INVESTIGATION OF FAVOURABLE OPERATING CONDITIONS FOR ELECTROCHEMICAL HYDROGEN COMPRESSORS BY SIMULATION

Michael Richter[1], Christoph Keuschnigg[1], Eva Wallnöfer-Ogris[1], Rebekka Köll[1], Alexander Trattner[1,2]

[1] HyCentA Research GmbH, Inffeldgasse 15, 8010 Graz, Austria

[2] Graz University of Technology, Institute of Thermodynamics and Sustainable Propulsion Systems, Inffeldgasse 19, A-8010 Graz, Austria

Motivation and Goals

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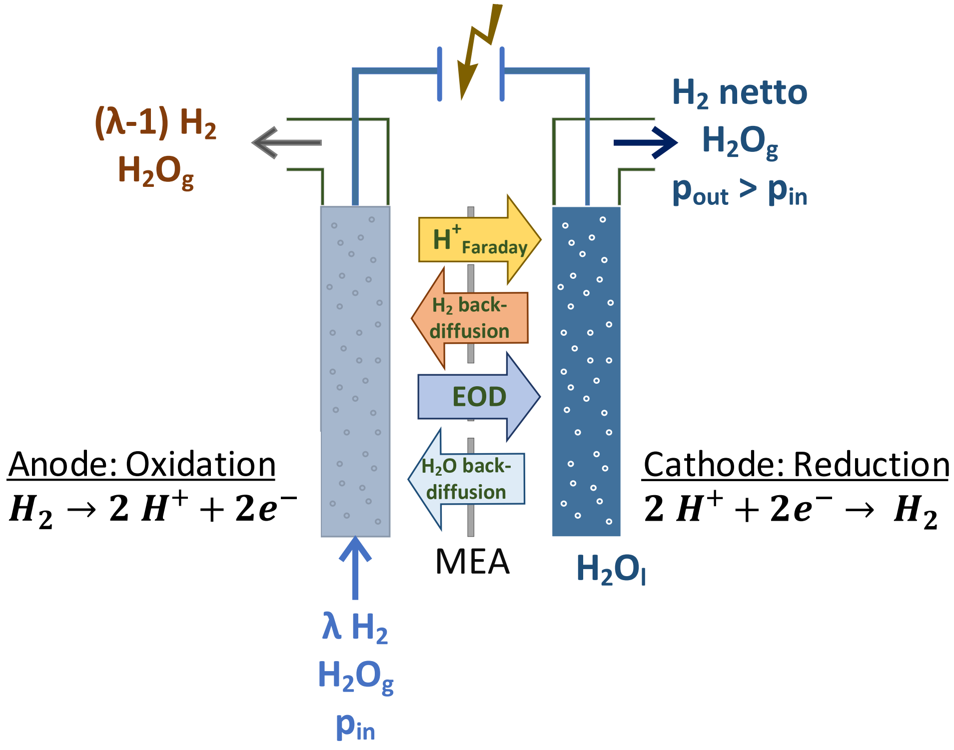
Electrochemical hydrogen compressor research

High level motivation

+ Noise & vibration free operation
+ High compression efficiencies & less required stages for low input pressures
+ Purification of gas mixtures to get > 99% H_2

Research needs & goals

- water transport phenomena in EHC-cells
- significant back-diffusion at high pressure gradients
- suitable material selection for stack development
- suitable operating conditions



Overview CFD-Modelling in Ansys Fluent

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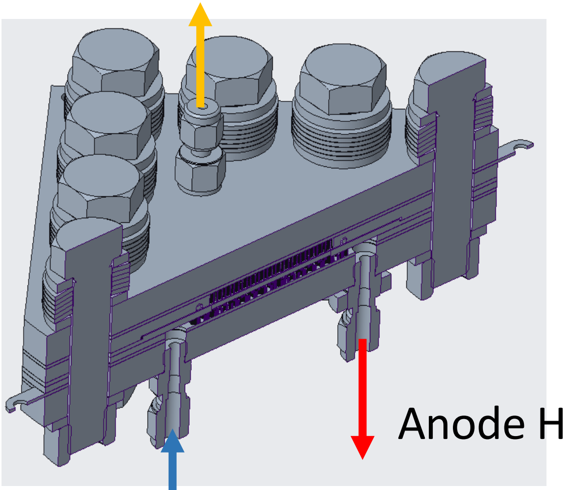
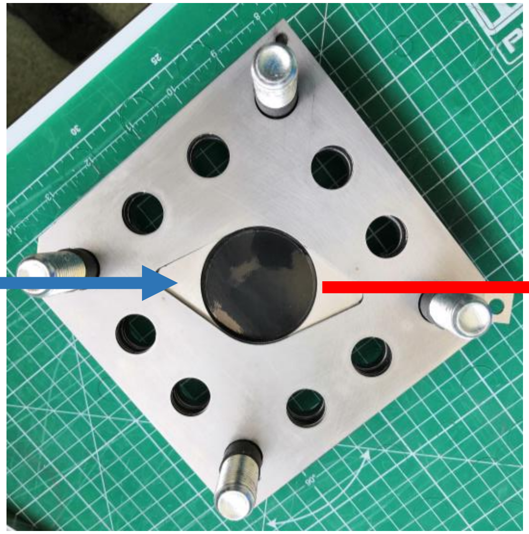
Single cell design





