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Quasi-2D Model of a PEM Electrolyser for Assessment of Dynamic Thermal Behavior

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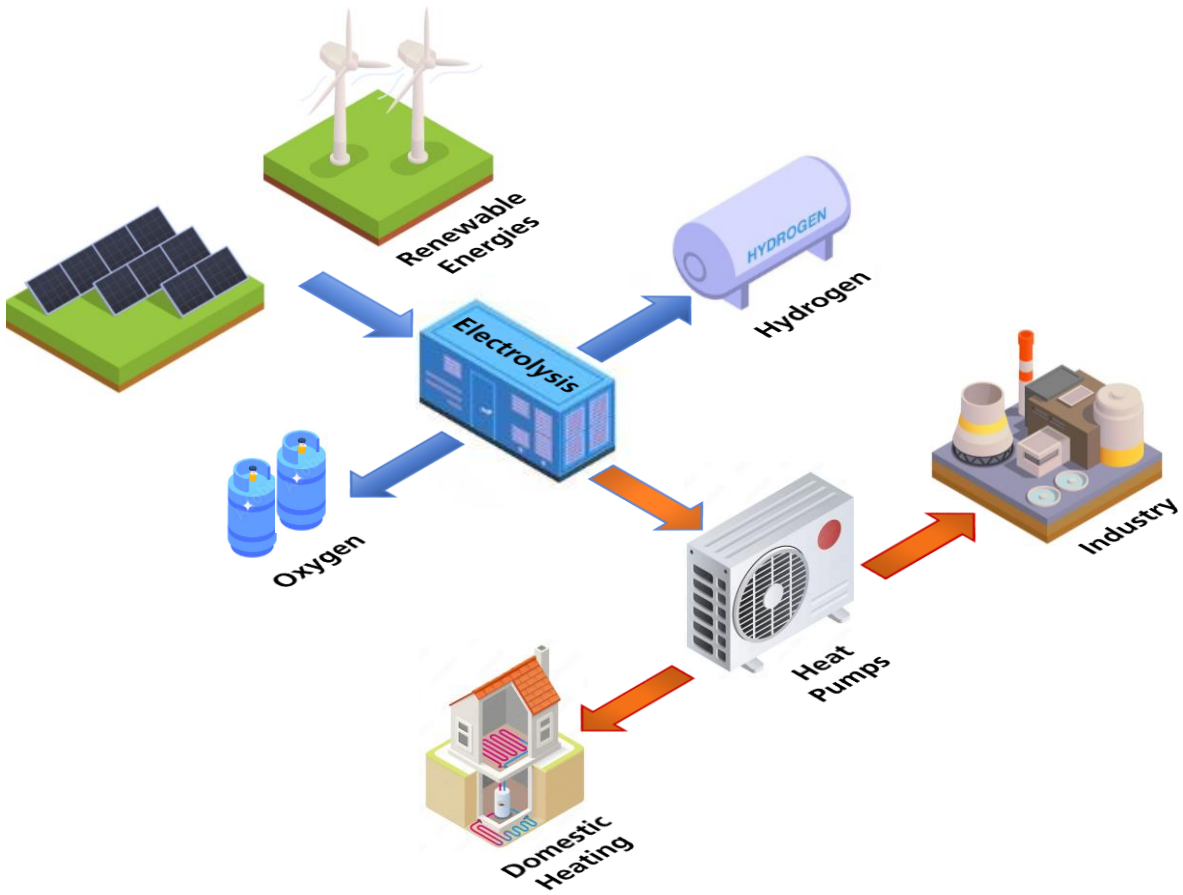
Agenda

1. Background & Motivation
2. Model Description
    1. General Structure
    2. Bipolar & End Plates
    3. Flow Channels
    4. Membrane Electrode Assembly (MEA)
3. Model Validation
4. Summary & Next Steps

Background & Motivation

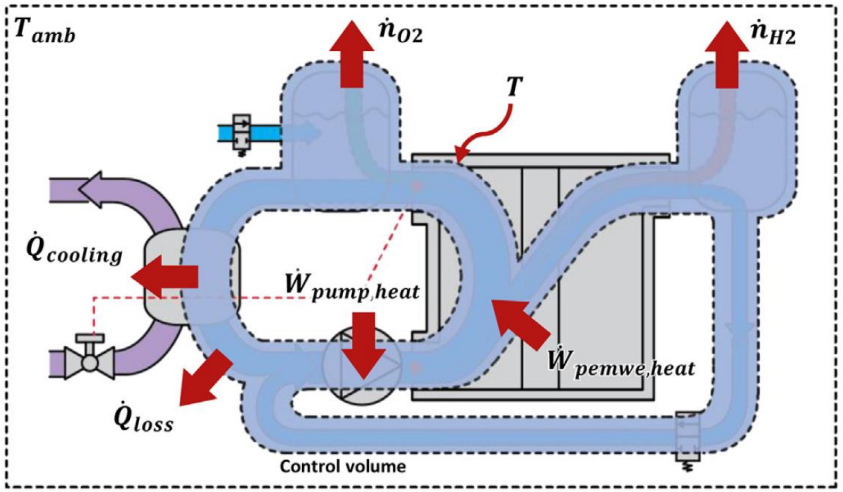
- Model development as part of the IntegrH2ate research project
- Aims to increase the economic viability of PEM electrolysis by utilizing the by-products heat and oxygen
- The waste heat is to be raised to a higher temperature level with a heat pump
- Control strategies are being developed for the coupled electrolyser-heat pump system
- For the development of control strategies, the dynamic thermal behavior of the PEM electrolyzer must be known



