Institute of Technical Thermodynamics

# Modeling and Simulation of Transport Processes in Reinforced Polymer Electrolyte Membranes

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## Motivation

PEMs for automotive applications require good performance and a high durability. Therefore, thin PTFE-reinforced membranes which exhibit reduced mechanical degradation are state-of-the-art. Since chemical degradation of the membrane is closely coupled to local species concentrations, a detailed transport model is needed to predict chemical aging and derive optimal operating conditions for a fuel cell under driving cycle conditions.

## Modeling Approach

Software:

- DuMu$^X$[1]:
  DUNE for Multi-{Phase, Component, Scale, Physics, ...} flow and transport in porous media

Transient 2D simulation of transport based on the model of Weber and Newman[2,3]:

- Interactions between $H^+$, $H_2O$ and the membrane
- $H_2$ and $O_2$ crossover depending on hydration
- Consideration of Schröder‘s „paradox“
- Influence of PTFE-reinforcement layer

Mathematical model:

- Charge balance (electroneutrality in the PEM):

$$\nabla \cdot \mathbf{i} = 0$$

$$\mathbf{i} = S\left(-\kappa\nabla\Phi - \frac{\kappa\xi_l}{F}\overline{V}_{H_2O}\nabla p_l\right) + (1-S)\left(-\kappa\nabla\Phi - \frac{\kappa\xi_v}{F}\nabla\mu_{H_2O}\right)$$

- Mass balances for water and gas species:

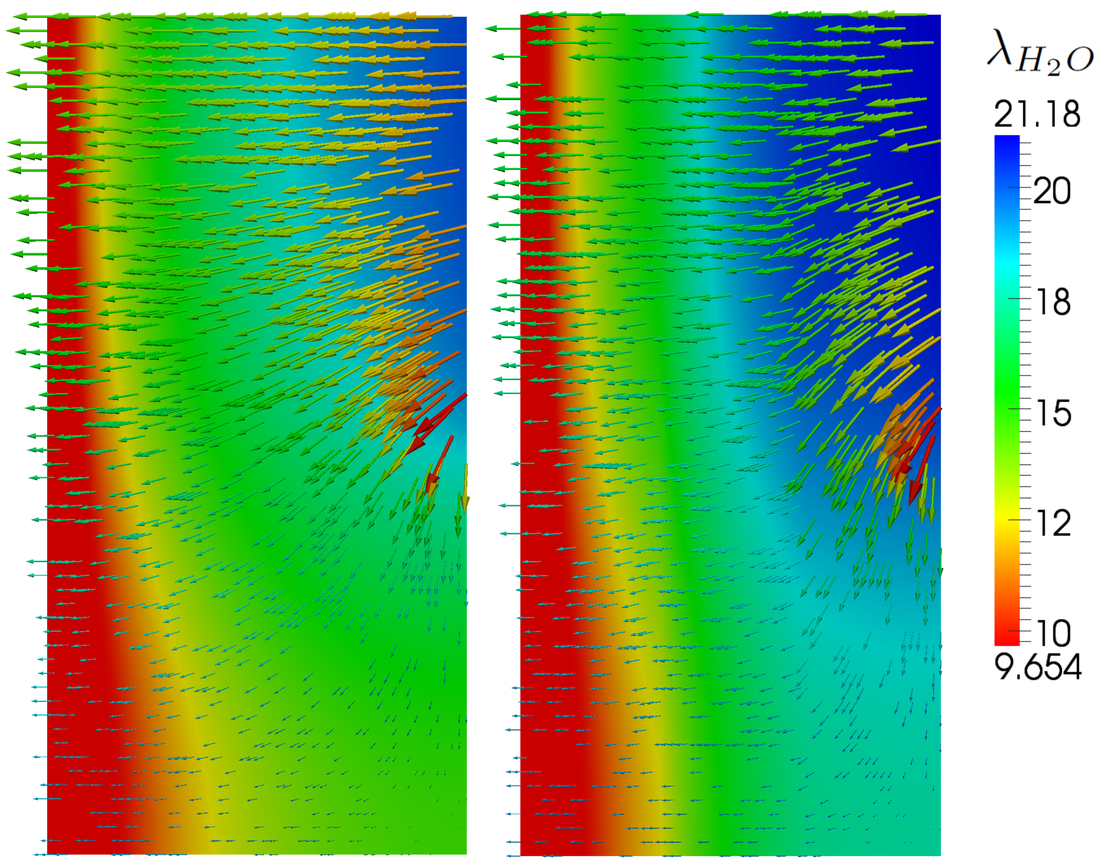
$$\phi\frac{\partial\rho_i}{\partial t} + \nabla\cdot\mathbf{N}_i = 0$$

