Fast and accurate:
Novel 2D/1D PEM fuel cell modelling

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The overall objective of the project is the analysis of PEM fuel cell degradation and the implementation of degradation models in AVL FIRE™

- In-Situ testing of fuel cells
- Analysis of local aging effects
- Analytical modeling of local aging effects
- Implementation of aging models in AVL FIRE™
- Validation using locally resolved measurement data

The tasks of the ZBT in the context of FC-DIAMOND

- In-Situ testing and aging of PEM fuel cells including locally resolved measurements
- Analysis of local aging effects
Why modelling for fuel cells?

Main reason for modelling is understanding!
- What happens inside of my black box
- If I treat my item different: How does it react?

Fuel cell modelling looks into different technology levels
- MEA / electrode structure
- Flow-field / cell level
- Stack level
- System level

Accuracy of modelling directly interrelates with
- Calculation time
- Effort to set up the model
- Effort to parametrize the model

The electrochemical model is based on the analytical model by A. Kulikovsky (2014)

\[
\frac{\partial j}{\partial x} = -2i_\ast \left( \frac{c}{c_{\text{ref}}} \right) \sinh \left( \frac{\eta}{b} \right)
\]

\[
j = -\sigma_i \frac{\partial \eta}{\partial x}
\]

\[
D \frac{\partial c}{\partial x} = \frac{j_0 - j}{4F}
\]


- Analytical solution of the differential equation system of the cathode catalyst layer considering catalyst layer thickness (in contrast to Butler-Volmer)
- The diffusion of the GDL of the cathode is solved with a linear approach
- The model was extended by a crossover and a membrane model

**Figure 1.** Schematic of the cathode catalyst layer and the shapes of proton \( j \) and electron \( j_e \) current densities, the local ORR overpotential \( \eta \) and oxygen concentration \( c \). Note that the proton current in membrane \( j_0 \) is the cell current and the total voltage loss in the system is \( \eta_0 \).
**PEM 1D-model: current voltage calculation**

**Model parameter**

- Most parameters are constant (physical) factors of the cell or the cell environment & operating condition.
- Four parameters of the Kulikovsky model as well as the crossover have to be calibrated to the individual cell materials.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Unit</th>
<th>Ex. Value</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{\text{cell}}$</td>
<td>measurable cell voltage</td>
<td>$V$</td>
<td>0 .. 1</td>
<td>result</td>
</tr>
<tr>
<td>$V_{\text{DC}}$</td>
<td>open circuit Voltage</td>
<td>$V$</td>
<td>1.23</td>
<td>common par</td>
</tr>
<tr>
<td>$R_{\Omega}$</td>
<td>ohmic resistance</td>
<td>$\Omega \text{ cm}^{-2}$</td>
<td>0.126</td>
<td>fit par</td>
</tr>
<tr>
<td>$j_0$</td>
<td>current density</td>
<td>$A \text{ cm}^{-2}$</td>
<td>0 .. 2</td>
<td>input</td>
</tr>
<tr>
<td>$b$</td>
<td>Tafel slope</td>
<td>$V$</td>
<td>0.03</td>
<td>common par</td>
</tr>
<tr>
<td>$i_*$</td>
<td>Volumetric exchange current density</td>
<td>$A \text{ cm}^{-3}$</td>
<td>0.817 $10^{-3}$</td>
<td>fit par</td>
</tr>
<tr>
<td>$\sigma_t$</td>
<td>CCL proton conductivity</td>
<td>$(\Omega \text{ cm})^{-1}$</td>
<td>0.03</td>
<td>common par</td>
</tr>
<tr>
<td>$c_h$</td>
<td>Oxygen concentration in the channel</td>
<td>mol $\text{ cm}^{-3}$</td>
<td>5.52 $10^{-6}$</td>
<td>operating condition</td>
</tr>
<tr>
<td>$c^*_h$</td>
<td>Oxygen concentration in the channel inlet</td>
<td>mol $\text{ cm}^{-3}$</td>
<td>7.36 $10^{-6}$</td>
<td>operating condition</td>
</tr>
<tr>
<td>$c_{\text{ref}}$</td>
<td>Reference oxygen concentration</td>
<td>mol $\text{ cm}^{-3}$</td>
<td>7.36 $10^{-6}$</td>
<td>par</td>
</tr>
<tr>
<td>$l_t$</td>
<td>Catalyst layer thickness</td>
<td>cm</td>
<td>0.001</td>
<td>common par</td>
</tr>
<tr>
<td>$l_b$</td>
<td>GDL thickness</td>
<td>cm</td>
<td>0.025</td>
<td>common par</td>
</tr>
<tr>
<td>$D$</td>
<td>Oxygen diffusion coefficient in the CCL</td>
<td>cm$^2$s$^{-1}$</td>
<td>1.36 $10^{-4}$</td>
<td>fit par</td>
</tr>
<tr>
<td>$D_b$</td>
<td>Oxygen diffusion coefficient in the GDL</td>
<td>cm$^2$s$^{-1}$</td>
<td>0.0259</td>
<td>fit par</td>
</tr>
</tbody>
</table>
The model parameters correlate with physical dependencies