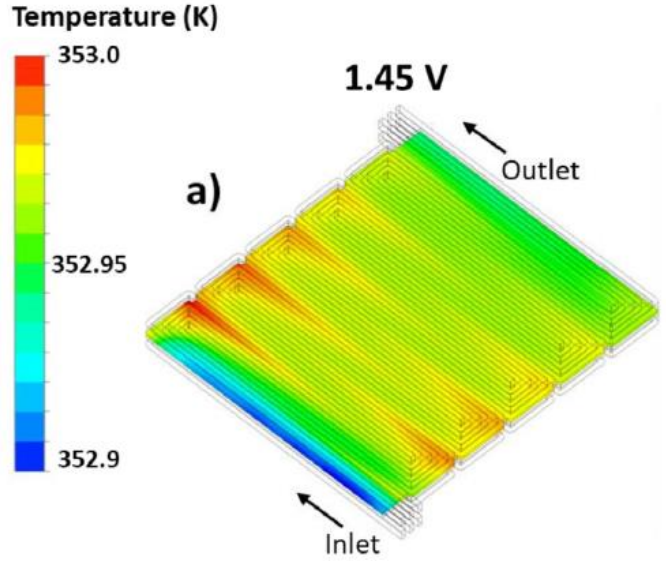
Source: www.flaticon.com

Background & Motivation

- So far, only highly simplified lumped parameter models[1] and very complex 3D finite volume approaches[2] exist to describe the (dynamic) thermal behavior
- Some quasi-2D approaches exist, but without description of heat transfer in the flow channels[3]
- Therefore, a quasi-2D simulation model with focus on the heat transfer processes in the individual cells has been developed



Source: Espinosa-Lopez et al. (2018)



Source: Ma et al. (2021)

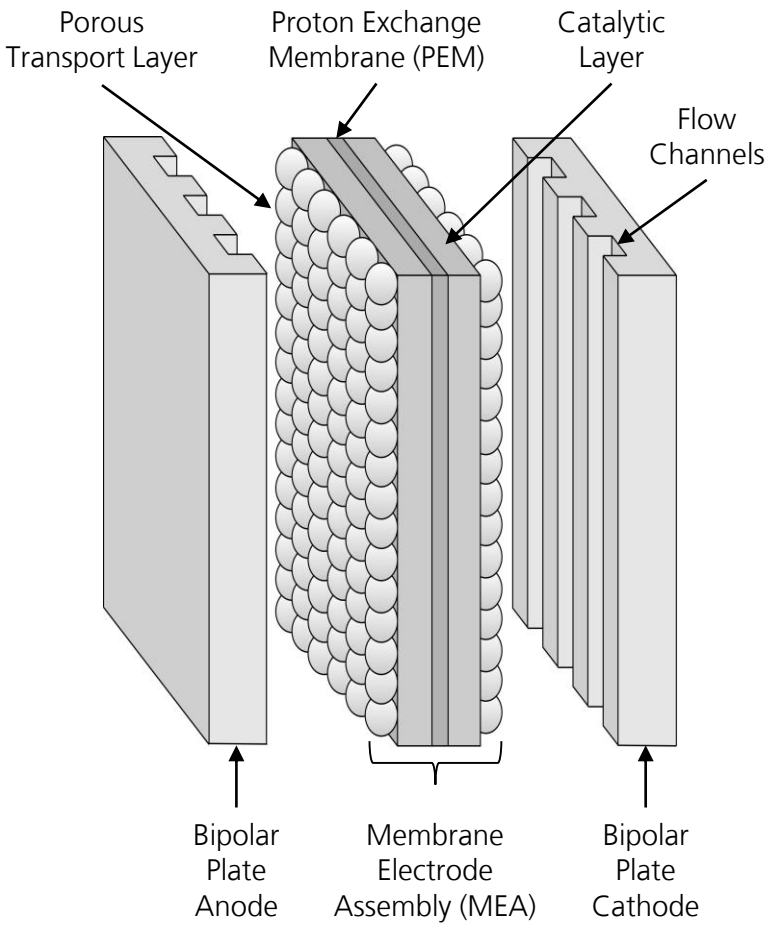
Literature:

[1] García-Valverde, R., N. Espinosa and A. Urbina. "Simple PEM Water Electrolyser Model and Experimental Validation." In: International Journal of Hydrogen Energy 37, no. 2 (2012): pp. 1927–38. DOI: 10.1016/j.ijhydene.2011.09.027.

