Zentrum für BrennstoffzellenTechnik

Fluid Flow and Current Density Distribution in Large-Area HT PEMFCs

G. Bandlamudi, C. Siegel, C. Heßke, A. Heinzel

ZBT GmbH
Carl-Benz-Straße 201
47057 Duisburg
Germany

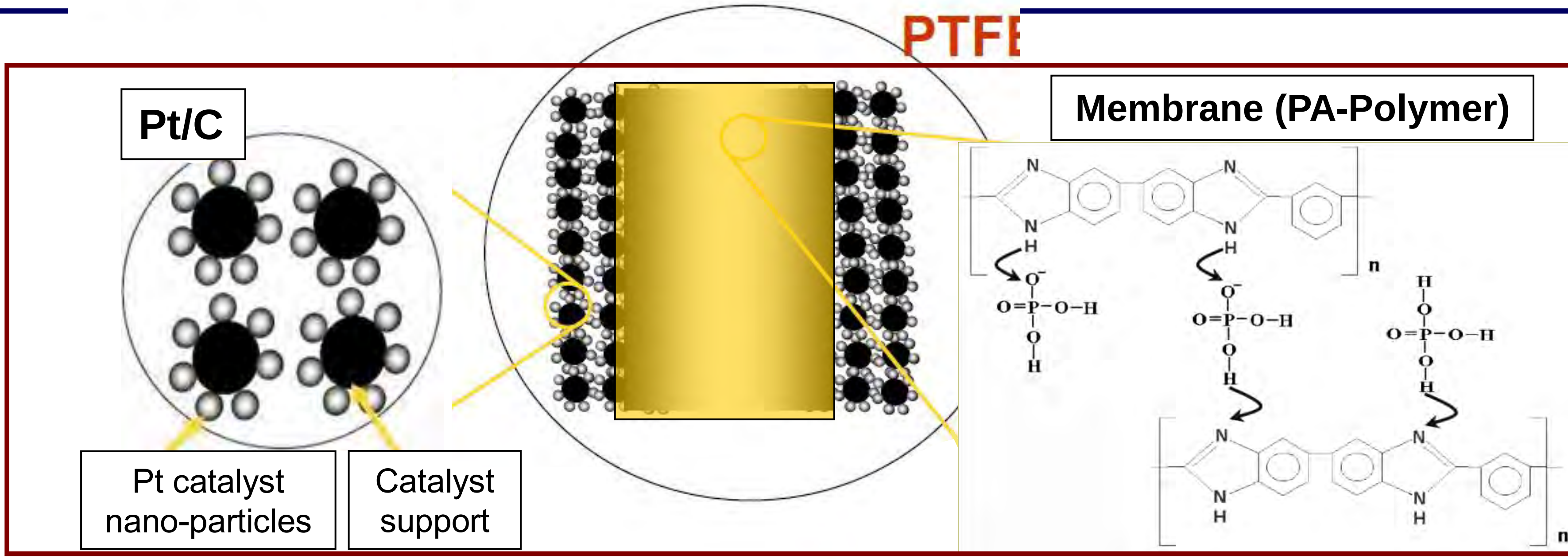
Telefon: +49-203-7598 1632
Telefax: +49-203-7598 2222
www.zbt-duisburg.de
g.bandlamudi@zbt-duisburg.de

SIEGEL SCHLEIMER
INGÉNIEURS-CONSEILS

Excerpt from the Proceedings of the 2011 COMSOL Conference in Stuttgart

Outline

1. Introduction to HT PEMFCs
2. Fluid flow and current density issues specific to HT PEMFCs
3. Approaches to studying large area fuel cells
4. Experimental investigations with large area HT PEMFCs
5. Modeling approach
6. Conclusions



bon particles

ii) Operational: Catalyst utilization, fuel/oxidant efficiency

ZBT

2. Performance limiting processes: Fluid Flow & Current Density

$$E_{OCV} = 1.166 - [2.4185E-04 + (1.1656E-07) * (T - 298.15)] * [T - 298.15] + [4.3084E-05 * T] * \ln \frac{[P_{H2}{}^{1}] * [P_{O2}{}^{0.5}]}{[P_{H2O}{}^{1}]}$$

•4 •4

$$\eta_{crossover} = \left[\frac{RT}{\alpha nF}\right]\left[\ln \frac{[i + i_{crossover}]}{[i_0]} - \ln \frac{[i]}{[i_0]}\right]$$

•3 •2

$$\eta_{ohmic} = iR$$

•2 •3

$$\eta_{fuel\ transport} = \left[\frac{RT}{nF}\right] \ln \left[1 - \frac{i}{i_L}\right]$$

