# Mathematical Polymer-Electrolyte-Membrane Fuel Cell Model

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***Abstract**. A non-isothermal model of a low temperature polymer-electrolyte-membrane fuel cell is presented. The model is based on conservation equations coupled along with physical, electrochemical and empirical expressions. The model focuses on the implemented electrical subsystem. Thermal and species behaviour are modeled to show that a cell can operate self-humidified under predefined operating conditions. The simulation results are compared with experimental life test investigations. The model can so be used for parametric studies on fuel cell performance and layout design.*

**Introduction**
Polymer-electrolyte-membrane fuel cells (PEMFC) are expected to play an important role in tomorrow's energy conversion devices. During the past few decades, researchers have focused on cell optimization, layout and design in order to be more competitive. In this context, mathematical modeling is an indispensable tool which helps predict the behaviour of a functioning self-humidified cell. Although computer models tend to be more idealistic, they do offer tremendous possibilities to arrive at reasonable conclusions while designing fuel cells.

**Basics – What is a fuel cell?**
Electrons and protons reach the cathode side through a bipolar plate, external load and proton conducting membrane respectively. In the meantime, water either in vapor or liquid phase is produced depending on the local operating conditions. Besides, heat is produced due to strong exothermic reaction when electrical power is drawn using the external load.

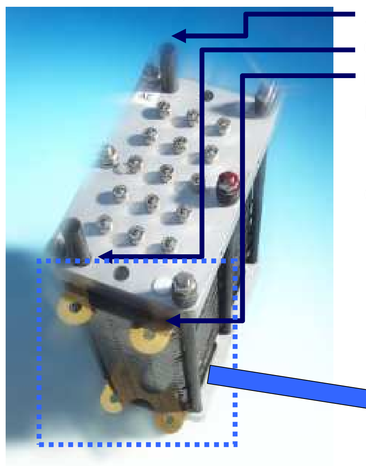


***Fig.1. ZBT standard low temperature PEM fuel cell***

**Internal electrochemical reactions**

$$2 \cdot H_2 \rightarrow 4 \cdot H^+ + 4 \cdot e^- + (Heat)$$

$$O_2 + 4 \cdot H^+ + 4 \cdot e^- \rightarrow 2 \cdot H_2O_{v,l} + (Heat)$$

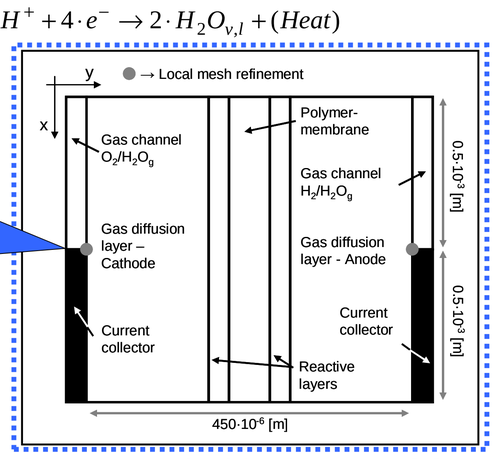


***Fig.2. 2D computational domain – 450·10-6 [m] by 1·10-3 [m] divided into five subdomains***

**Assumptions and simplifications**
- Ideal gases behaviour
- Two-dimensional sandwich model
- Constant, steady-state working conditions
- Single-phase considerations for water flow
- Momentum equation reduced to Darcy's law
- Homogeneous and isotropic material parameters
- No potential drop caused by contact resistances (i.e. constant electrical boundary potential)

**About fuel cell modeling**
Fuel cell modeling is solving for all conservation equations coupled with electrochemical, empirical equations and material parameters. Conservation laws are generally represented by the following general partially differential equation

$$d_1 \cdot \frac{\partial^2 \Psi}{\partial t^2} + d_2 \cdot \frac{\partial \Psi}{\partial t} = -\frac{\partial j_x}{\partial x} - \frac{\partial j_y}{\partial y} - \frac{\partial j_z}{\partial z} + S$$

**Focusing the electrical subsystem**
Volumetric anode and cathode current density

$$j_a = a_a \cdot i_{a,0} \cdot \left( c_{H_2} \cdot c_{H_2^{ref}}^{-1} \right)^{0.5} \cdot \frac{F}{R \cdot T} \cdot (\phi_s - \phi_m)$$

$$j_c = a_c \cdot i_{c,0} \cdot \left( c_{O_2} \cdot c_{O_2^{ref}}^{-1} \right) \cdot e^{\frac{F}{R \cdot T} \cdot (U_0 - \phi_s + \phi_m)}$$