- Single cell geometry modelled in PTC-Creo
- Cell operation with humidified H_2 via bubbler

EHC-cell

- **active area:** ~20 cm²
- **membrane:** Nafion® 117 (178 µm)
- **catalysts:** Pt/Pt (0,55 mg/cm²)
- **Flowfield:** expanded metal sheets
- **Gas diffusion layer:** sintered Ti + carbon cloth/paper

Overview CFD-Modelling in Ansys Fluent

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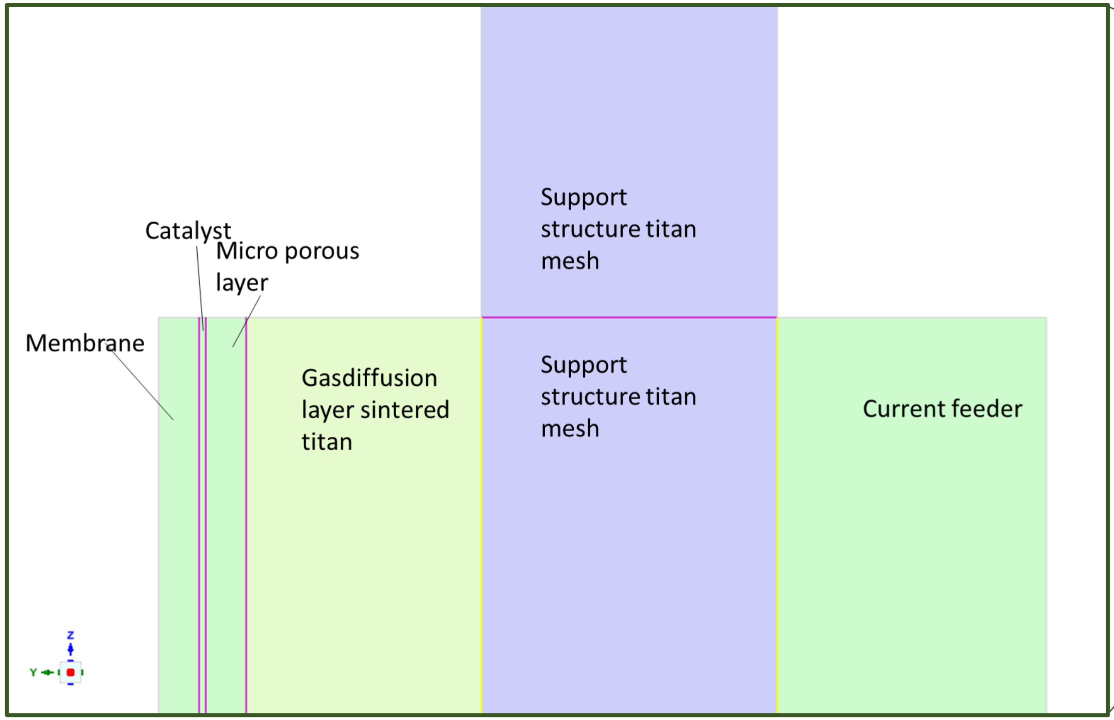
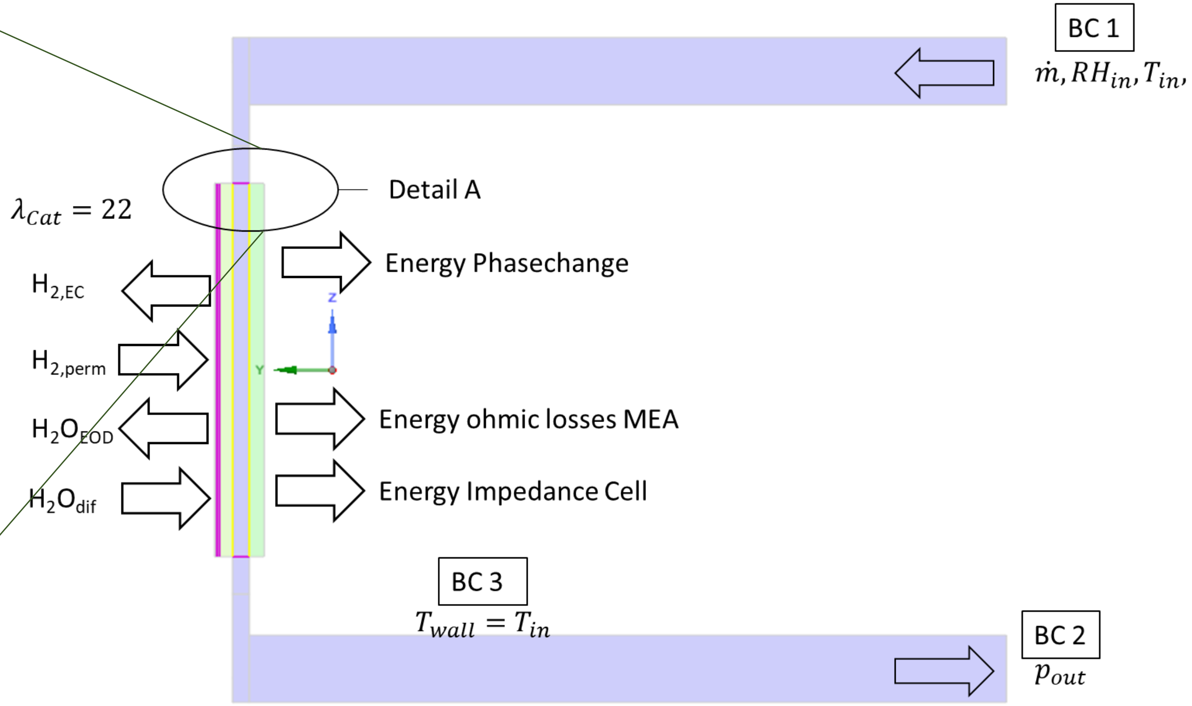
Cell layers, sinks & sources