•1 •1

$$\eta_{act} > 50mV$$

$$\eta_{act} = \left[\frac{RT}{\alpha nF}\right] \ln \frac{[i]}{[i_0]}$$

i_0 and α = kinetic parameters

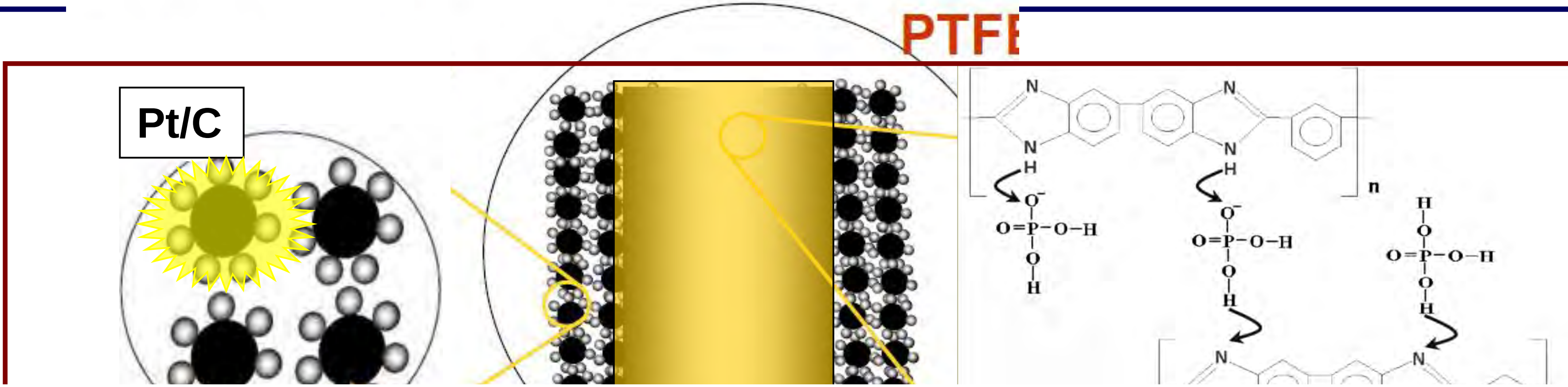
$$\eta_{act} < 10mV$$

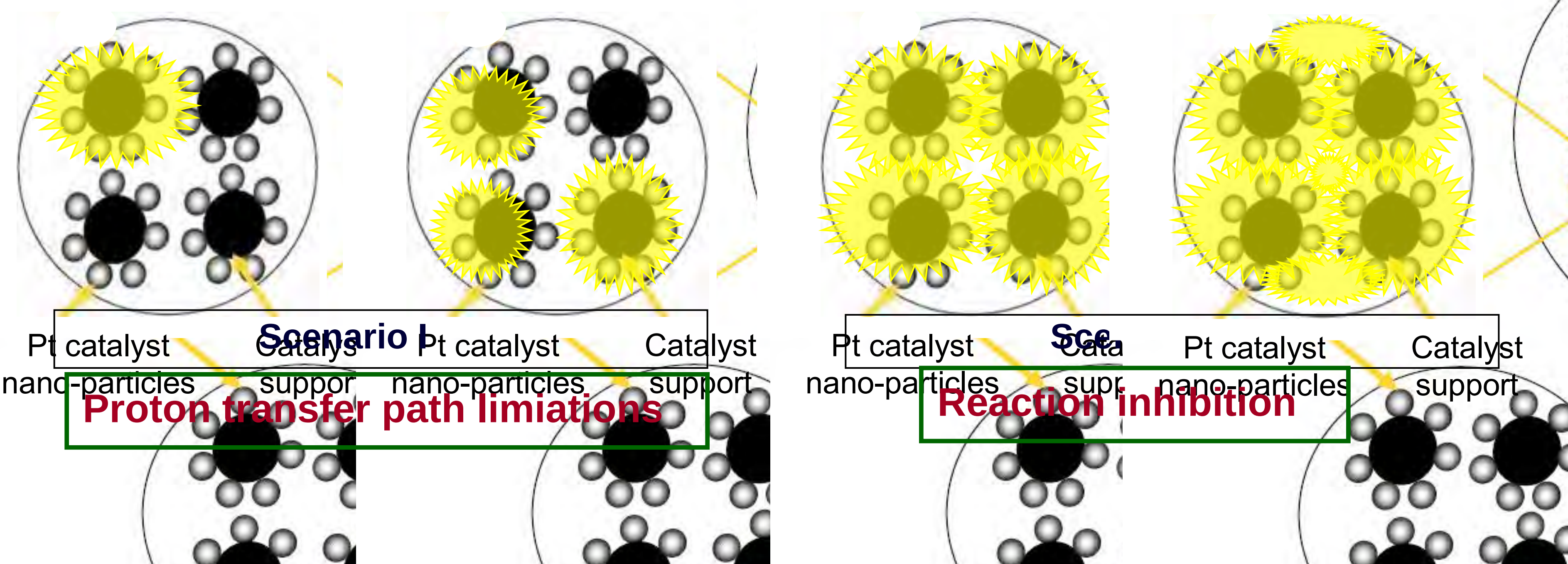
$$\eta_{act} = \left[\frac{RT}{\alpha nF}\right] \frac{[i]}{[i_0]}$$

R_{ct}

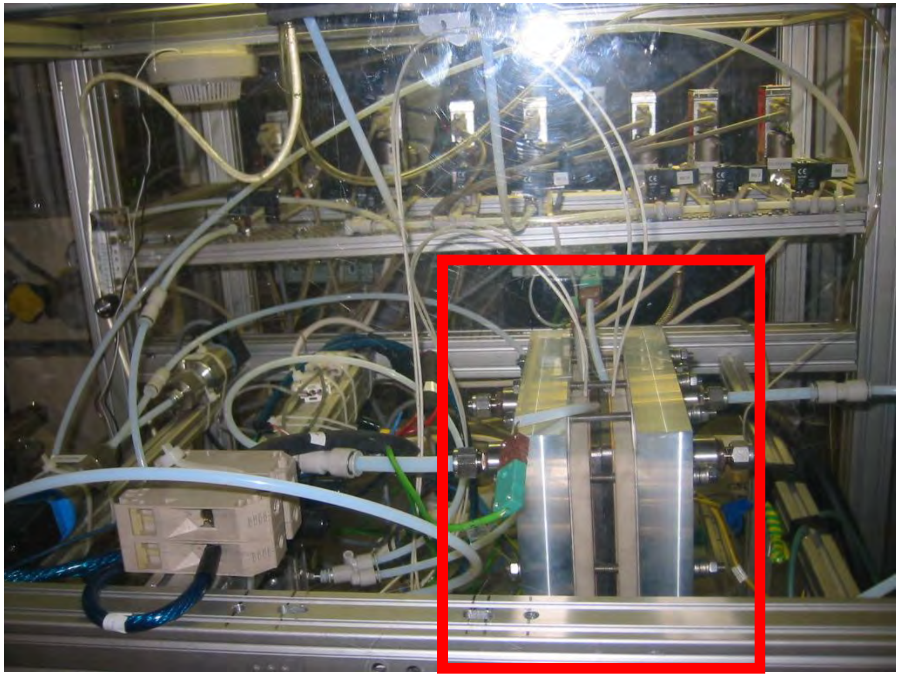
(AECD)