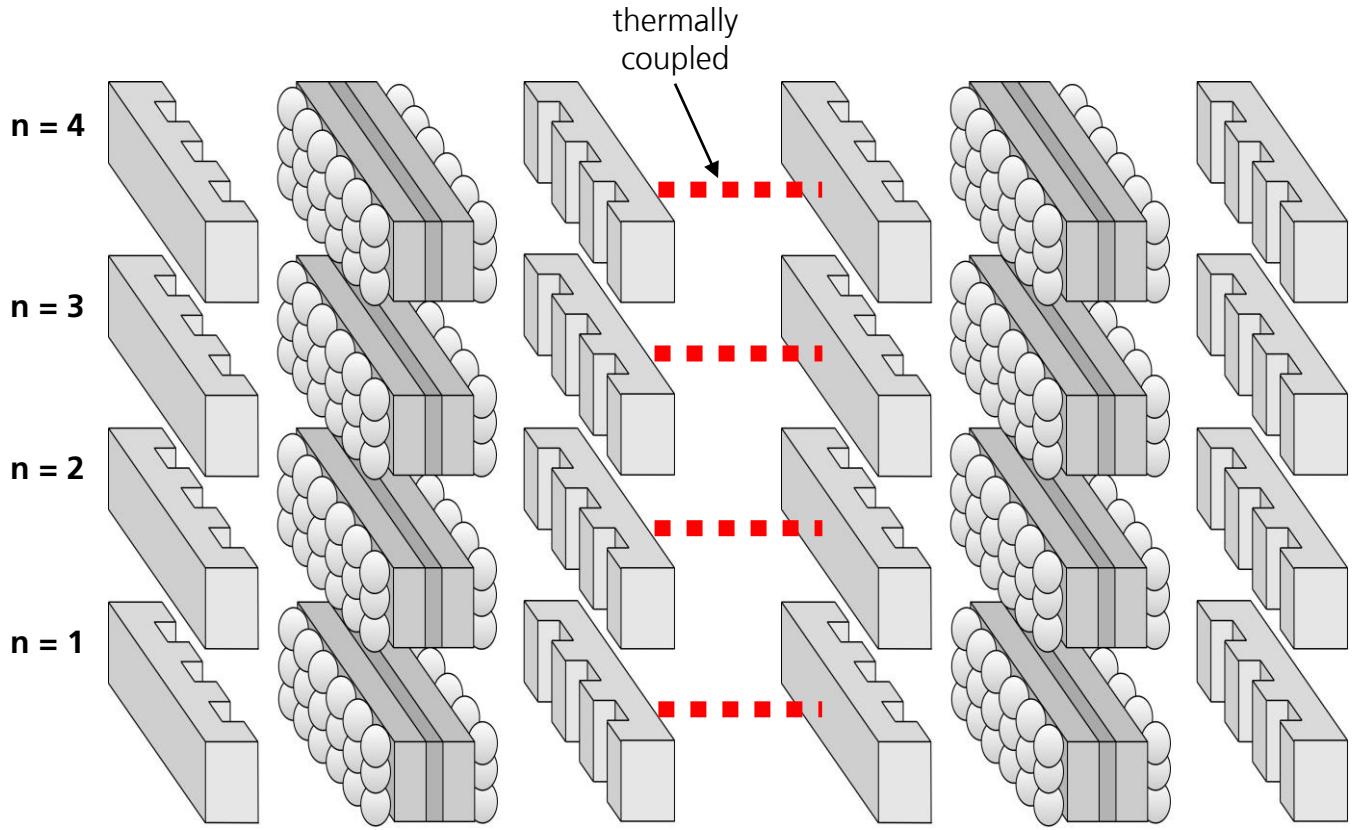
[2] Ma, Z., L. Witteman, J. A. Wrubel and G. Bender. "Comprehensive Modeling Method for Proton Exchange Membrane Electrolyzer Development." In: International Journal of Hydrogen Energy 46, no. 34 (2021): pp. 17627–43. DOI: 10.1016/j.ijhydene.2021.02.170.

[3] Lin, N. and J. Zausch. "1D Multiphysics Modelling of PEM Water Electrolysis Anodes with Porous Transport Layers and the Membrane." In: Chemical Engineering Science 253 (2022): p. 117600. DOI: 10.1016/j.ces.2022.117600.

Model Description – General Structure



Discretization



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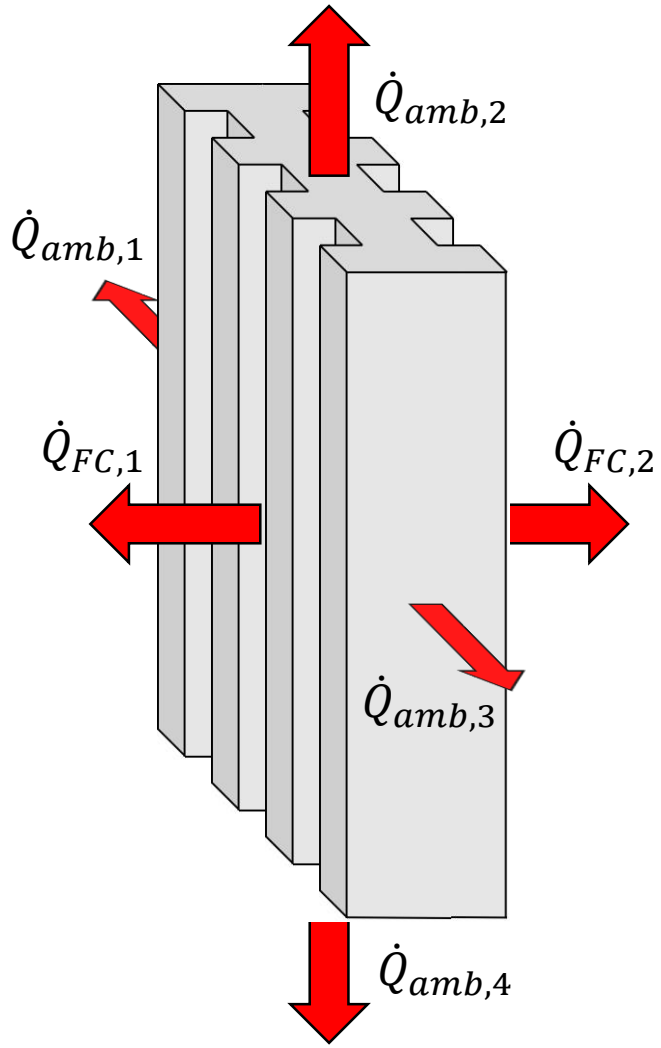
Model Description – Bipolar & End Plates