Sources and sinks:

- mass transfer processes
- Energetic terms (ohmic heat + condensation heat)

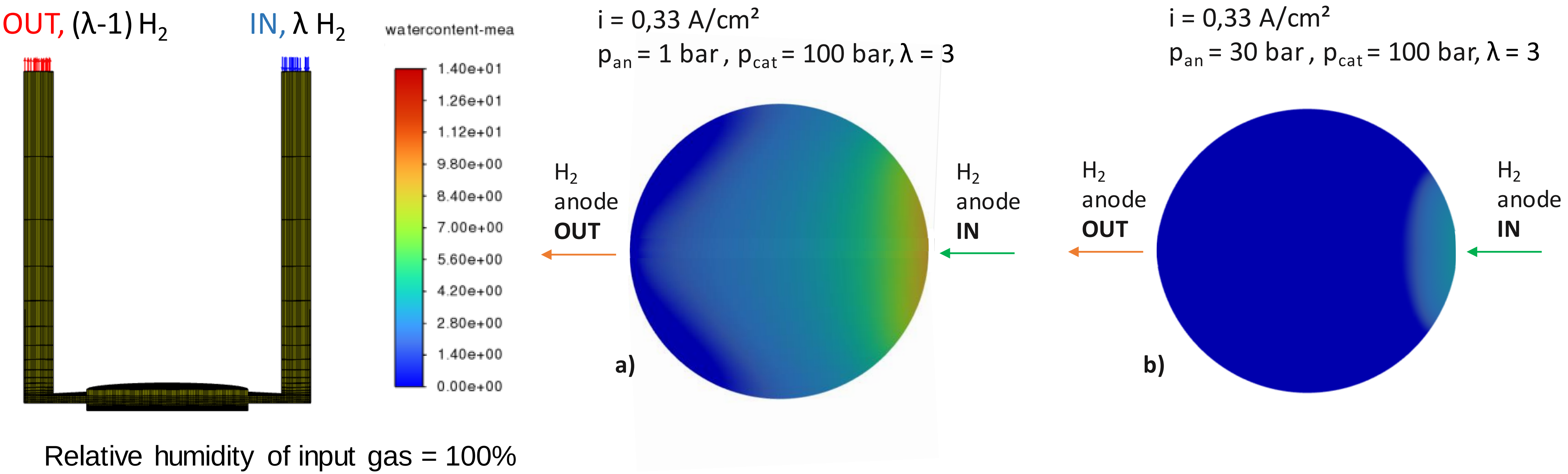
Numerical simulation at **anodic path**

Cathode path implemented via boundary conditions:

- relative humidity = 100% (due to high gas pressure)
- $\lambda_{MEA,\ cat}$ = 22 due to contact with liquid water