catalyst utilization



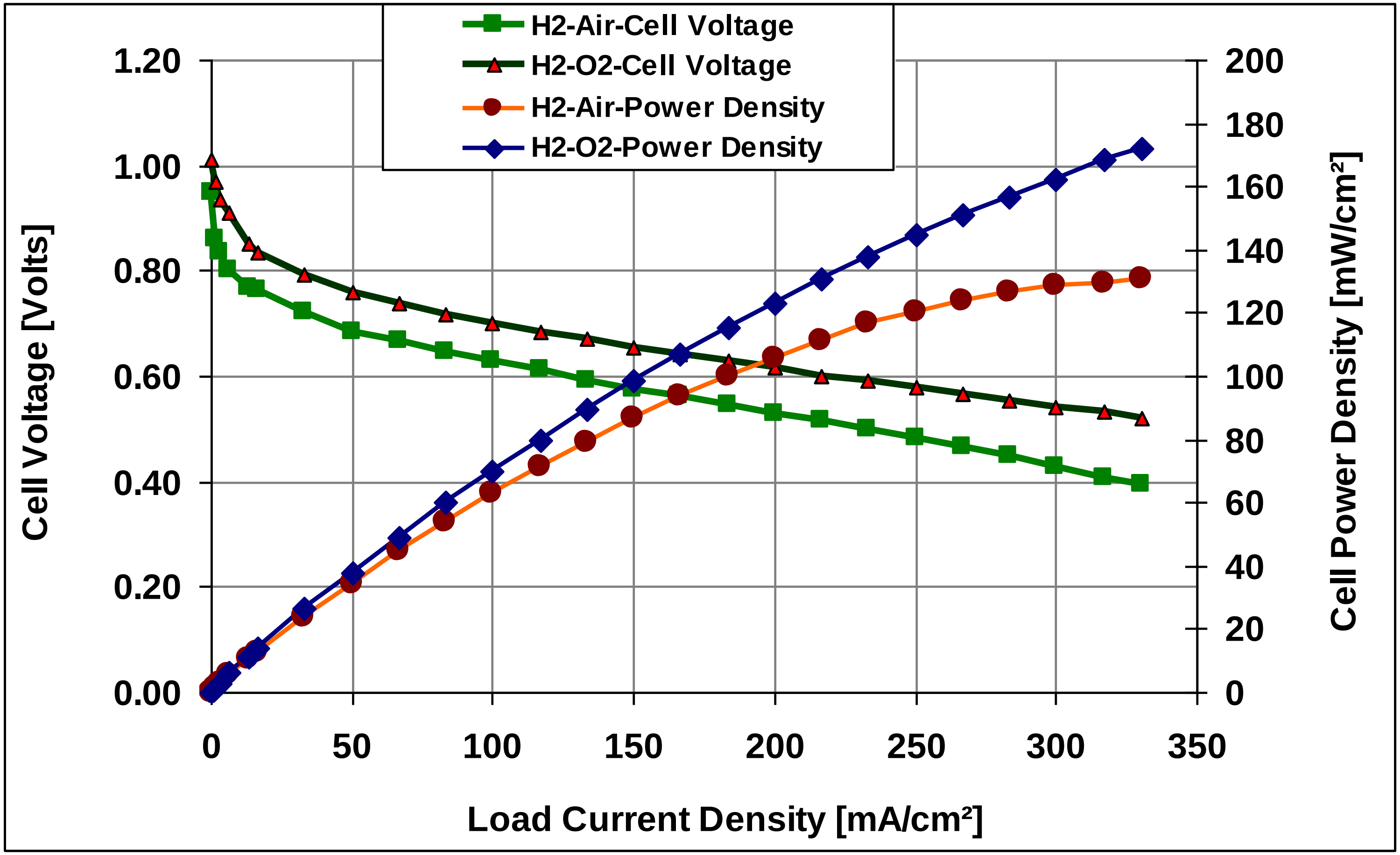


4. Large area HT PEMFC – Experimental investigations



- Cell‘s active area: 300 cm²
- Total geometrical area: 503 cm²
- BPHP: Graphite compound

HT PEMFC – current voltage curves



H_2/Air: 1.35/2.5; Temp.: 170°C

H_2/O_2: 1.35/2.5; Temp.: 170°C

- Pressure drop (Anode): 0.3 kPa
- Pressure drop (Cathode): 2.4 kPa

Large area HT PEMFC: Cell facts and performance loss break-up

• σ (Membrane)	= 0.08 S/cm
• Catalyst	= 1 mg/cm²
• σ (Flow field plate)	= 50 S/cm

• HFR (Cell)	= 423 mΩ·cm² (160°C)
	= 416 mΩ·cm² (180°C)
• Ohmic loss	= 140 mV (330 mA/cm²)
• Activation loss	= 206 mV
• Cell voltage	= 520 mV
• Fuel transport	= 146 mV

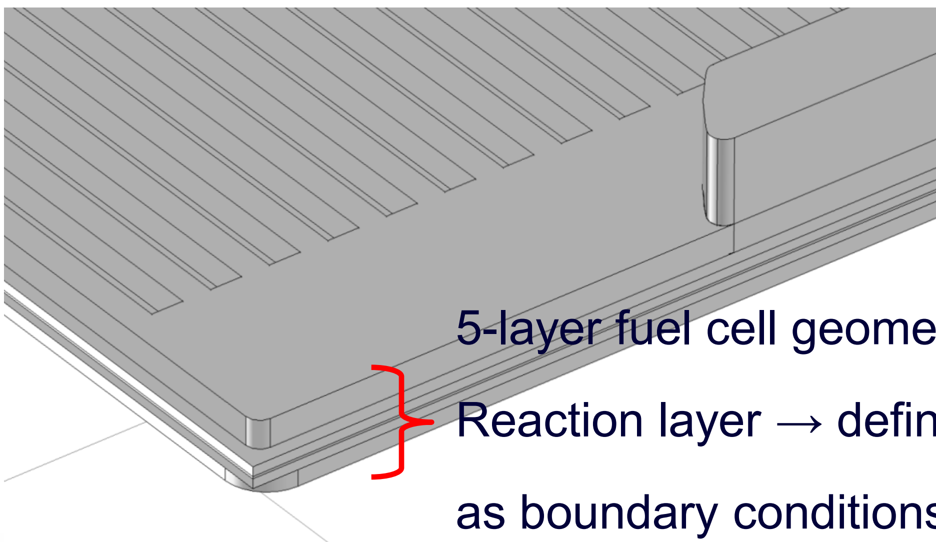
5. Modeling approach: 3D computational geometry

2D geometry in x-y-plane (CAD file) →

extrude in z-direction (3D) geometry

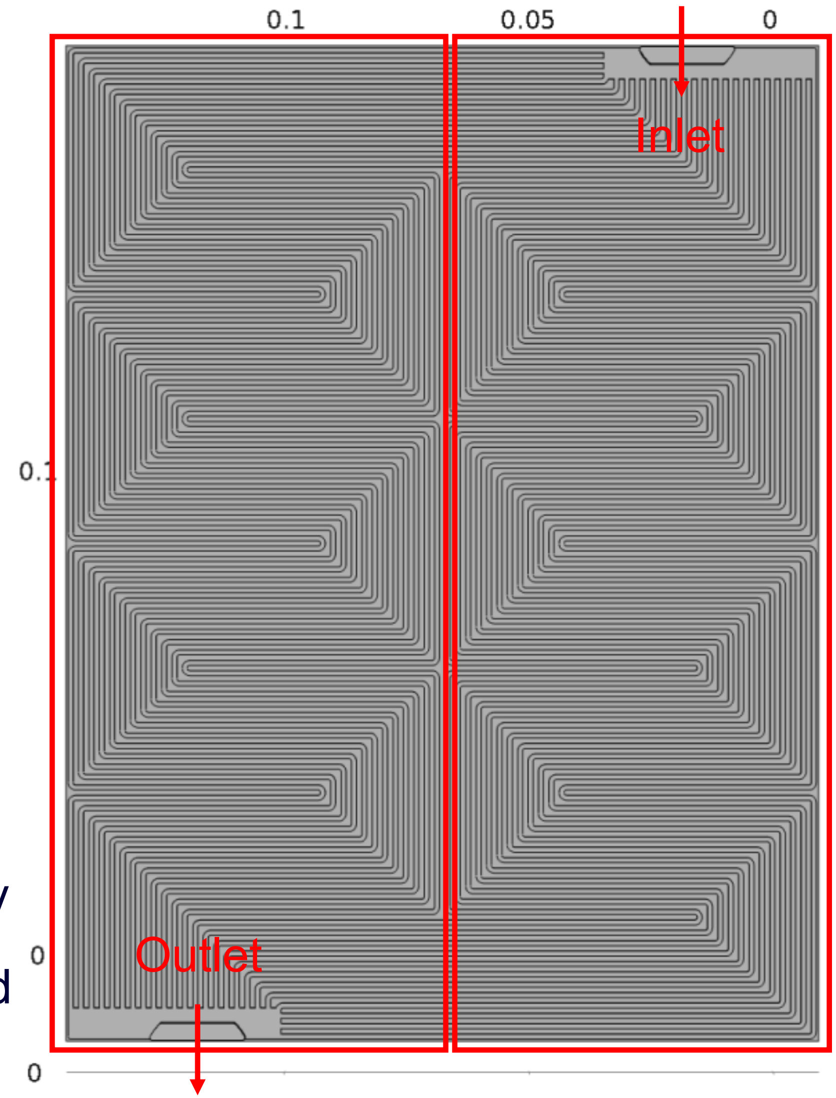
24 channel parallel serpentine flow field