- Bipolar and end plates are treated as lumped capacitance masses with a uniform temperature at each timestep:

$$\overbrace{C_{th}\frac{dT}{dt}}^{\substack{enthalpy\\ change\ BP}} = \overbrace{\sum_j \dot{Q}_{FC,j}}^{\substack{heat\ flows\\ to\ FC}} + \overbrace{\sum_i \dot{Q}_{amb,i}}^{\substack{heat\ flows\\ to\ ambient}}$$

$$\dot{Q}_{FC/amb} = A \cdot \alpha \cdot (T_{FC/amb} - T)$$

- The material is assumed to be titanium
- End plates are considered separately because of their larger volume



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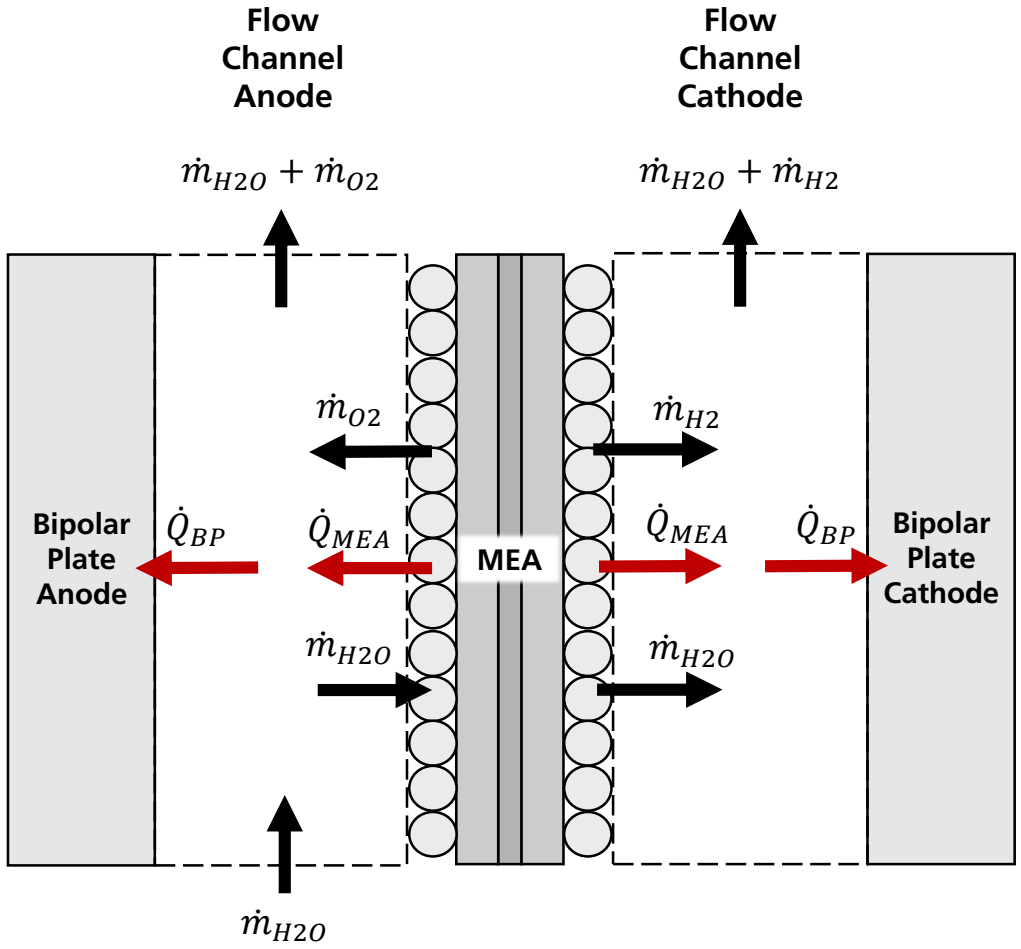
Model Description – Flow Channels