Results

water content λ_{MEA} at p_{in} = 1 bar vs. 30 bar



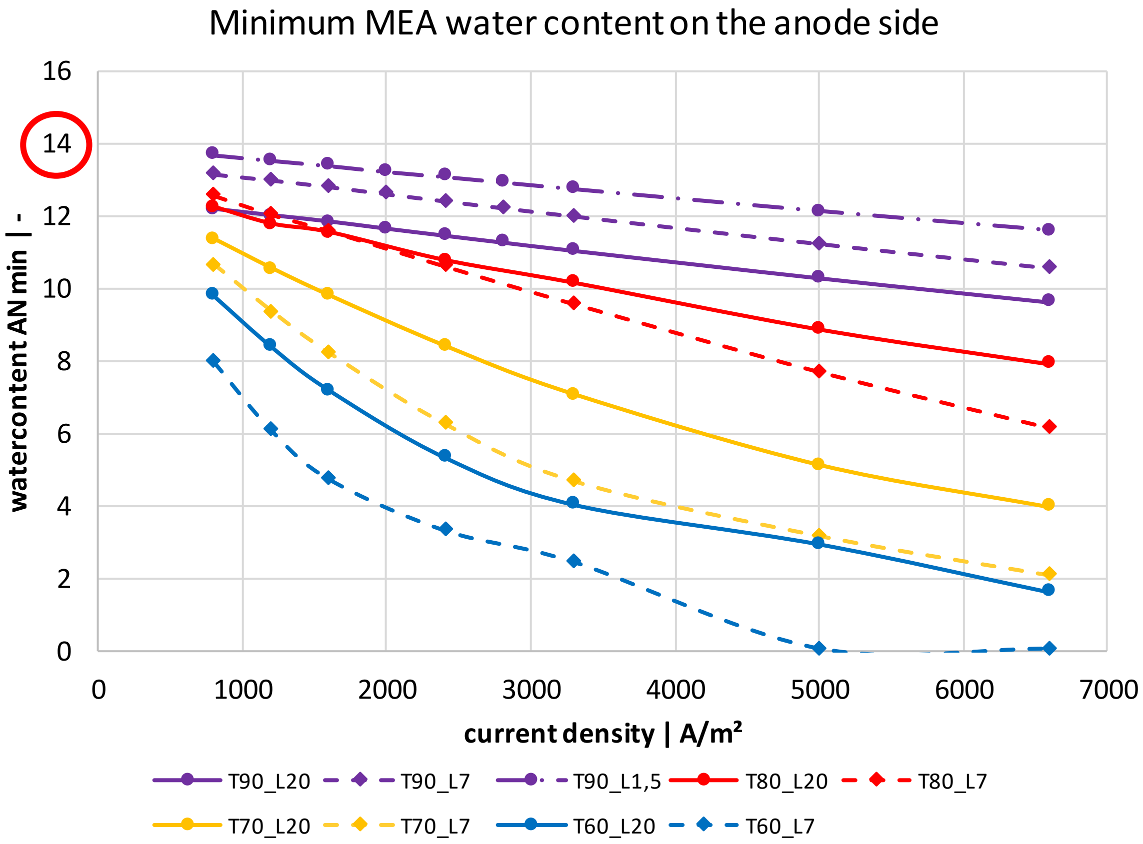
Relative humidity of input gas = 100%

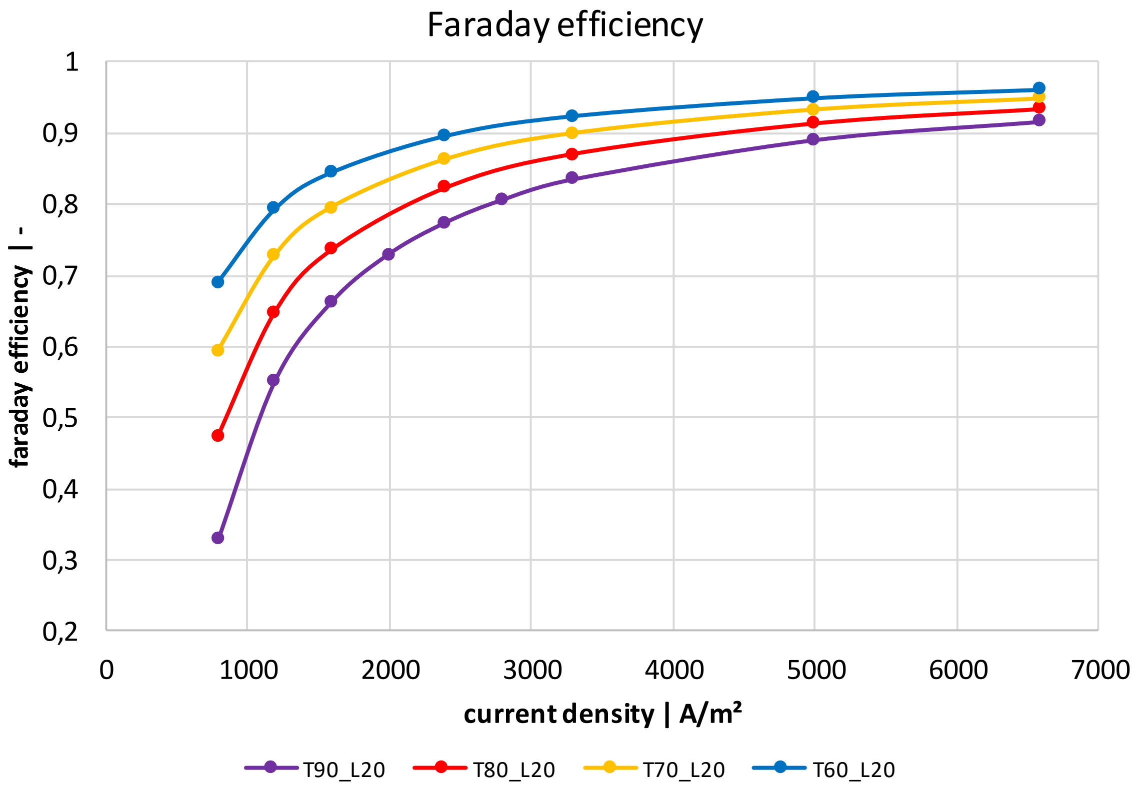
with higher input pressure (high partial pressure of H_2) → amount of water vapour in gas stream is too low to comply with induced electrochemical drag

→ significant lack of humidification with higher input pressures

Results

Water content λ_{MEA} & Faraday efficiency, p_{in} = 1 bar, p_{out} = 100 bar





$$\lambda_{MEA} = 0{,}043 + 17{,}81 * a - 39{,}85 * a^2 + 36{,}0 * a^3$$ [1]

if saturated: a = 1 → λ_{MEA} = 14

$$\eta_F = \frac{\dot{n}_{H_2 net}}{\dot{n}_{H_2 theoretical}} = \frac{\dot{n}_{H_2 theoretical} - \dot{n}_{H_2 backdiff}}{\dot{n}_{H_2 theoretical}}$$

[1] Springer, T.E.; Zawodzinski, T.A.; Gottesfeld, S.; Polymer Electrolyte Fuel Cell Model, J. Electrochem. Soc. 1991, 138, 2334