→ (two 'blocks')



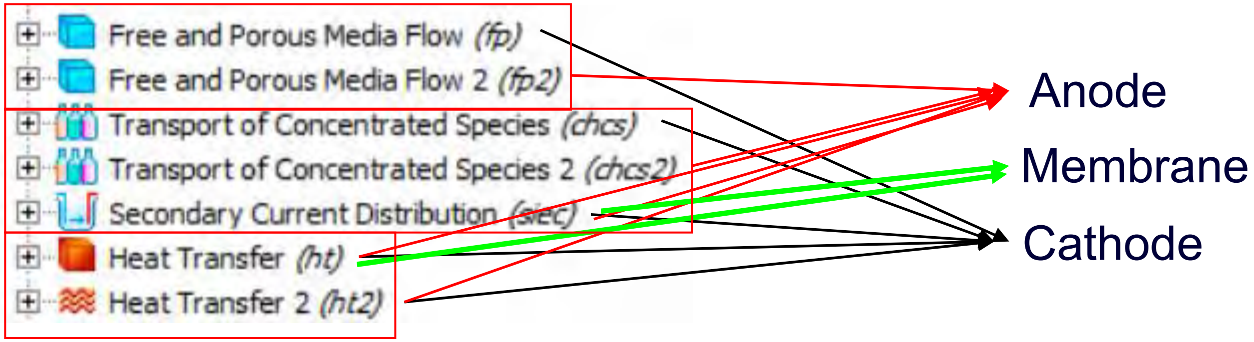
5-layer fuel cell geometry

Reaction layer → defined as boundary conditions



The governing equations*

Application modes in the ‘batteries and fuel cells module’ (V4.2.0.187)



Boundary conditions according to experimental set-up

Initial conditions generated with several ‘dummy’ simulations

Number of degrees of freedom: ca. 20 million (19,692,625)

→ Highly coupled system to be solved together with boundary and initial conditions

*see: Siegel, C., Bandlamudi, G., Heinzel, A, A Systematic Characterization of a PBI/H3PO4 Sol-Gel Membrane – Modeling and Simulation, *J. Power Sources*, **196**, 2735-2749 (2010)