- The dynamic energy balance is calculated using the specific enthalpy of the water-gas mixture:

$$\overbrace{m\frac{dh_{FC}}{dt}}^{\substack{enthalpy\\change\ FC}} = \overbrace{\sum_i \dot{m}_{in,i}\, h_i}^{\substack{enthalpy\\flows\ in}} - \overbrace{\sum_j \dot{m}_{out,j} h_j}^{\substack{enthalpy\\flows\ out}} + \dot{Q}_{MEA} - \dot{Q}_{BP}$$

$$h_{FC} = \left(1 - X_g\right) \cdot h_{H2O} + X_g \cdot h_g$$

$$X_g = \frac{\dot{m}_g}{\dot{m}_g + \dot{m}_{H2O}}$$



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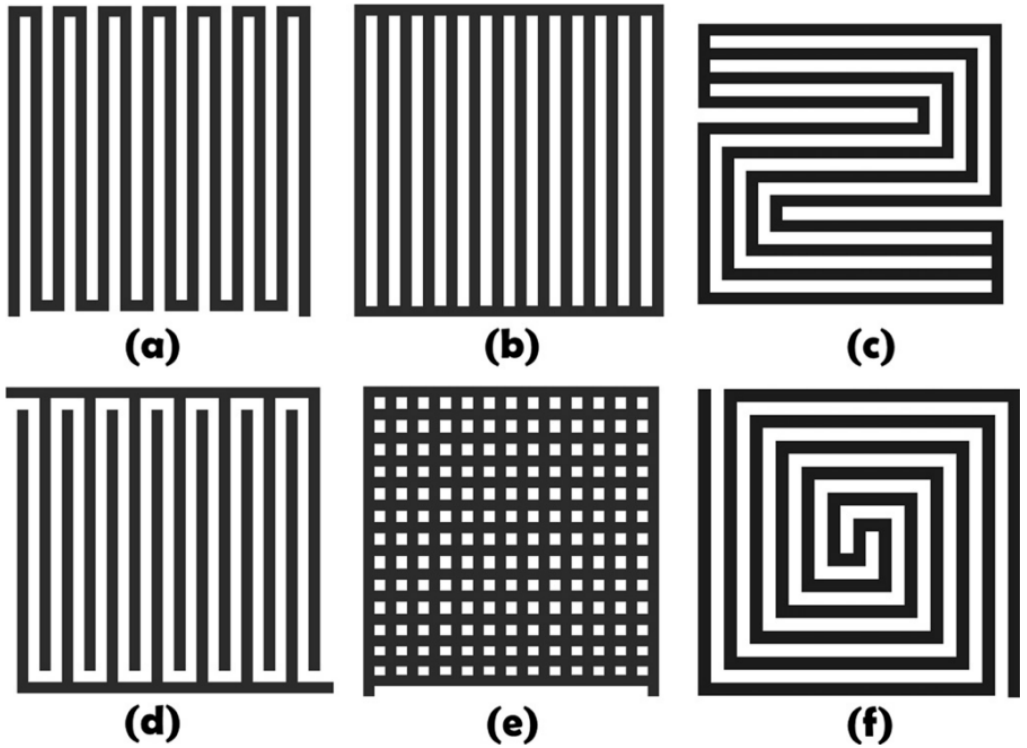
Model Description – Flow Channels

- Parallel flow field is assumed with rectangular flow channels
- Heat transfer coefficient is calculated using a general correlation for heat transfer in vertical channels with gas-liquid flow[1]
- Pressure loss is calculated using a universal approach for frictional pressure drop in mini/micro-channels with gas-liquid flow[2]



Source: Arvay et al. (2013)

Literature:

[1] Shah, Mirza M. "General Correlation for Heat Transfer to Gas–Liquid Flow in Vertical Channels." In: Journal of Thermal Science and Engineering Applications 10, no. 6 (2018). DOI: 10.1115/1.4040652.

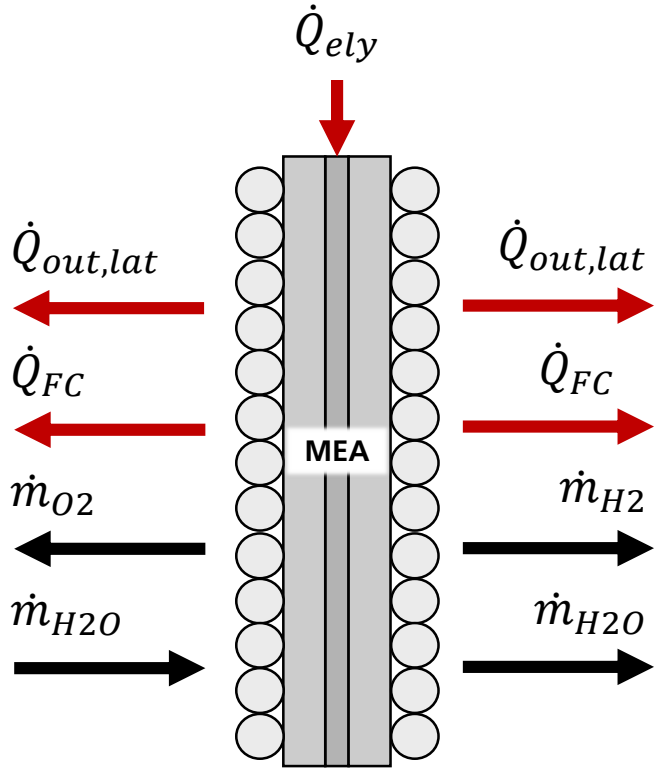
[2] Kim, S.-M. and I. Mudawar. "Universal approach to predicting two-phase frictional pressure drop for adiabatic and condensing mini/micro-channel flows." In: International Journal of Heat and Mass Transfer 55, no. 11-12 (2012). DOI: 10.1016/j.ijheatmasstransfer.2012.02.047.