Results

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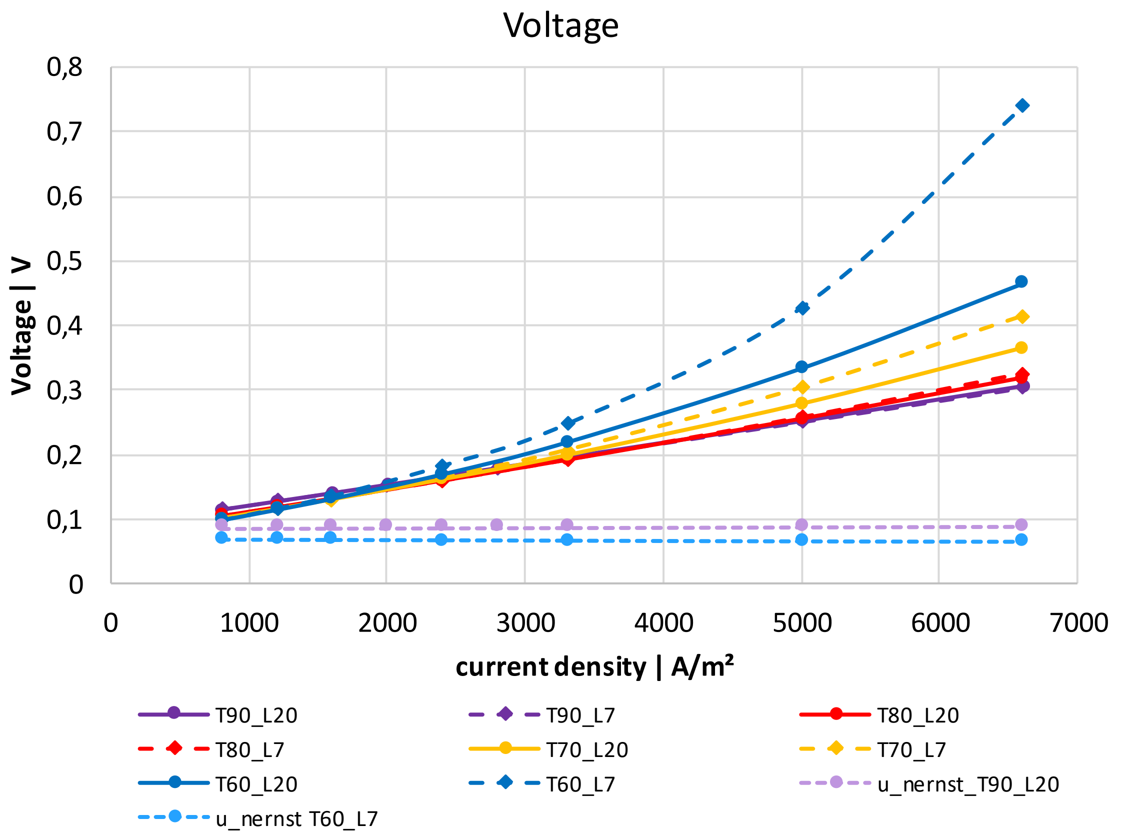
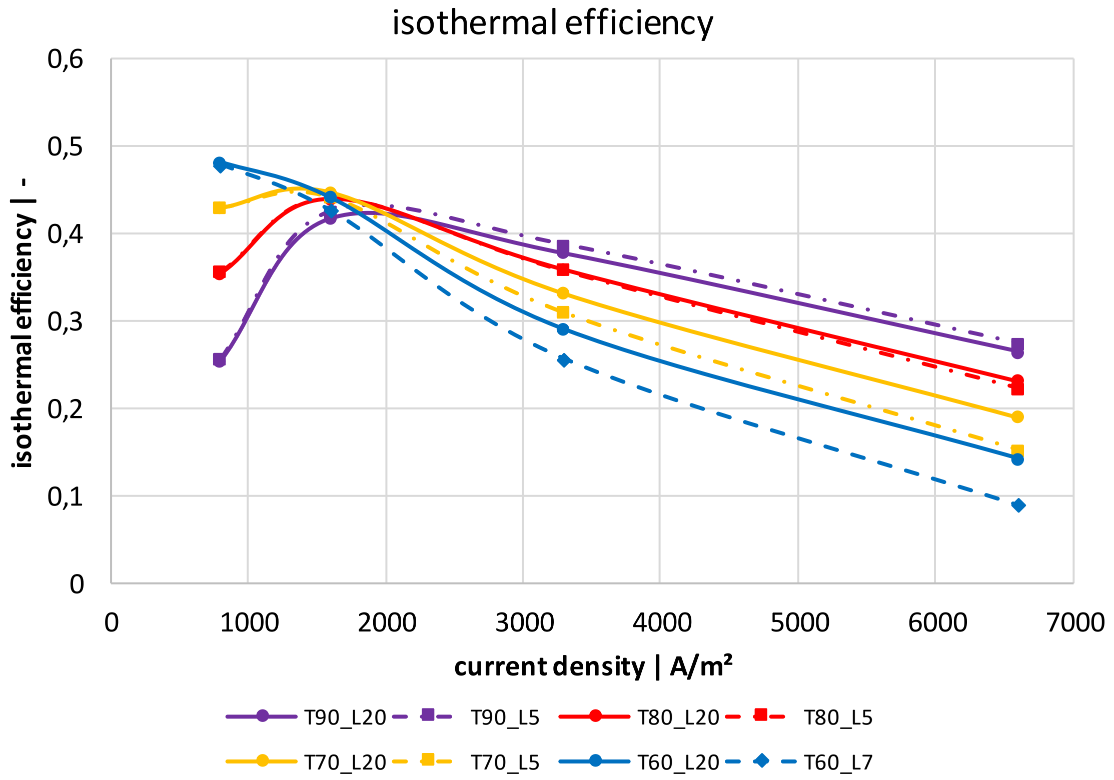
Voltage & isothermal efficiency, p_{in} = 1 bar, p_{out} = 100 bar