The computational mesh

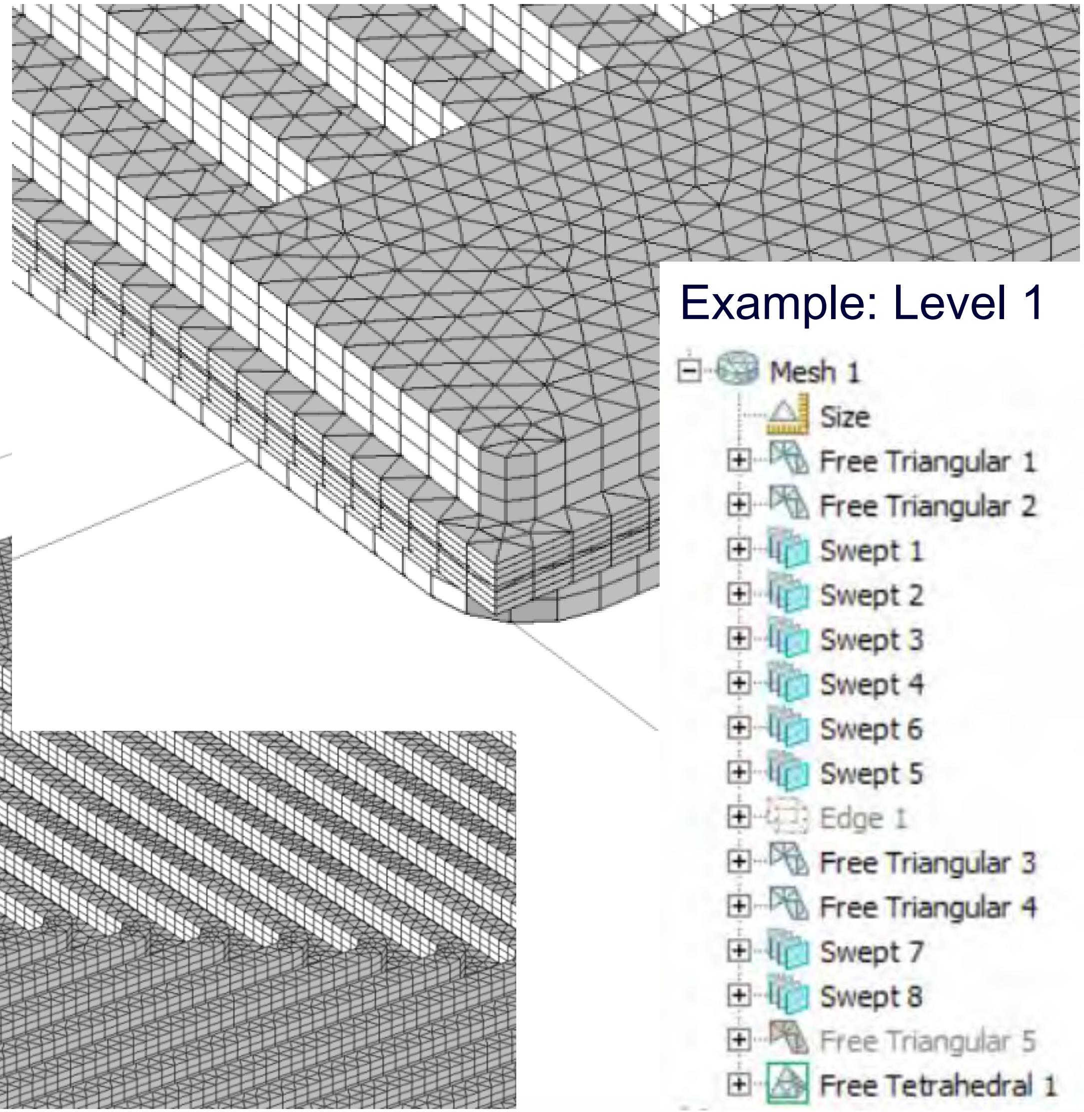
Manual mesh generation →

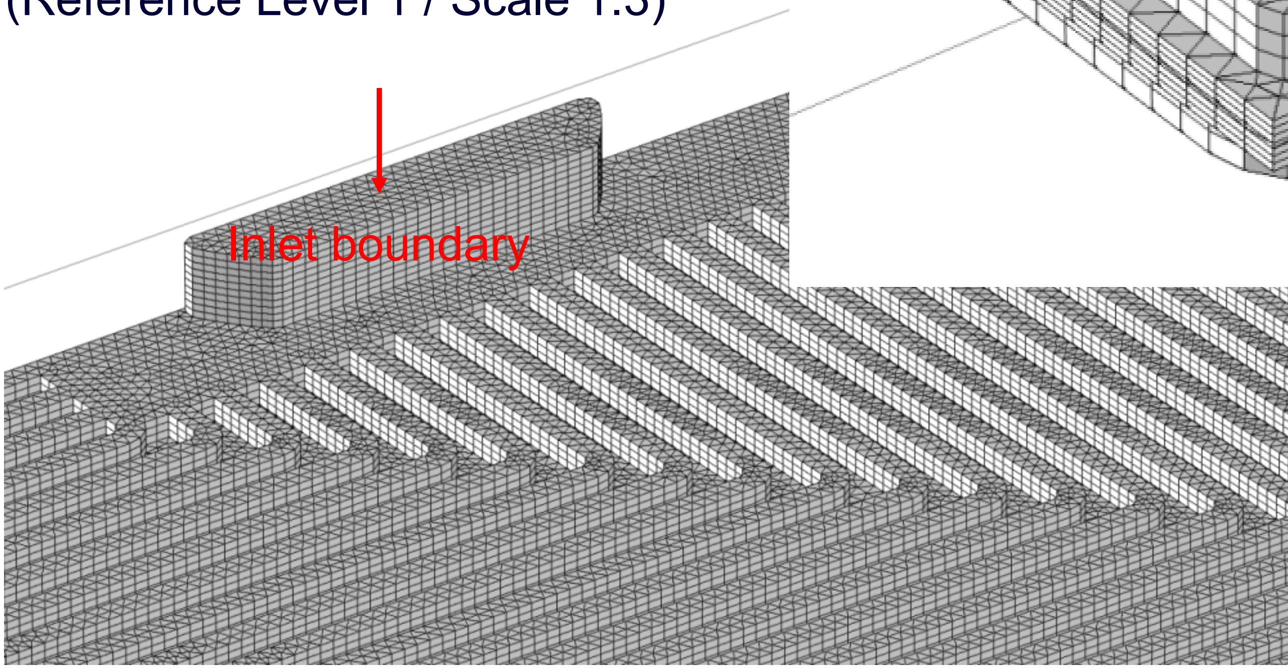
different mesh levels generated

Level 1: 2,190,900 Elements

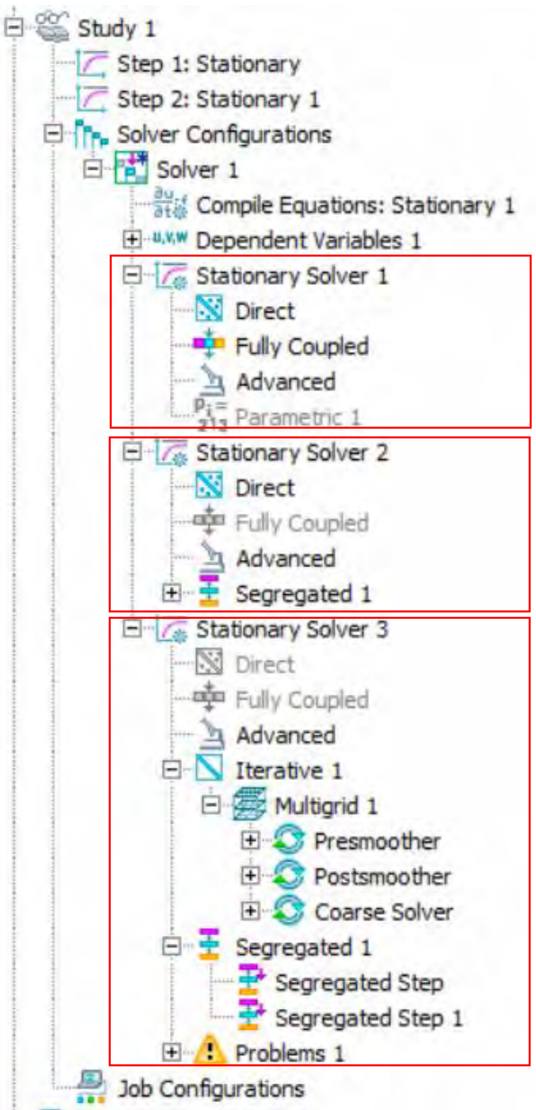
Level 2: 1,402,404 Elements

(Reference Level 1 / Scale 1.3)





Manual set-up of the solvers



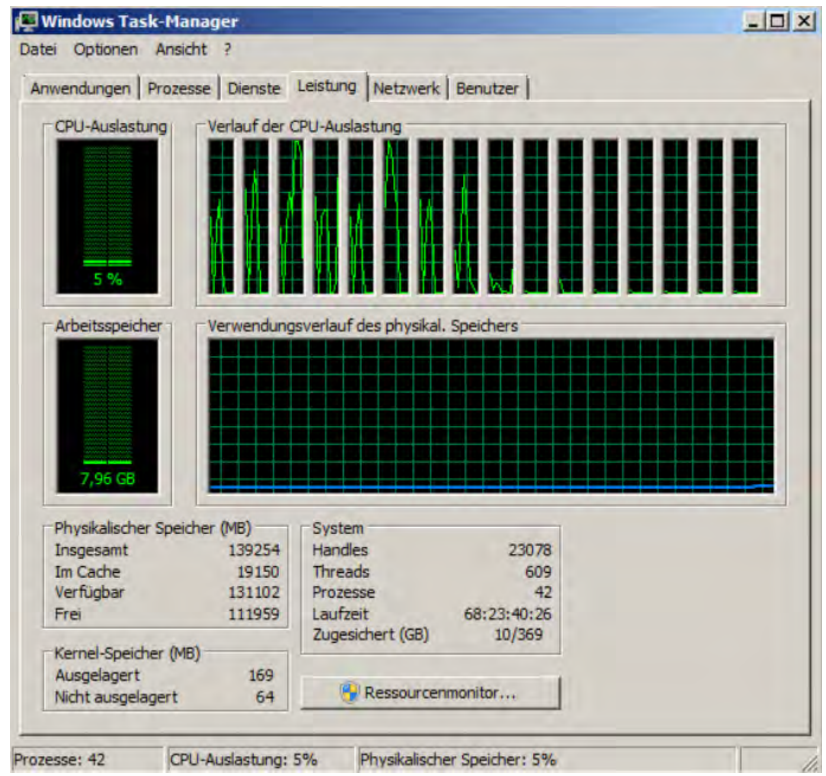
Different solvers used for different solution steps

→ cathode and anode side (momentum/mass)

