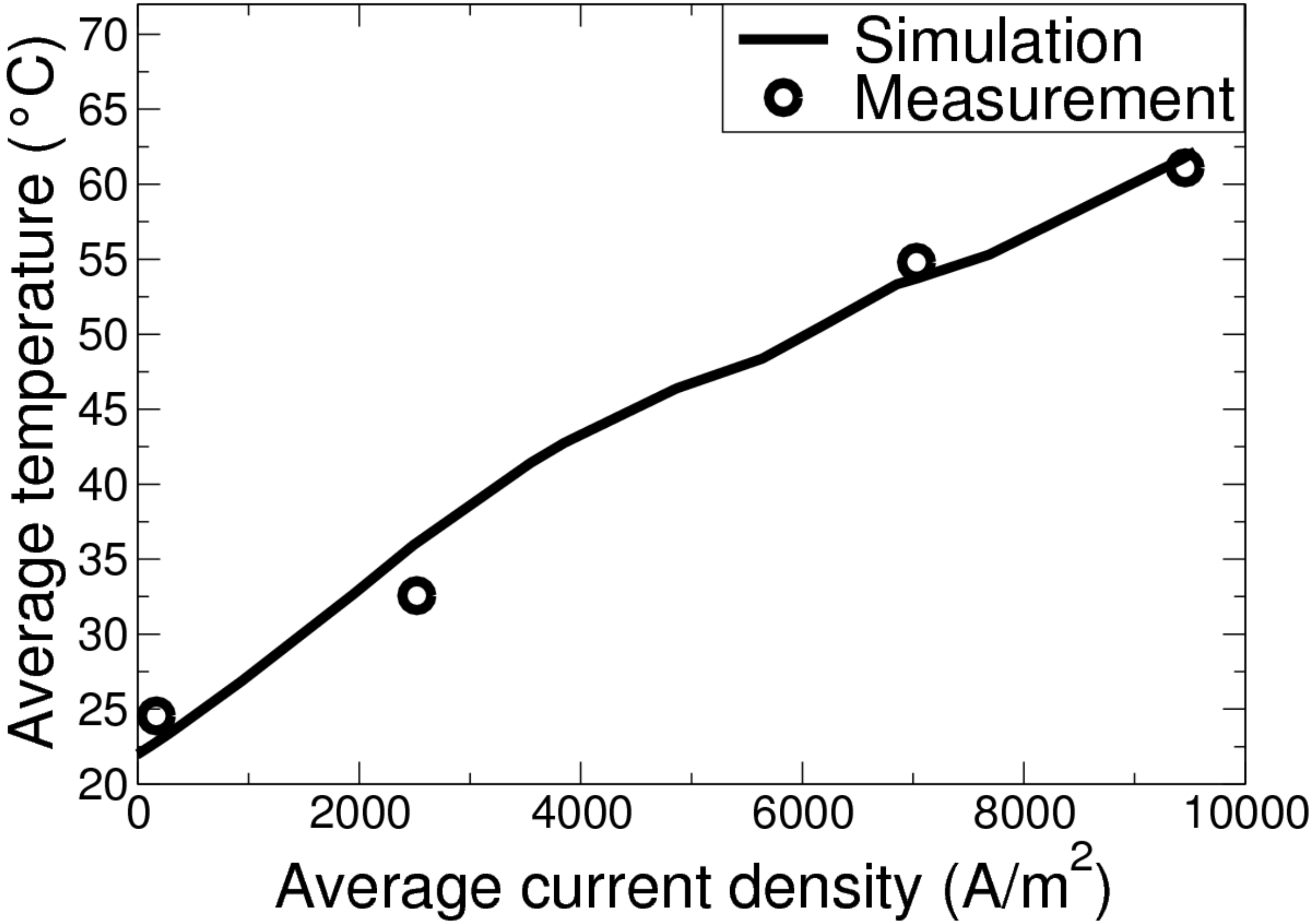




- Current density prediction very good, predicted temperature