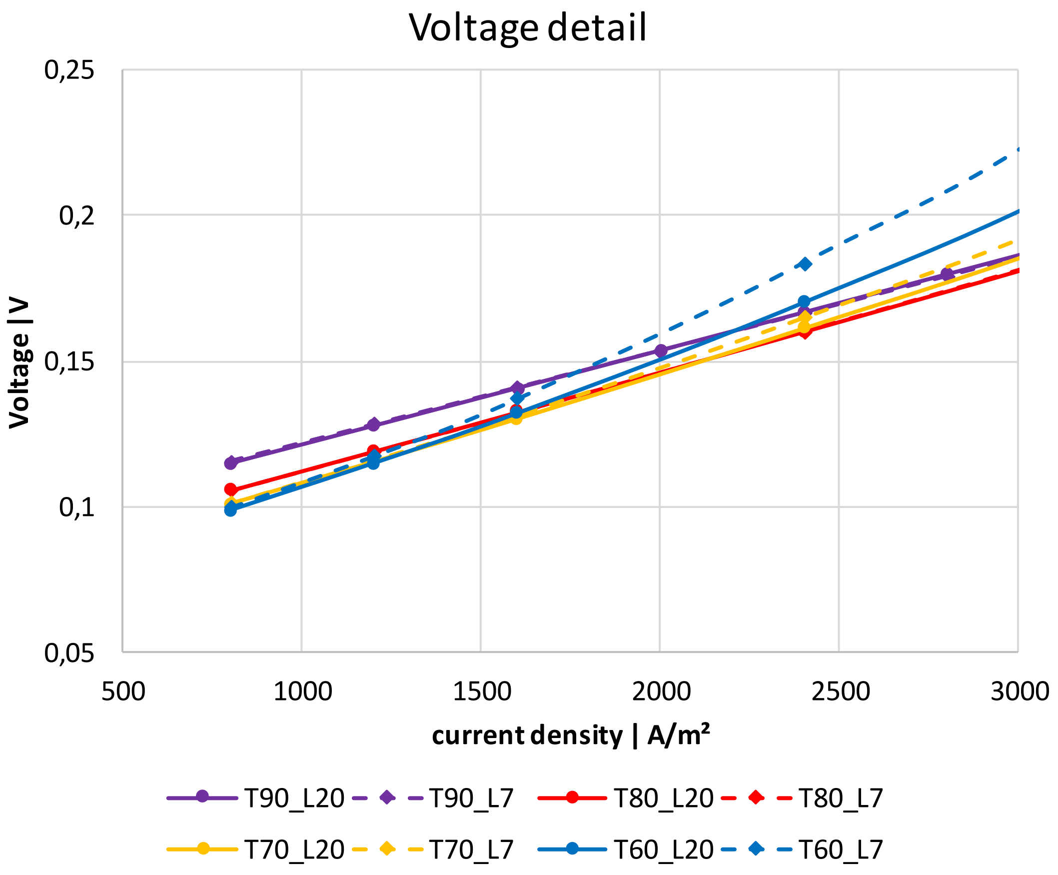
$$U_{cell} = U_{Nernst} + U_{act} + U_{ohmic} + U_{mass-transfer} + U_{back-diffusion}$$