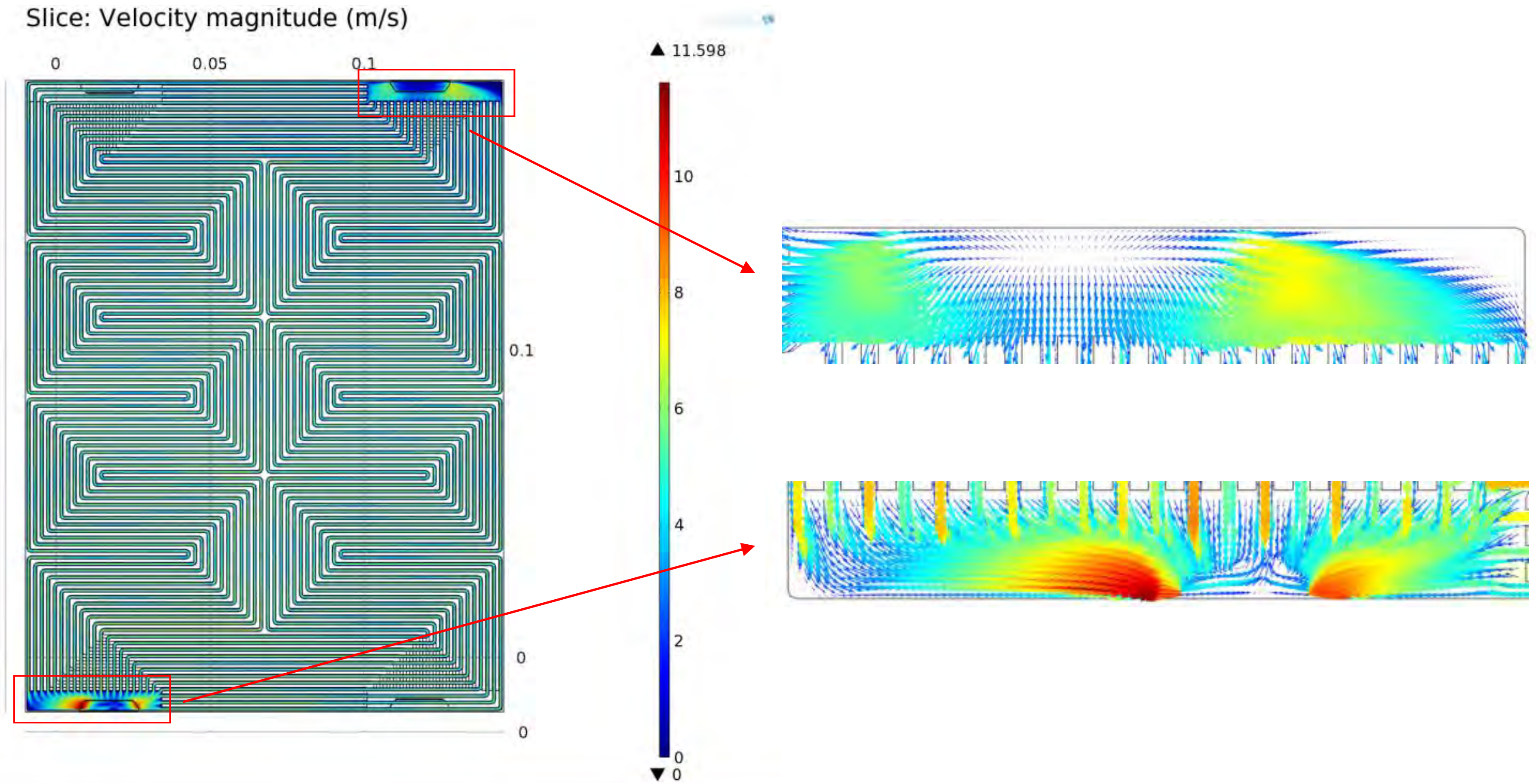
→ anode and cathode side (species/charge)

→ anode and cathode side (temperature 2x)

Hardware:16-core machine with a total of 144 GB RAM



Cathode side fluid flow (slice plot and arrow plot in x-y-plane)

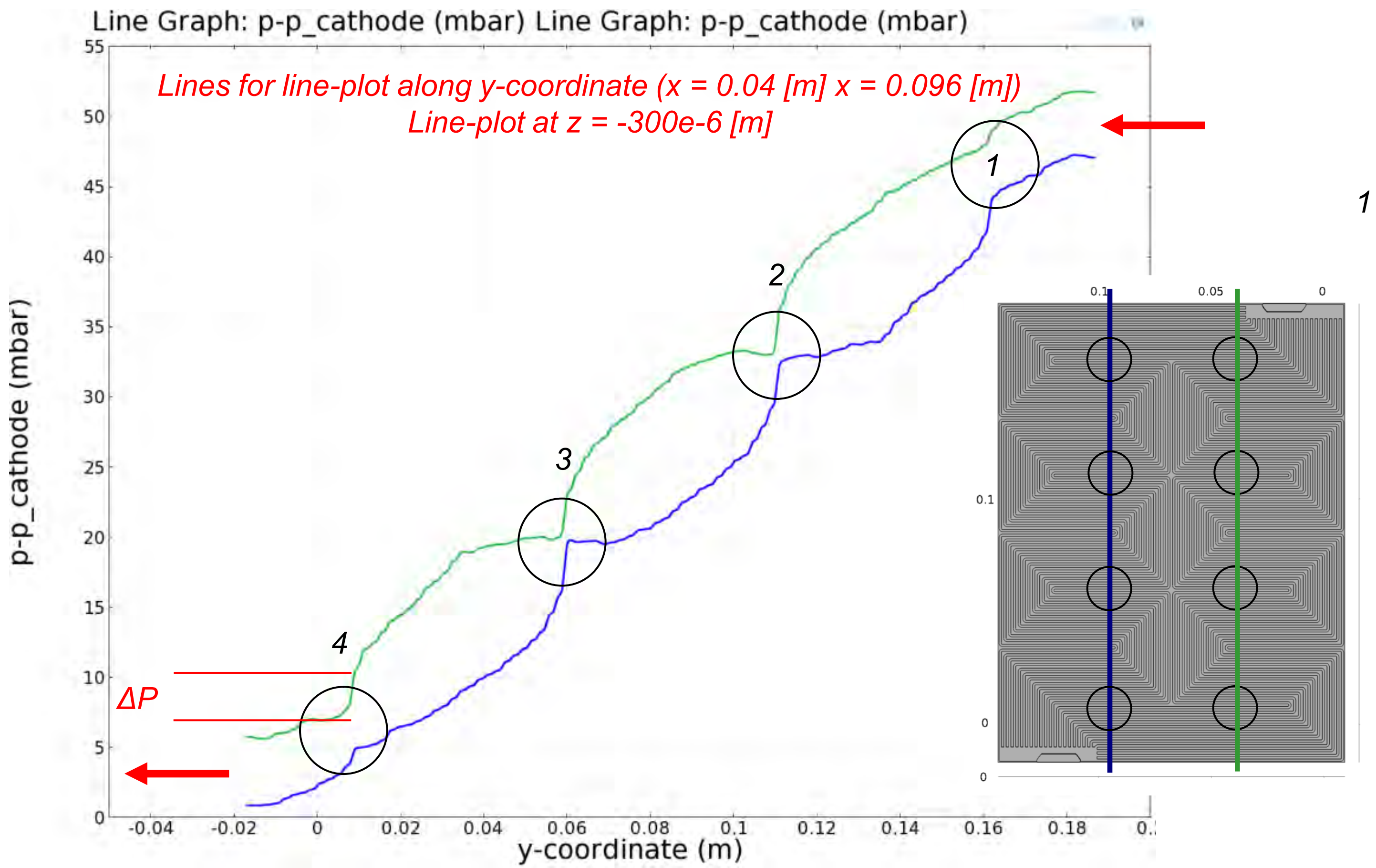


Operating conditions: 120 A, cell voltage U = 0.6 V, Ts = 160°C, Tf = 21°C, H_2/air operation

Gas flow rates according to desired load current of I = 120 A, stoichiometries of 1.35 (anode) and 2.5 (cathode), no backpressure.