gradient too small

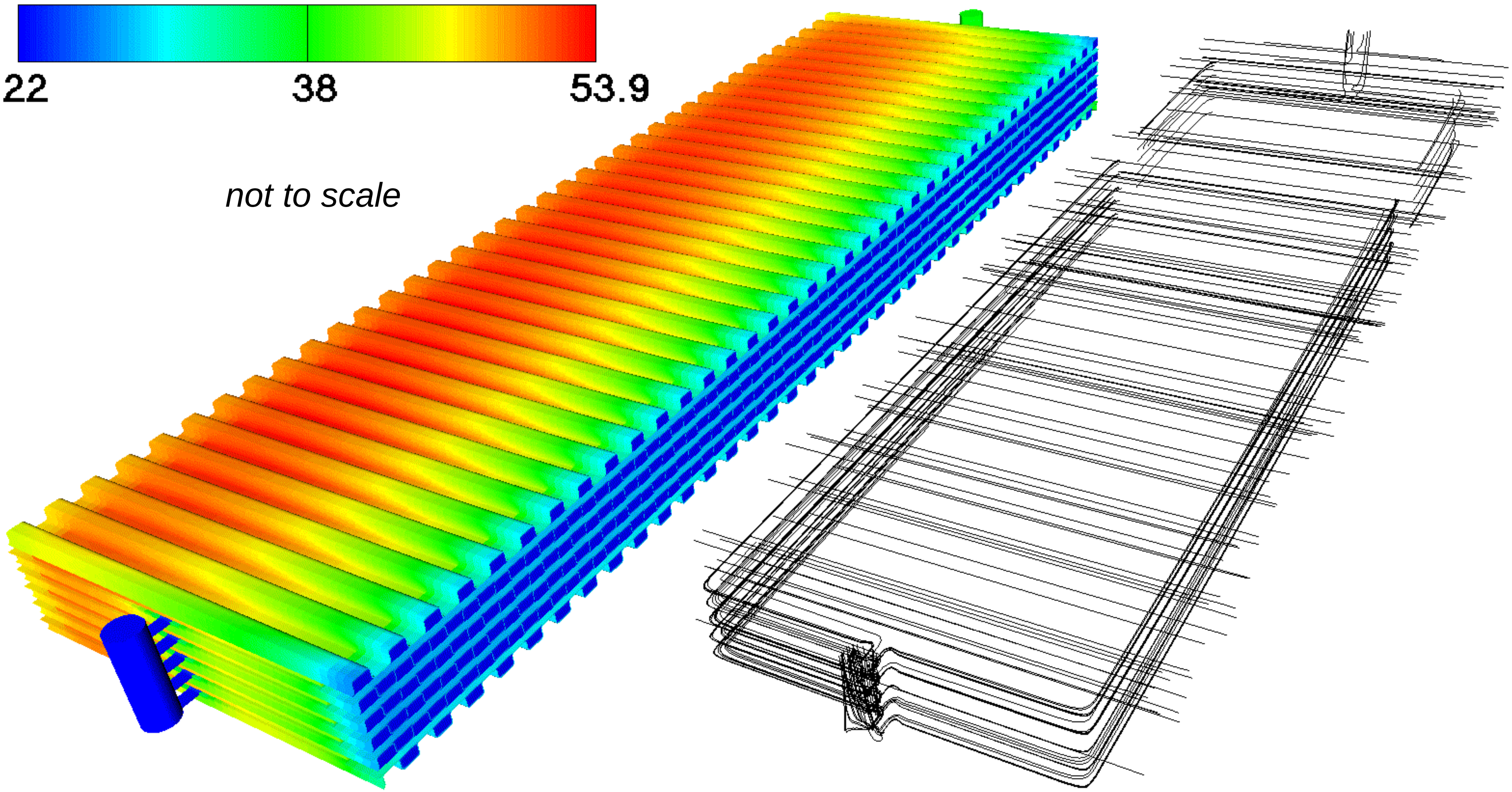
Simulation of AC64-5 stack – healthy (new) stack