- Volumetric exchange current density dominates low current operation
- Diffusion resistance of micro layer CCL already has influence at medium current
- Diffusion resistance of the GDL shows stronger influence on higher currents
- Ohmic resistance has linear influence

→ Accurate modelling possible
PEM 1D-model: current voltage calculation

degradation analysis – ECSA / catalyst aging

~ 3.000.000 calculated polarization curves
Intel i7 5820k 3,3 GHz \( \rightarrow \) \(~ 2 \text{ min total calc. time}

SoH02 / SoHMuSDaSS MEA
PtCo-catalyst gradient free operation in Baltic 25

Volumetric exchange current density and the electrochemical surface area (ECSA) mainly describe the same physical property of the catalyst layer
PEM 1D-model: current voltage calculation limitation

- Appropriate results for the model are verified
  - Gradient free operation
  - Small area cells
- Real life:
  - Complex flow fields / large areas
  - Anode / cathode humidity varies
  - Oxygen content reduces to the end
- Local conditions vary significantly
- Gradients along the channels have to be valued

→ Segmentation of the model

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2D-1D-model: cell modelling
symmetric segmentation of the cell

Bipolar plate
Cathode path
Anode path

18 segments
2D-1D-model: cell modelling model structure

- Within the active area basic macroscopic structures can be emulated
- Correlation of anode segments to cathode segments is described by tables (example: 1 – 17 / 2 – 18 / 3 – 15 / 4 – 16 / … / 18 – 2)
  → Emulation of different flow field setups and co-flow, counter-flow, meander-flow or double-U-flow fields is possible
- In every segment electrochemical calculation is made based on segment-state and input from neighbouring cells
- Electrochemical model based on 2014 Kulikovsky model
- Water transport calculation through the membrane based on osmotic drag and diffusion

\[^1\text{A Physically-Based Analytical Polarization Curve of a PEM Fuel Cell; A. A. Kulikovsky; Journal of The Electrochemical Society, 161 (3) F263-F270 (2014) }\]
2D-1D-model: cell modelling
water transport

2D physical – water transport through the membrane

- Models for electroosmotic drag and diffusive water transport included
- Different water concentrations for every segment along the channel
- Individual diffusive water transports for every segment

\[ \text{c}_{\text{H}_2\text{O}} = \text{saturation concentration} \]

\[ W_{\text{Prod}} = \text{produced water} \quad W_{\text{Osm}} = \text{osmotic drag} \quad W_{\text{Diff}} = \text{diffusion} \quad W_{M} = \text{net transport through the membrane} \]
2D-1D-model: validation
polarization curve / calibration

2D parametrization
- Cell average current & voltage as fitting goals

![Graph showing polarization curve with various markers for different components.]

- $U_{Mess}$
- $U_{Sim}$
- $U_{Act}$
- $U_{\Omega}$
- $U_{Diff,CCL}$
- $U_{Diff,GDL}$

$T_{FC}$: 65 [°C]
Pressure $C/A$: 1.3 / 1.5 [bar g]
Stoic $C/A$: 1.5 / 1.3
Rel humid $C/A$: 30 / 50 [%]
2D-1D-model: validation current density distribution

Model validation
- Single cell measurement including S++ segmented cell
- Model shows good conformity in all segments and for current variation

**Measurement**
- Single cell measurement including S++ segmented cell
- Model shows good conformity in all segments and for current variation

**Simulation**
- Avg. 2.00 [A cm\(^{-2}\)]
- Avg. 1.60 [A cm\(^{-2}\)]
- Avg. 1.20 [A cm\(^{-2}\)]
- Avg. 0.80 [A cm\(^{-2}\)]
- Avg. 0.40 [A cm\(^{-2}\)]
- Avg. 0.10 [A cm\(^{-2}\)]

Temperature: \(T_{CC} = 65 \, ^\circ\text{C}\)
Pressure: \(C / A: 1.3 / 1.5 \, \text{bar g}\)
Stoic C / A: 1.5 / 1.3
Relative humid C / A: 30 / 50 [%]
2D-1D-model: validation membrane resistance (HFR)

Model validation
- Even the high frequency resistance shows a good conformity for the whole polarization curve
- Differences identified to result from thermal contact resistances
Alignment with AVL FIRE™ simulation results
Computational mesh of ZBT cell (exploded view)

- Membrane
- Catalyst layer
- Gas diffusion layer
- Flow channels
- Segmented bipolar plate
- Segments
- Measurement plate
- Bipolar plate with cooling channels
- Cooling channels
- Collector plate
- End plate

27 million elements
Alignment with AVL FIRE™ simulation results validation: current density distribution

- Also good agreement with measurement data
- Deviations at the cathode inlet

3D results in mid-plane of membrane @ 1,4 A cm⁻²
Alignment with AVL FIRE™ simulation results validation: membrane water content

- Also good agreement with measurement data.