Selected results

Cathode side pressure losses (line-plot)

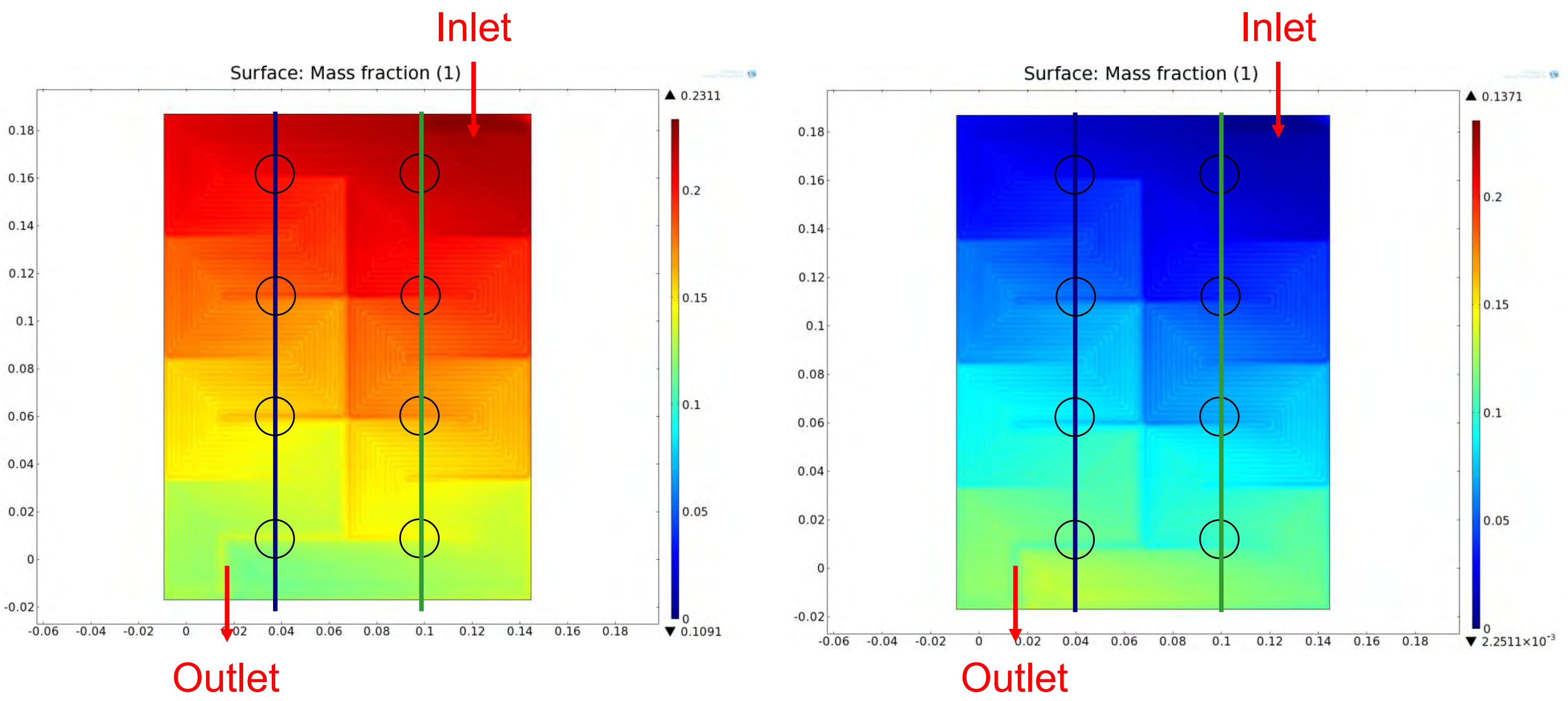


Operating conditions: 120 A, cell voltage *U* = 0.6 V, *T*s = 160°C, *T*f = 21°C, H_2/air operation

Gas flow rates according to desired load current of *I* = 120 A, stoichiometries of 1.35 (anode) and 2.5 (cathode), no backpressure.

Selected results

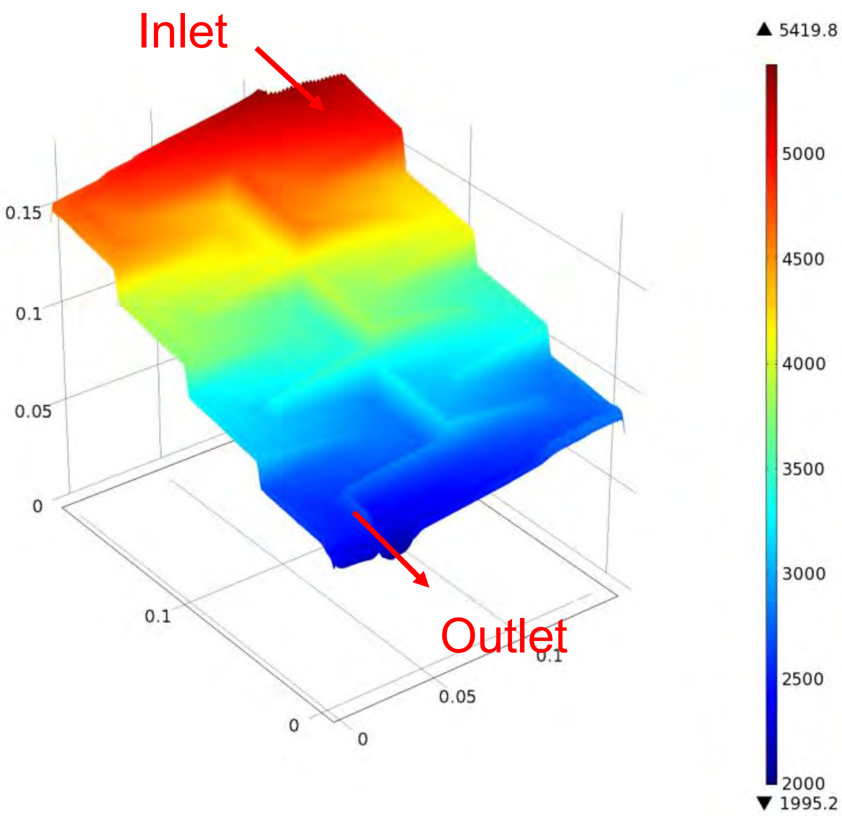
Cathode side mass fractions in 2D x-y-plane