Model Description – Membrane Electrode Assembly (MEA)

- MEA is treated as a lumped capacitance mass with the porous transport layers being considered the only relevant thermal mass:

$$\overbrace{C_{th,MEA}\frac{dT_{MEA}}{dt}}^{\substack{enthalpy\\change\ MEA}} = \overbrace{\sum_i \dot{m}_{in,i}\,h_i}^{\substack{enthalpy\\flows\ in}} - \overbrace{\sum_j \dot{m}_{out,j}h_j}^{\substack{enthalpy\\flows\ out}} + \dot{Q}_{ely} - \dot{Q}_{FC} - \dot{Q}_{out,lat}$$

- The material is assumed to be titanium with a porosity of $\Phi = 0.37$
- It is assumed that the outgoing mass flow temperatures are equal to the MEA's operating temperature
- Gas Crossover is described with formulations from Afshari et al. (2021)[1]



Literature:

[1] Afshari, E. et al. "Performance assessment of gas crossover phenomenon and water transport mechanism in high pressure PEM electrolyzer." In: International Journal of Hydrogen Energy 46, no. 19 (2021). DOI: 10.1016/j.ijhydene.2020.10.180.

Model Description – Membrane Electrode Assembly (MEA)

- Steady-State Cell voltage is calculated in the MEA:

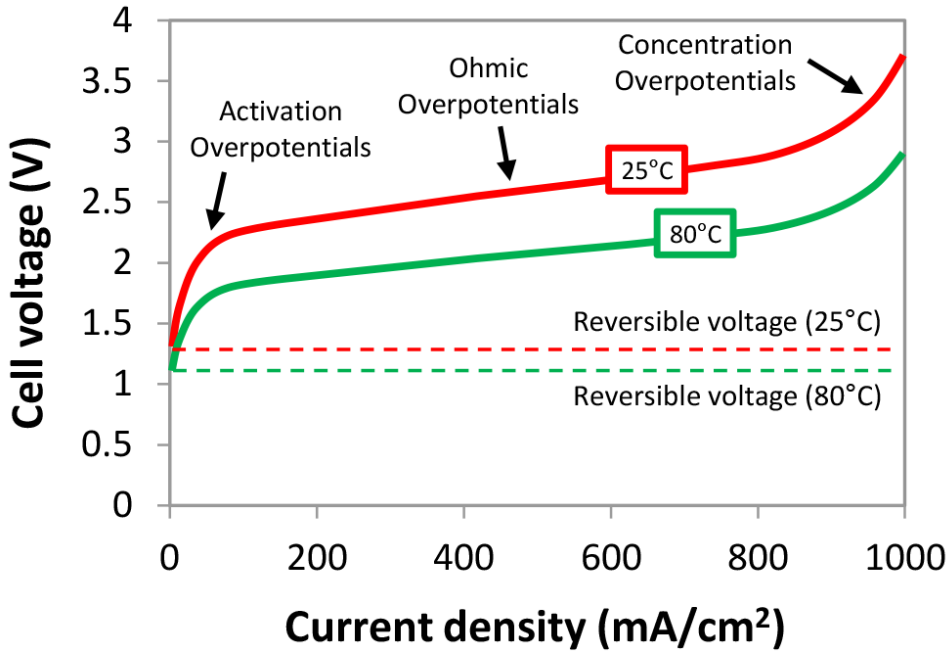
$$V_{cell} = V_{rev} + V_{act} + V_{ohm}$$

V_{rev}: Reversible voltage

V_{act}: Activation overpotential

V_{ohm}: Ohmic overpotential

- Concentration overpotential is neglected because of its minimal effects at typical operating current densities



Source: Amores et al. (2017)

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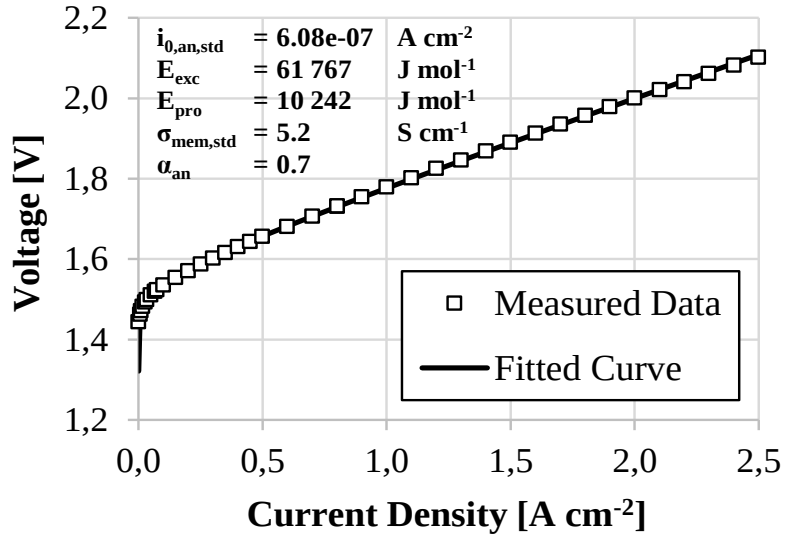
Model Validation

- Experimental data from a 1 kW PEM electrolysis test stand was used
- Data was not ideal due to lack of load steps but could be use to test the general model functionality
- Missing parameters for modeling the electrochemical behavior were determined with a non-linear least squares analysis

Parameter	*Value*	*Unit*
Max. Power	1.88	kW
Max. Current	75	A
Max. Voltage	25	V
Number Cells	10	-
Cell Area	30	cm^2
Pressure Anode	1	bar
Pressure Cathode	5	bar