Average temperature vs. average current density in reaction layer



Simulation of AC64-5 stack – healthy (new) stack

Temperature (°C) and streamlines of whole stack at 0.66 V



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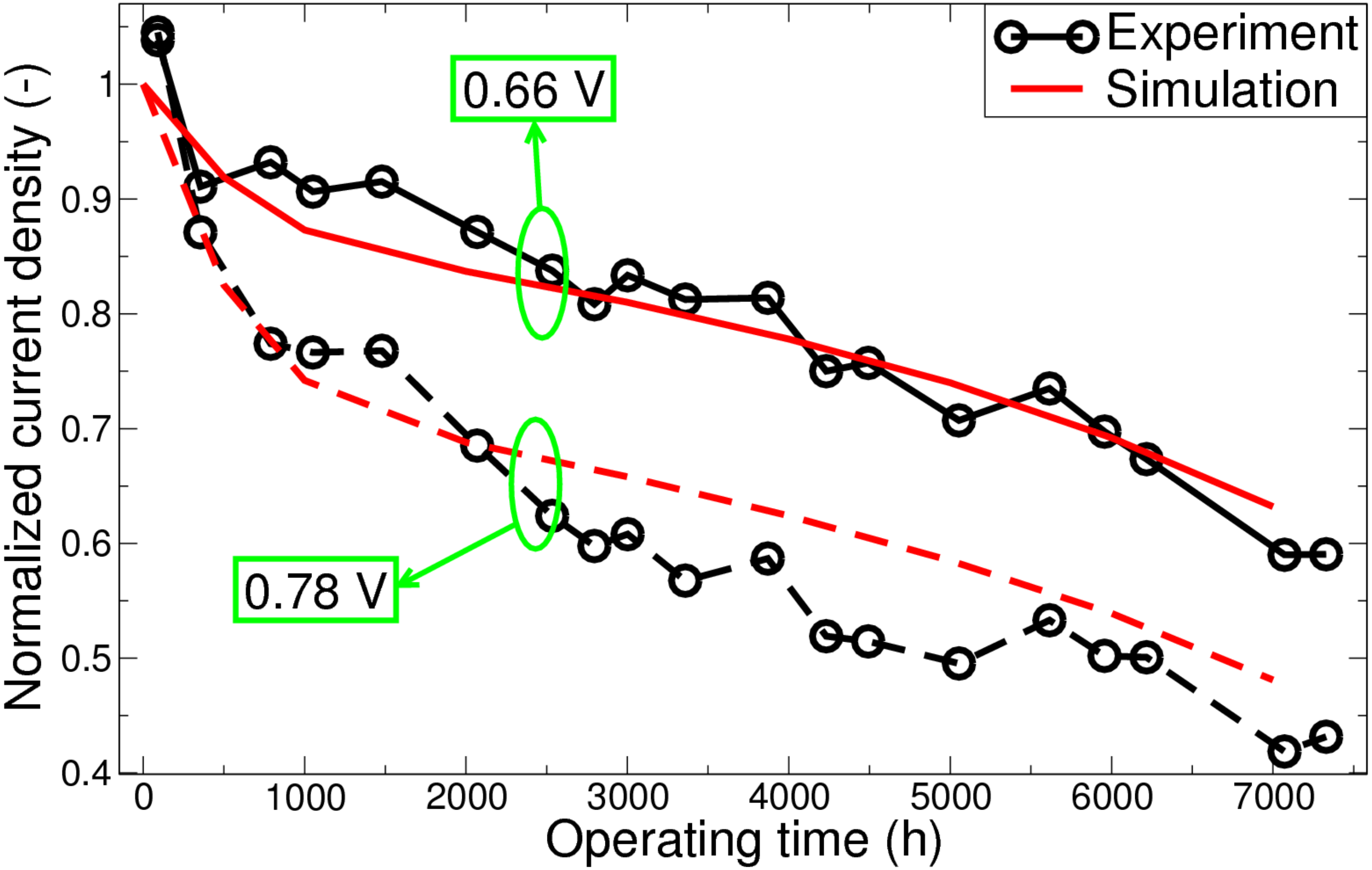
Simulation of AC64-5 stack – degraded (used) stack

Comparison between calculated and measured current density drop vs. operating time for two different cell voltages in AC64 stack