- The electrical subsystem is the backbone of the given model set-up. In fact, the quantity *j* in provides a strong coupling between all variables.
- By solving the model sequentially fundamental data are delivered for the remaining conservation laws

**e.g.: Charge conservation**

$$-\nabla \cdot \left( \sigma_s^{eff} \cdot \nabla \phi_s \right) = \pm j_{a,c}$$

$$-\nabla \cdot \left( \sigma_m^{eff} \cdot \nabla \phi_m \right) = \pm j_{a,c}$$

**Numerical methods**
COMSOL Multiphysics (FEMLAB) is used to solve for this model. The modeling domain is discretized using a finite element method (FEM). The resulting base mesh consists of 5,406 triangular elements with a two local refinements as can be seen in Fig.2. The extended mesh consisted of 58,820 degrees of freedom (minimum element quality 0.6873). The model is solved in stages using a robust UMFPack direct solver. Owing to the strong nonlinearity of the charge conservation, one has to solve this equation first in order to use the solution as an initial guess for the next step.

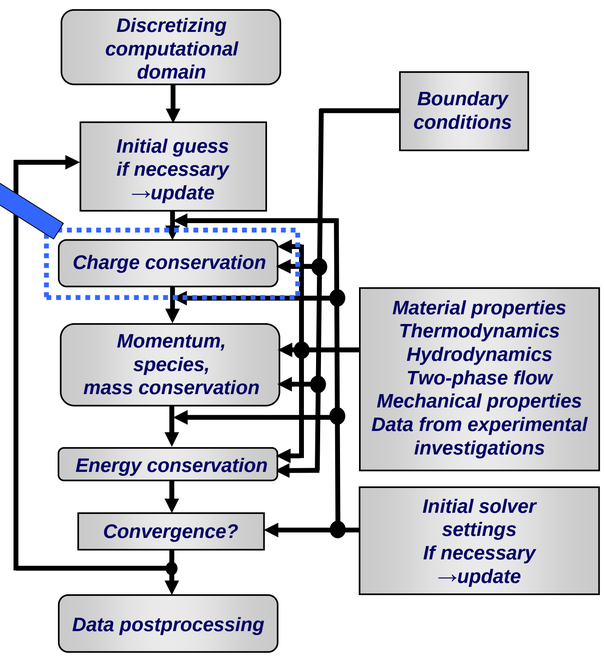


***Fig.3. Sequentially solution procedure***

A grid-independence test is carried out and showed that there is no notable difference in quantities behaviour. For the standard case (single phase calculations), the solution time was around 3,000 seconds on a Windows PC platform (1GBRAM) to obtain a converged solution within 76 iteration steps. Solving for two-phase flow (see Fig.7) dramatically increases the complexity of the equation system and 279 iterations are needed for a converged solution. In order to get more stability into the highly nonlinear equation system, non-ideal constrains are used for the membrane water transport equation and for pore saturation calculations.

**Simulating the electrical subsystem**
The following plots do show various quantities related to the electrical subsystem. Conservation of charge needs to be solved for electrical and ionic phase potential.