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Model Validation

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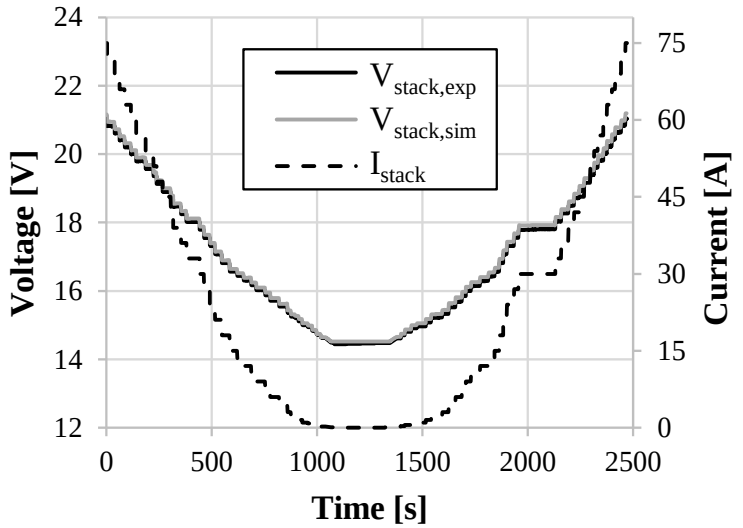
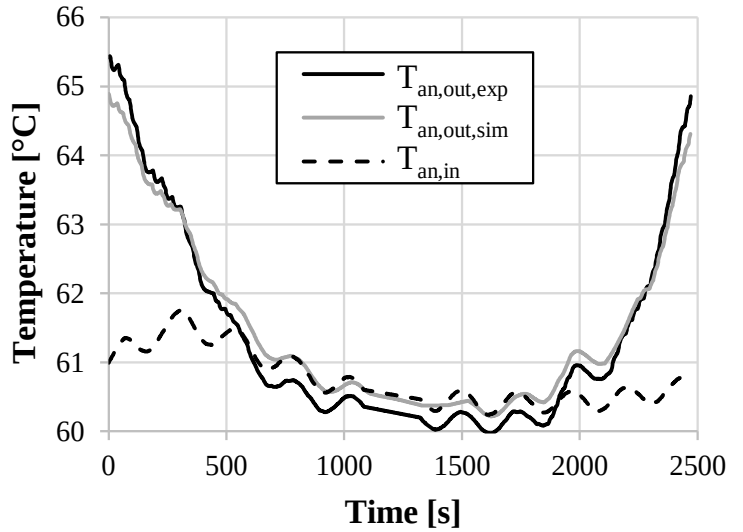
- Data was not ideal due to lack of load steps but could be use to test the general model functionality
- Missing parameters for modeling the electrochemical behavior were determined with a non-linear least squares analysis
- Results:
  - Voltage Deviation: $\Delta V_{MAE} = 0.088$ V
    $\Delta V_{max} = 0.40$ V
  - Temperature Deviation: $\Delta T_{MAE} = 0.24$ K
    $\Delta T_{max} = 0.63$ K





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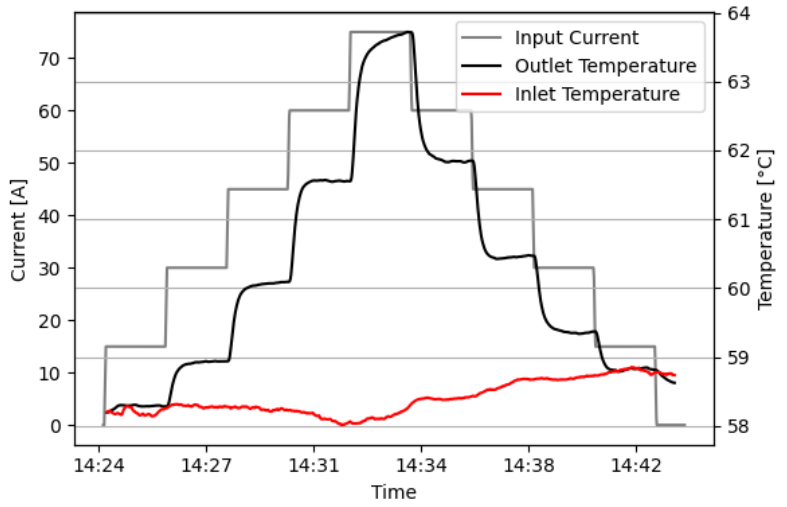
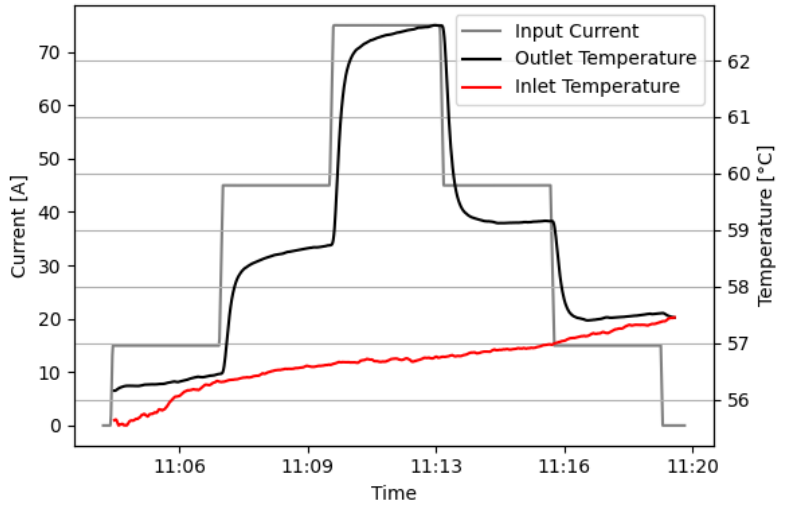
Summary