3D results in mid-plane of membrane @ 1.4 A cm⁻².

![Graph showing membrane water content with 3D visualization and measurement data comparison.]

- T_Fc: 65 [°C]
- Pressure C / A: 1.3 / 1.5 [bar g]
- Stoic C / A: 1.5 / 1.3
- Rel humid C / A: 30 / 50 [%]
2D-1D-model application: analysis of different flow fields / supply strategies

- It is possible to design and connect fuel cells in different ways
- Most base geometries can be emulated with the 2D-1D ZBT model
- The model can thus be used to analyze the influence of these geometries and flow paths on the performance and water management
- The following three designs have been analyzed

**co-flow**

**counter-flow**

**double-U-flow**
2D-1D-model: water management

- Similarities of water transports for co-flow and double-U-flow
- Counter-flow with great differences

$T_{ic} 66 \, ^\circ C$
$0,4 \, A \, cm^2$

cath: stoic 2.0, dry
anode: ≙ recirculation system

$\mathbf{W}_{\text{Prod}} = \text{produced water}$
$\mathbf{W}_{\text{Osm}} = \text{osmotic drag}$
$\mathbf{W}_{\text{Diff}} = \text{diffusion}$
$\mathbf{W}_{\text{M}} = \text{net transport through the membrane}$

calculated water transport within the fuel cell
2D-1D-model: water management

- Similarities of water transport for co-flow and double-U-flow
- Counter-flow with great differences

- Similarities of water concentrations for co-flow and double-U-flow
- Counter-flow with great differences

$T_{fc} 66^\circ C$
$0,4 A cm^2$

cath: stoic 2.0, dry
anode: $\triangle$ recirculation system

$W_{Prod}$ $W_{Osm}$ $W_{Diff}$ $W_M$

$W_{Prod}$ $W_{Osm}$ $W_{Diff}$ $W_M$

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$W_{Prod}$ $W_{Osm}$ $W_{Diff}$ $W_M$

$W_{Prod}$ $W_{Osm}$ $W_{Diff}$ $W_M$
2D-1D-model: water management

- Similarities of water transports for co-flow and double-U-flow
- Counter-flow with great differences

- Similarities of water concentrations for co-flow and double-U-flow
- Counter-flow with great differences
- The highest low-water concentration can be found in the double-U-flow

$T_{fc} \ 66 \, ^\circ C$
$0.4 \, A \cdot cm^{-2}$
cath: stoic 2.0, dry
anode: $\triangleq$ recirculation system

- $W_{Prod}$
- $W_{Osm}$
- $W_{Diff}$
- $W_M$

- $K_K$
- $K_E$
- $A_E$
- $A_K$
- $C_{sat}$

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2D-1D-model: comparison of the results

- Similarities for co-flow and double-U-flow
- Current density distribution for co-flow and double-U-flow more homogeneous
- Counter flow with significant differences and high peaks in the center region
2D-1D-model: comparison of the results

- Counter flow results in the highest performance
- Possibly the more homogeneous current density distribution and the higher “low humidity” results in lower degradation rates

![Polarization Curve](image1)

- co-flow
- counter-flow
- double-U-flow
2D-1D-model: conclusions

- Model with high accuracy regarding gradients along the flow field channels
- **Split second calculation time for every equilibrium state**
  - integration in system modelling
  - 2D resolution is essential for the system water management
- Capable for numerical degradation analysis
  - numerical calibration of model parameters is possible
  - adaption of model to degradation measurements
  - analysis of degradation possible through evaluation of model parameters
2D-1D-model: next steps

- Split second calculation time for every equilibrium state
  - integration in system modelling
  - 2D resolution is essential for the system water management

FVV-Project

“Fuel cell system simulation - Membrane humidification management “
→ optimization regarding runtime
→ expansion by dynamic behavior (e.g. thermal, membrane humidity)
→ expansion by stack behavior
2D-1D-model: next steps
Integration in Cruise-M Environment

FUEL CELL SYSTEM MODELLING

- TRANSMISSION SYSTEM
- ELECTRIC SYSTEM
- SUSPENSION SYSTEM
- STEERING SYSTEM
- AIR DELIVERY SYSTEM
- FUEL CELL STACK
- COOLING SYSTEM
- BRAKING SYSTEM
- FUEL DELIVERY SYSTEM
- HVAC SYSTEMS

AVL CRUISE™ M
2D-1D-model: next steps
Integration in Cruise-M Environment
2D-1D-model: next steps
Integration in Cruise-M Environment

FUEL CELL SYSTEM modelling
2D-1D-model: next steps
Integration in Cruise-M Environment

FUEL CELL SYSTEM modelling
2D-1D-model: next steps
Integration in Cruise-M Environment
Thank you for your attention!

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