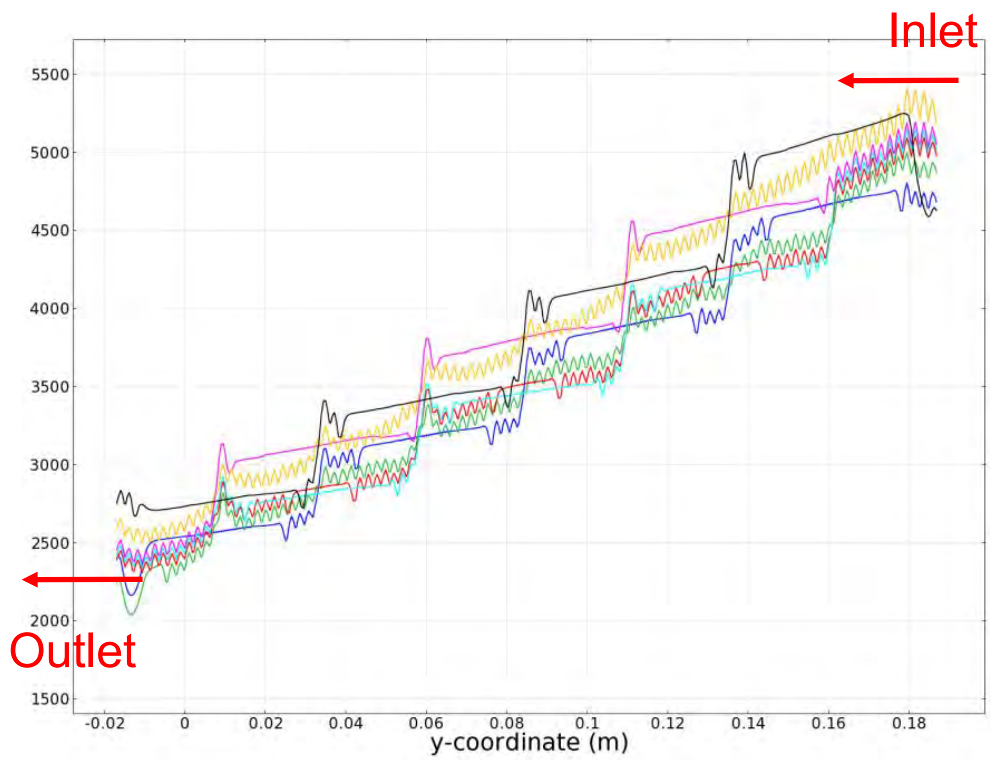


Operating conditions: 120 A, cell voltage *U* = 0.6 V, *T*s = 160°C, *T*f = 21°C, H_2/air operation

Gas flow rates according to desired load current of *I* = 120 A, stoichiometries of 1.35 (anode) and 2.5 (cathode), no backpressure.

Current density distribution in 2D x-y-plane (with height expression) and line-plot

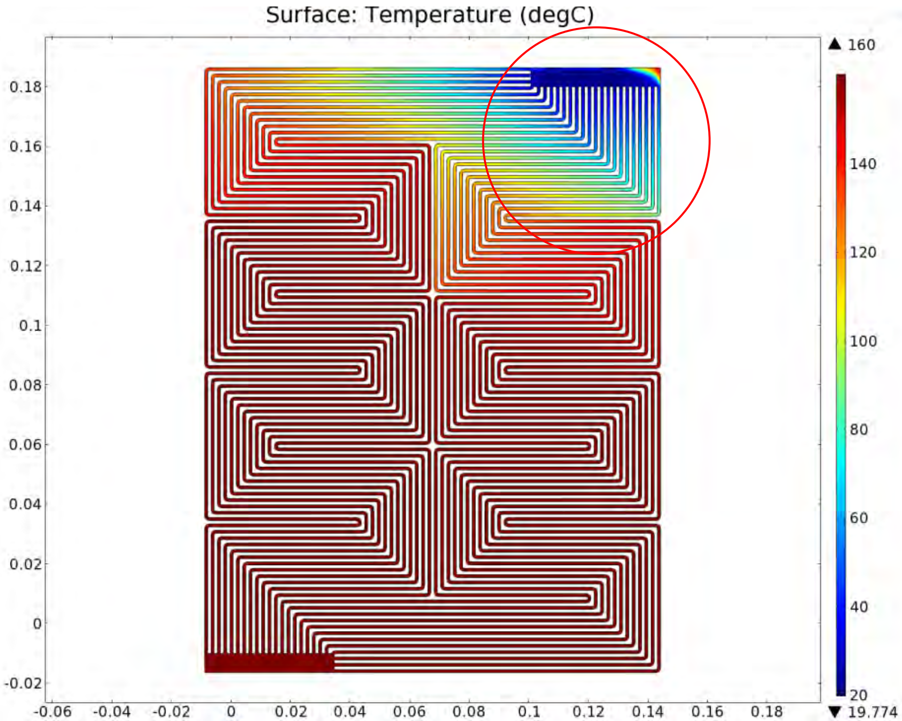


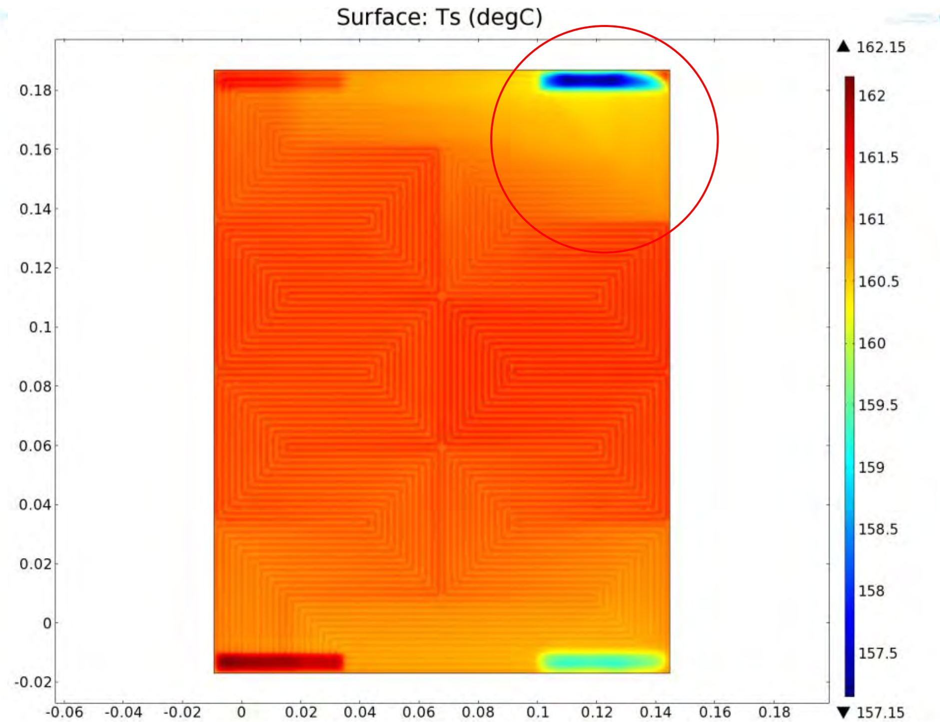


Operating conditions: 120 A, cell voltage *U* = 0.6 V, *T*s = 160°C, *T*f = 21°C, H_2/air operation

Gas flow rates according to desired load current of *I* = 120 A, stoichiometries of 1.35 (anode) and 2.5 (cathode), no backpressure.

Temperature distribution in 2D x-y-plane





Operating conditions: 120 A, cell voltage U = 0.6 V, Ts = 160°C, Tf = 21°C, H_2/air operation

Gas flow rates according to desired load current of I = 120 A, stoichiometries of 1.35 (anode) and 2.5 (cathode), no backpressure.

6. Conclusion and outlook

Conclusions:

In large area HT-PEMFCs,

- Fuel cell simulations with 300-400 cm^2 MEA possible with adequate hardware (full 3D geometry with 20 million DOF)
- Flooded electrodes, low Pt-utilization, local O_2 PP dictates performance (CD, ΔP)
- EIS behaviour is different from small area HT PEMFCs (Mass transport dominates)
- Gradients: T, P, variations in local profiles of oxidant and fuel PP are large.

Outlook:

- Validation of the modeling approach
- EIS simulations (currently under investigation)
- Iterative update of the current flow field layout
- Fuel cell stack layout