- Many assumptions have been made which need to be substantiated
  - Flow field design
  - Applied materials
  - …
- Experimental data was not ideal for assessing dynamic thermal behavior
- New data acquisition with larger load steps last week, evaluation will take place in the near future
- Construction of our own experimental setup next year





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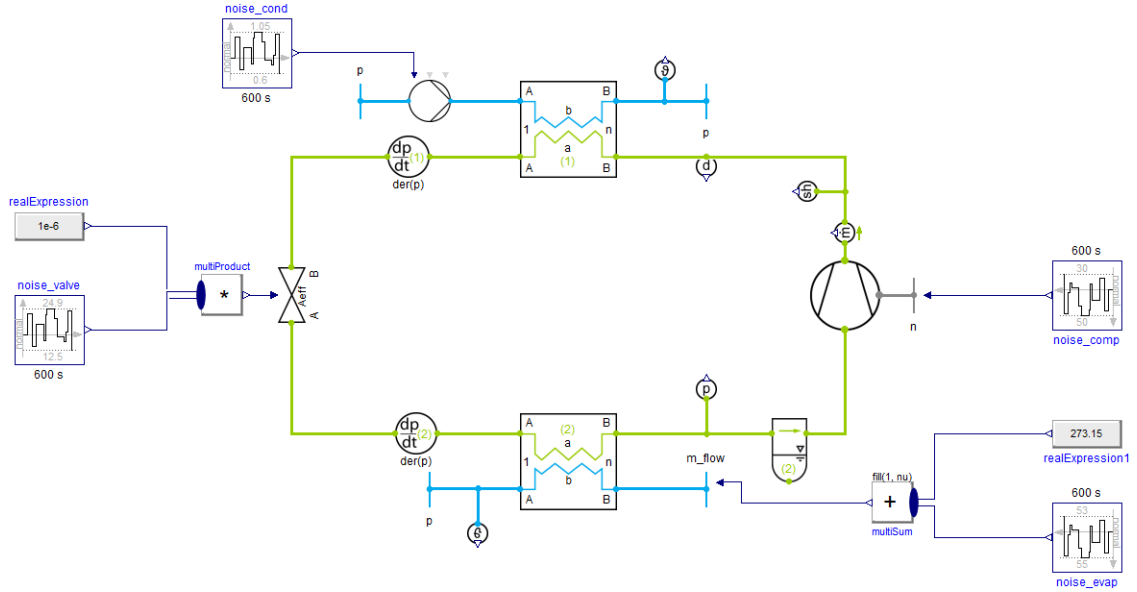
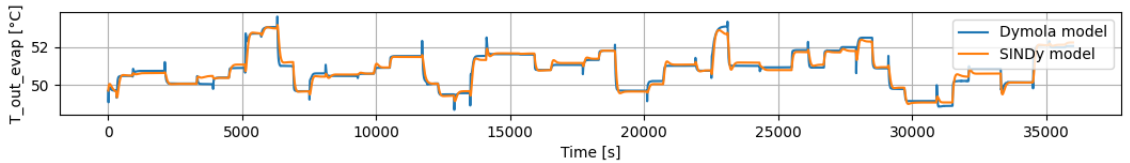
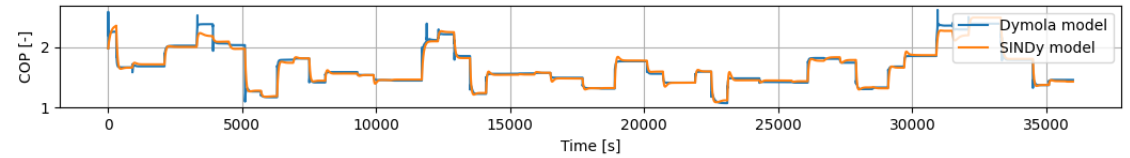
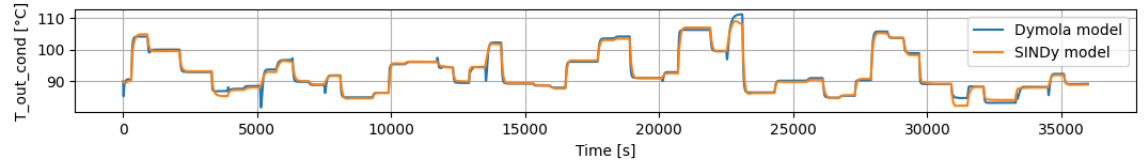
Next Steps

- Goal: Development of a control strategy for the coupled electrolyser-heat pump system
- System identification based on the complex simulation model in Modelica
- Design of a model predictive controller (MPC) based on the identified dynamic model of the coupled system
- Comparison with a classical PID control system









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Thank you for your attention!

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