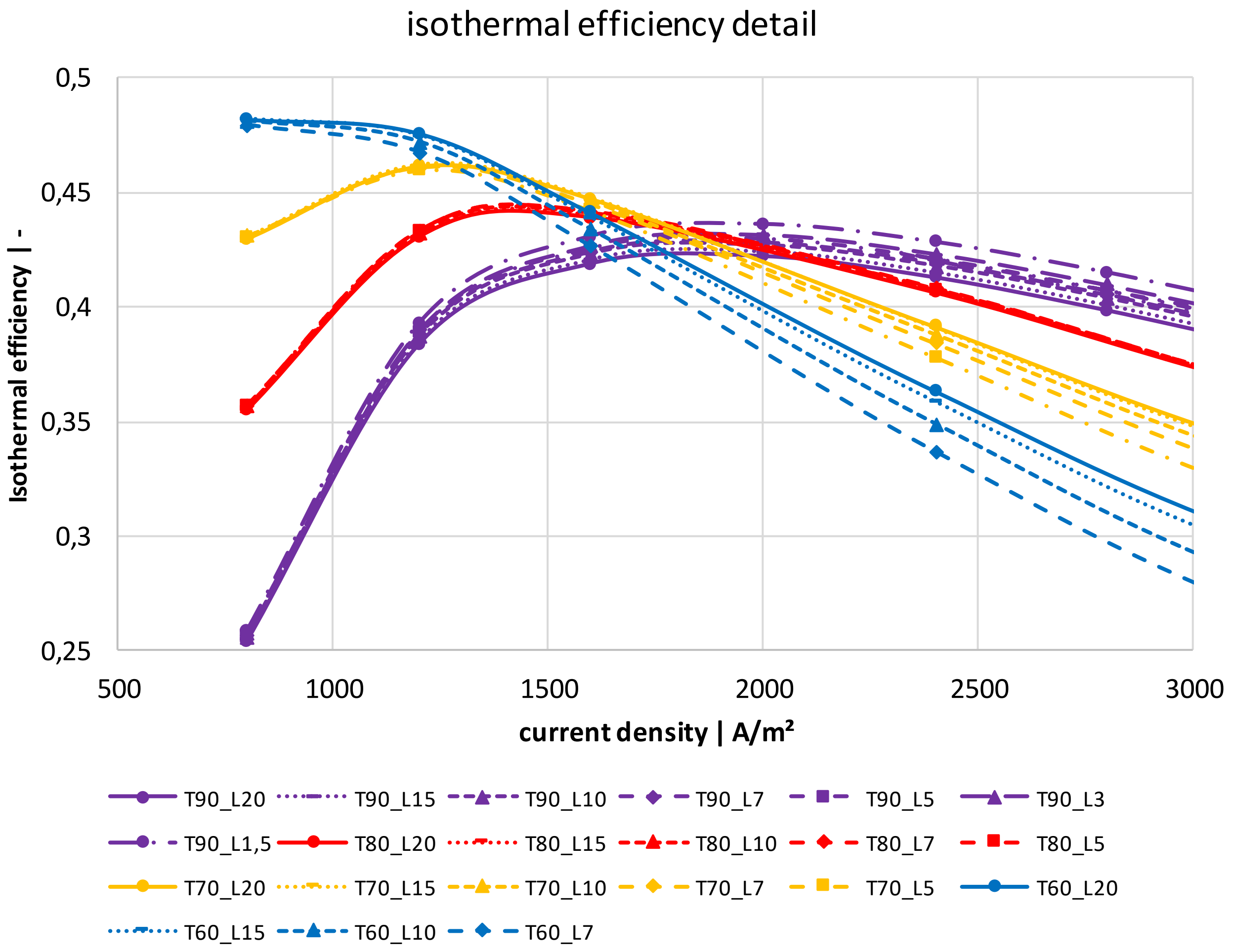
$$U_{cell} = \frac{R*T}{2*F} * \ln\left(\frac{p_{H2_{cat}}}{p_{H2_{an}}}\right) + \frac{R*T}{2*\alpha_{0,H2ox}*F} * \ln\left(\frac{i}{i_{o_{an}}}\right) + \frac{R*T}{2*\alpha_{0,H2red}*F} * \ln\left(\frac{i}{i_{o_{cat}}}\right) + R_{el} * i$$

$$\eta_{EHC,th} = \frac{W_{ideal}}{W_{actual}} = \frac{n_n RT \ln\left(\frac{P_c}{P_a}\right)}{U_{cell}(2Fn_f)}$$

Results

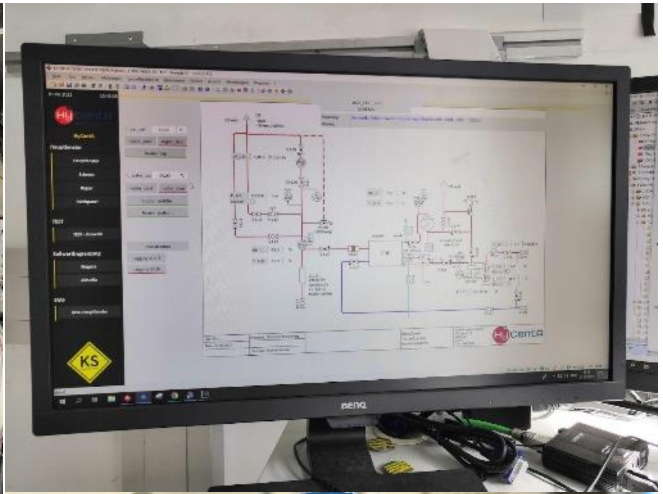
Voltage & isothermal efficiency, p_{in} = 1 bar, p_{out} = 100 bar



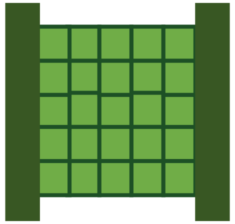


Outlook

Single cell testing of EHC-prototype: EIS and segmented cell testing



- 2nd Cell design appropriate for segmented cell testing in preparation
  - Current density distribution
  - Temperature distribution



Segmented cell measurement device

- Current design used for material tests with:
  - GDL
  - Membrane + catalyst loadings
  - Flat gaskets
  - Gas mixture separation (CH_4/H_2)

EHC-cell

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- **membrane:** Nafion® 117 (178 µm)
- **catalysts:** Pt/Pt (0,55 mg/cm²)
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Thank you!

Acknowledgments

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HYTECHONOMY

HYTECHONOMY HYFACILITY

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move2zero

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DI Michael Richter
richter@hycenta.at

HyCentA Research GmbH
Inffeldgasse 15
A-8010 Graz

www.hycenta.at