Abstract. For the past 15 years, a lot of models have been developed to simulate a conventional low-temperature PEM fuel cells (HTPEM). However, models related to high-temperature polymer membrane (HTPEM) fuel cells (operating at temperatures of NTF5C−150°C) are rather new and still much work needs to be done to realize the same. Based on the HTPEM fuel cells and the phosphoric acid fuel cell (PAFC) modeling equations, the present work shows methods and possibilities for simulating operating and quantifying behaviour of HTPEM fuel cells using a PBI/H3PO4 (phosphoric acid − PA) based membrane. At higher operating temperatures one does not need to account for two-phase water behaviour within the vital parts of the cell, which strongly simplifies the complexity of the problem. On the other hand, detailed energy conservation should be addressed, e.g., a two-equation system could be introduced to separately account for gaseous and liquid (aqueous) phase behavior. Moreover, certain inferences could be drawn from the phosphoric acid fuel cell (PAFC) modeling, more particularly, the catalyst layer related parameters. Further, the PBI/H3PO4 membrane conductivity and transport mechanisms should be taken into account along with the consideration of gas properties. Yet another important modeling related question is the evaluation of cathode side reaction kinetics. Simulative case studies were performed at the University of Duisburg-Essen using a commercial available CFD-software tool.

1. The HTPEM fuel cell

Fuel cells convert energy stored in a fuel and oxidant into electricity according to the well known reaction:

\[ \text{Fuel} + \text{Oxidant} \rightarrow \text{Electrolyte} \]

For a fuel cell operating at a temperature of 150°C, the liquid water (porous media partial flooding), sluggish cathode electrode kinetics, low carbon monoxide tolerance of the catalyst, and electrochemical and power density constraints make the detailed energy conservation a must. In the present study, two models were compared: the LTPEM (similar PAFC when assuming aqueous phase reaction (gas dissolving)) and HTPEM (similar PAFC when assuming solid phase reaction (no gas dissolving)). Main modeling aspects:

- Gas-phase equals solid-phase temperature (thermal equilibrium)
- Evaluation of gaseous to aqueous reaction kinetics
- Detailed reaction layer considerations (volumetric fluxes)
- Concentration of dissolved species (Henry’s law)

2. HTPEM modeling aspects – Combining LTPEM and PAFC governing equations

Based on the principles of conservation, HTPEM modeling especially requires detailed reaction layer and membrane modeling which are supposed to be different from traditional governing equations whereas the computational domain is very similar to the LTPEM (e.g.: 1D, 2D (sandwich and along-channel), 3D, coupled dimensions, ...)

2.1 Bipolar-plate and gas channel (flow-field) considerations

ZBT in-house developed high temperature, compound based bipolar-plates

Main modeling aspects:

- Material parameters at elevated temperatures (e.g. thermal, electrical)
- Mechanical aspects (e.g. localized fluid-structural interactions)
- Membrane electrode assembly compression (e.g. clamping pressure distribution, gas diffusion layer deflection) (see case study in Fig. 2)

Fig.1. HTPEM modeling aspects regarding LTPEM and PAFC governing equations

2.2 Gas diffusion layer considerations

Gas diffusion layer → similar to LTPEM

Main modeling aspects:

- Two-equation system to separately account for gas and solid phase temperature within the porous media
- Heat exchange between \( \Gamma \) and \( \Gamma^* \) using a volumetric heat transfer coefficient \( \lambda \)

Fig.4. Gas diffusion layer – Energy conservation (two-equation system)

2.3 Reaction layer considerations

Reaction layer modeling → similar LTPEM when assuming gaseous phase reaction (often used)

Main modeling aspects:

- Gas-phase equals solid-phase temperature (thermal equilibrium)
- Evaluation of gaseous to aqueous reaction kinetics
- Detailed reaction layer considerations (volumetric fluxes)
- Concentration of dissolved species (Henry’s law)

Fig.5. Reaction layer modeling subdomain (gaseous phase reactions)

2.5 PBI/H3PO4 membrane considerations

Main modeling aspects:

- Proton conduction (e.g. Grothuss hopping, contribution of amorphous H3PO4)
- Possible water transfer (based on concentration gradients at anode and cathode reaction layer)
- Material fractions (PBI fraction, H3PO4 fraction, H2O fraction)
- Predicting local H3PO4 concentrations

Fig.7. PBI/H3PO4 membrane modelling

Conclusion

Several aspects and possibilities for HTPEM modeling using a PBI/H3PO4 membrane were presented. All computational domains nearly remain the same for HTPEM as it is the case for LTPEM models. When focusing the different subdomains, one can conclude that especially the reaction layer and the PBI/H3PO4 membrane need further investigation traditional modeling aspects. Volume fractions must be precisely defined. Moreover, free or unbound phosphoric acid and possible water content may have a major influence on the performance and should be incorporated when modeling HTPEM fuel cells.

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