Hierarchical Modeling of Polymer Electrolyte Membrane Fuel Cells

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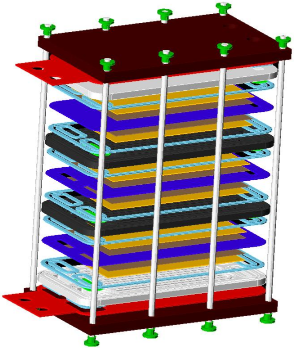
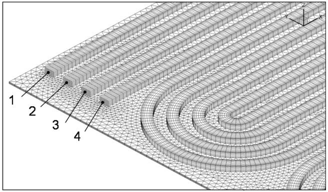
Motivation

- Detailed numerical model of fuel cell
- Include all the significant processes (species transport, electrochemical processes,...)
- Analysis performed on the level of the whole cell
- Fast and stable numerical code

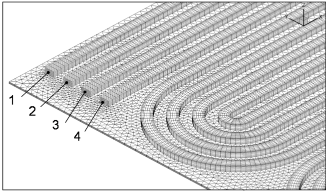


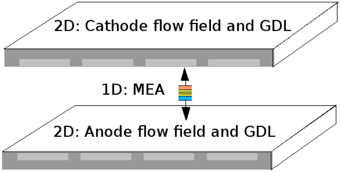
3D model drawbacks



- large area to thickness ratio of PEMFCs
- numerous coupled physical and electrochemical processes
- 3D analysis of the whole cell computationally very expensive

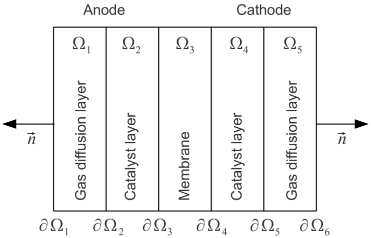
3D = 2D + 1D





- 3D = 2D + 1D + coupling → SESES + C code
- 2D: Species and charge transport in FF and GDL → SESES
- 1D: through plane response of MEA → $\underbrace{\text{COMSOL}}_{\text{model development}}$, C code

MEA model overview



- gradual building of model in several stages
- adding new fields: $3 \longrightarrow 5 \longrightarrow 7 \longrightarrow 8$
- using state-of-art parametrization from literature

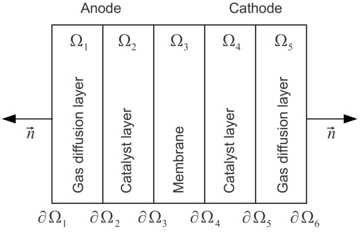
Model with 7 fields

- PDEs

$$\nabla \cdot j_{field}^{\Omega_i} = q_{field}^{\Omega_i}$$

- Fluxes

$$\begin{aligned}
j_e^{\Omega_i} &= -\sigma_e^{\Omega_i} \nabla \varphi_e, \\
j_p^{\Omega_i} &= -\sigma_p^{\Omega_i} \nabla \varphi_p, \\
j_T^{\Omega_i} &= -\kappa^{\Omega_i} \nabla T, \\
j_\lambda^{\Omega_i} &= n_{drag} \frac{j_p}{F} - \frac{D_\lambda^{\Omega_i}{}^{1.5}}{V_m} \nabla \lambda, \\
j_v^{\Omega_i} &= -D_v^{\Omega_i} \nabla c_v, \\
j_{O_2}^{\Omega_i} &= -D_{O_2}^{\Omega_i} \nabla c_{O_2}, \\
j_{H_2}^{\Omega_i} &= -D_{H_2}^{\Omega_i} \nabla c_{H_2},
\end{aligned}$$



Field	Ω_1	Ω_2	Ω_3	Ω_4	Ω_5
φ_e	X	X		X	X
φ_p		X	X	X	
T	X	X	X	X	X
λ		X	X	X	
c_v	X	X		X	X
c_{O_2}				X	X
c_{H_2}	X	X			