$$\mathbf{N}_{H_2O} = S\left[-\frac{\kappa\xi_l}{F}\nabla\Phi - \left(\alpha_l + \frac{\kappa\xi_l^2}{F^2}\right)\overline{V}_{H_2O}\nabla p_l\right] + (1-S)\left[-\frac{\kappa\xi_v}{F}\nabla\Phi - \left(\alpha_v + \frac{\kappa\xi_v^2}{F^2}\right)\nabla\mu_{H_2O}\right]$$

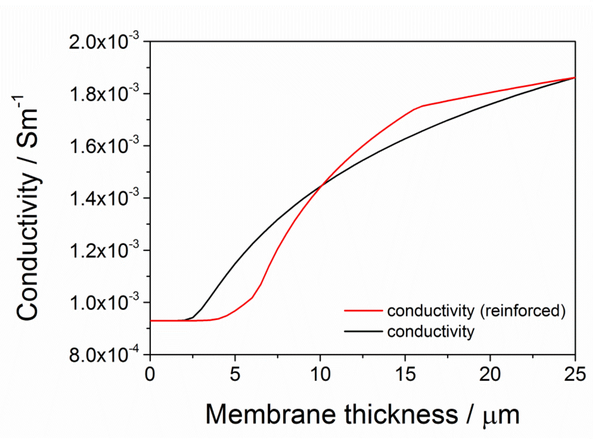
$$\mathbf{N}_{H_2} = -\psi_{H_2}\nabla p_{H_2} \qquad \mathbf{N}_{O_2} = -\psi_{O_2}\nabla p_{O_2}$$

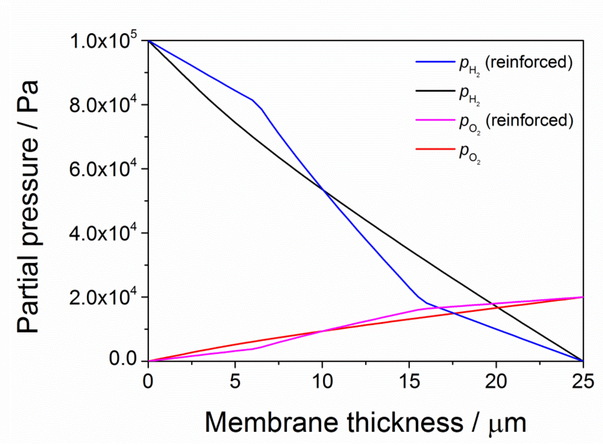
## Results

- Influence of reinforcement on membrane hydration:




- Influence on conductivity and gas crossover:




## Summary and Outlook

A transient 2D numerical model for the transport of water, protons and gases through a reinforced PEM has been established.

Future work:

Incorporation of chemical degradation, influence of chemical degradation on the performance, coupling to a complete cell model, derivation of optimal operating conditions avoiding degradation.

## References

[1]: Flemisch, B., Darcis, M., Erbertseder, K. et al. (2011). DuMu$^x$: DUNE for Multi-{Phase, Component, Scale, Physics, ...} Flow and Transport in Porous Media. *Advances in Water Resources* 34(9): 1102-1112.
[2]: Weber, A. Z., & Newman, J. (2003). Transport in Polymer-Electrolyte Membranes I. Physical model. *Journal of the Electrochemical Society*, *150*(7), A1008.
[3]: Weber, A. Z., & Newman, J. (2004). Transport in Polymer-Electrolyte Membranes II. Mathematical Model. *Journal of the Electrochemical Society*, *151*(2), A311.

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