Simulation of AC64-5 stack – degraded (used) stack

Current density distribution (A/m^2) for various operating times at 0.66 V

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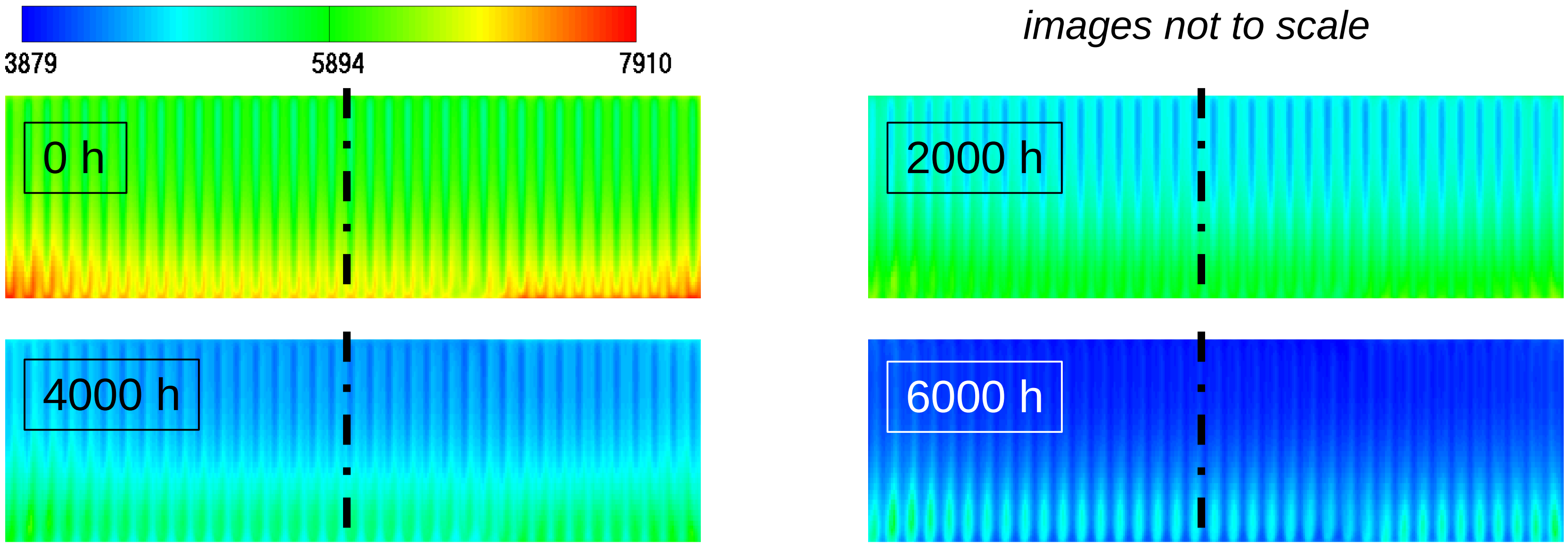