- Dirichlet BCs: $\partial\Omega_1$ and $\partial\Omega_6$
- Neumann BCs: at $\partial\Omega_2$ - $\partial\Omega_5$

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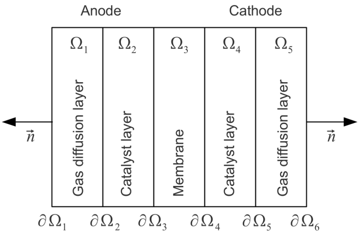

Field	Ω_1	Ω_2	Ω_3	Ω_4	Ω_5
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T	X	X	X	X	X
λ		X	X	X	
c_v	X	X		X	X
c_{O_2}				X	X
c_{H_2}	X	X			

- **Model can predict liquid water formation, but the actual field is not included.**

- Dirichlet BCs: $\partial\Omega_1$ and $\partial\Omega_6$
- Neumann BCs: at $\partial\Omega_2$ - $\partial\Omega_5$

Model with liquid water field

- Liquid water flux

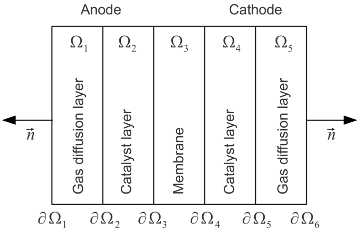
$$j_s = -\frac{K_{abs}^{\Omega_i} K_{rel}}{\mu_w} \frac{\partial p_c}{\partial s} \nabla s,$$

- Van Genuchten model

$$K_{rel}(s) = s^{\eta_k} \left(1 - (1-s)^{1/m_k}\right)^{2m_k},$$
$$s(p_c) = 1 - \left(1 + \left(\frac{p_c + p_{atm}^{std}}{p_{cb}}\right)^m\right)^{-n},$$

- Coupling with water vapor field

$$q_v^{\Omega_1} = Q_{pc}, \qquad q_s^{\Omega_1} = -Q_{pc},$$
$$q_v^{\Omega_2} = Q_{pc} - Q_{dv}, \qquad q_s^{\Omega_2} = -Q_{pc},$$
$$q_v^{\Omega_4} = Q_{pc} - Q_{dv}, \qquad q_s^{\Omega_4} = -Q_{pc},$$
$$q_v^{\Omega_5} = Q_{pc}, \qquad q_s^{\Omega_5} = -Q_{pc}$$

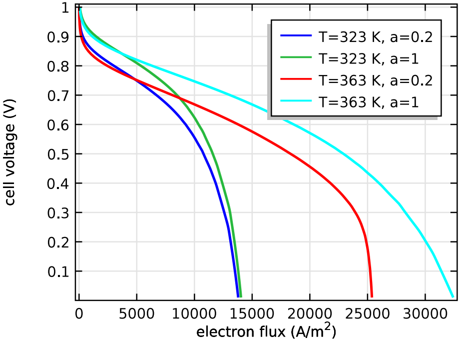


Field	Ω_1	Ω_2	Ω_3	Ω_4	Ω_5
φe	X	X		X	X
φp		X	X	X	
T	X	X	X	X	X
λ		X	X	X	
c_V	X	X		X	X
c_{O_2}				X	X
c_{H_2}	X	X			
c_S	X	X		X	X

- Dirichlet BCs: $\partial\Omega_1$ and $\partial\Omega_6$
- Neumann BCs: at $\partial\Omega_2$ - $\partial\Omega_5$

Results

- Extensive parametric study was carried out with Model with 7 fields
- The results of this model were compared with experimental data obtained at Paul Scherrer Institute, Villigen, Switzerland
- Current voltage curve



Conclusion and Future Work

- **1D MEA model including 7 fields was developed in COMSOL and verified by experiments.** ✓
- 1D model is used as a part of 2D + 1D simulation of the whole cell. ✓
- We are developing the model with one additional field for liquid water.

Thank you for your attention!