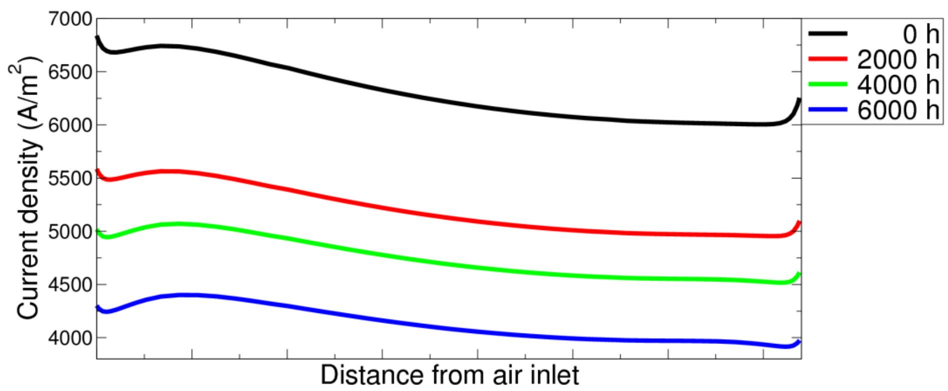

Simulation of AC64-5 stack – degraded (used) stack

Temperature distribution (°C) for various operating times at 0.66 V

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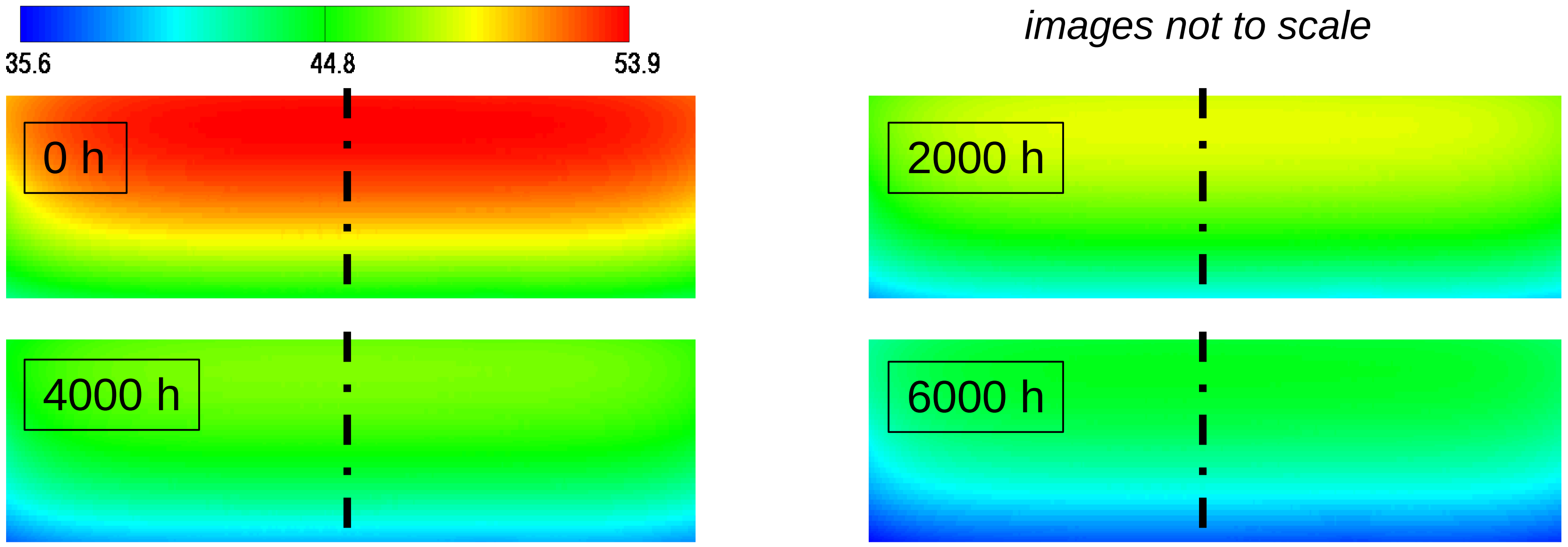

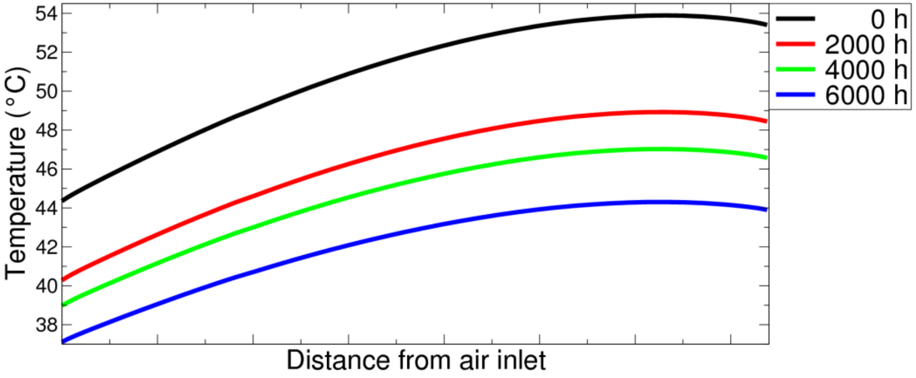

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- Excellent agreement between simulation and experiment in VI-curve, high frequency losses and average temperature
- Good agreement in current density distribution
- Predicted temperature gradient too small $\Rightarrow$ further investigations required
- Performance decrease with operating time is predicted with high accuracy

Outlook

- Extension of catalyst layer model from 0D to 3D
- Implementation of transient effects for PEM fuel cell simulation (load changes, dead end/purge mode)
- Chemically based degradation models for PEM fuel cells

Thank you for your attention!

"The research leading to these results has received funding from the Austrian Research Promotion Agency (FFG), Project A3-FALCON (Advanced 3D Fuel cell AnaLysis and CONdition diagnostics), No. 835811 ."