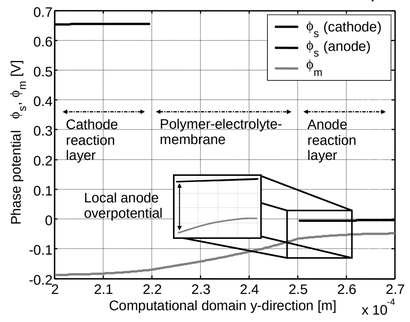


***Fig.4. Solid and ionic phase potential***

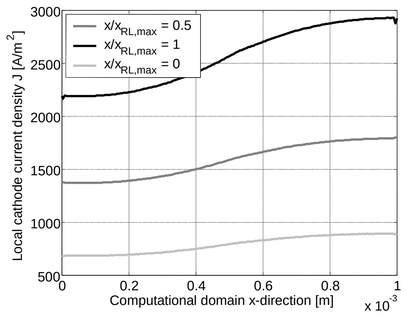


***Fig.5. Reaction layer current density***

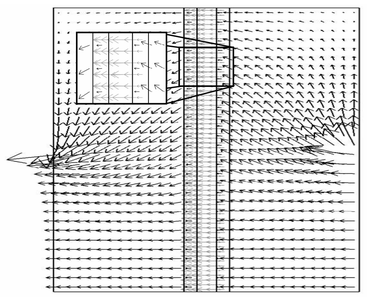

***Fig.6. Electrical and ionic current density distribution***

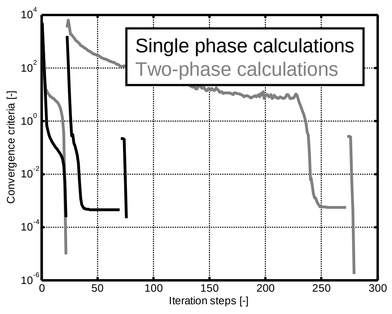


***Fig.7. Model convergence behaviour***

**Model validation against experimental investigations**
To validate the model set-up, the simulations are compared to a life test investigation. All experimental investigations were run at ZBT facility (Fig.8) in a life test over a longer period of time using a commercially available MEA. As for the cell layout a channel-to-land ratio of 1/1 was used for the flow-field design. The active area was 0.005 [m²].

**Operating conditions**
Gases are feed at room temperature with a relative humidity of 10 [%] (hydrogen) and 40 [%] (air) respectively. To maintain self-humidification, the cell runs at a voltage of 0.65 [V]. The operating temperature is maintained at a temperature of 313.15 [K]. Fig.5. shows the comparison of the polarization curves. The low current density results from the low cell voltage level and operating conditions and is predestined for such life test investigations. Now, back-diffusion of water in the membrane of the cell overcomes the electro-osmotic drag resulting in a net water flux from cathode to anode

***Fig.8. Center for Fuel Cell Technology (Zentrum für BrennstoffzellenTechnik (ZBT) gGmbH) in Duisburg/Germany***

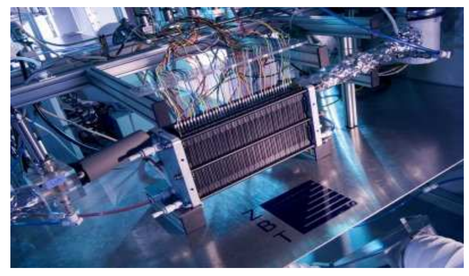

***Fig.9. Typical fuel cell teststand at ZBT***

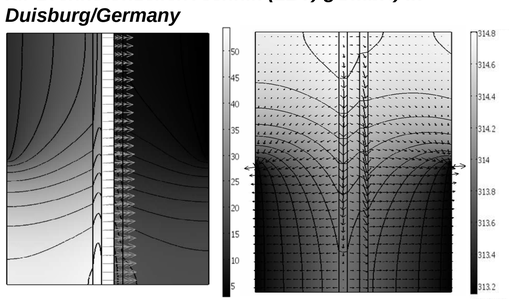

***Fig.10. Simulation of life time operating condition (Relative humidity and temperature distribution over the computational domain)***

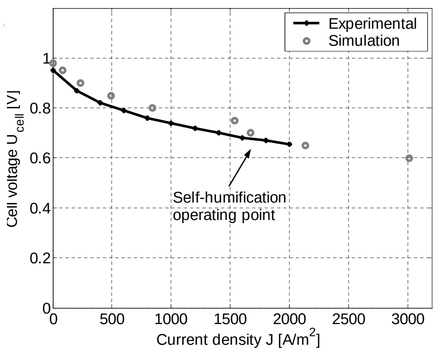


***Fig.11. U-I-Curve***

**Conclusion**
- A two-dimensional, non-isothermal PEMFC model is presented and validated
- The electrical subsystem is integrated as the backbone for this CFD study as it delivers fundamental data for solving remaining conservation laws.
- Phase potential and local current density distribution are presented and match with open literature data
- It is shown that a significant self-humidification effect occurs within PEMFC under precise operating conditions
- Water flux is balanced in a way that anode dry-out and cathode flooding is avoided

$$\nabla \cdot \left( \frac{n_{drag} \cdot I \cdot M_{H_2O}}{F} - D_{H_2O} \cdot \nabla c_{H_2O} - c_{H_2O} \cdot u_{H_2O} \right) = 0$$

- The simulated temperature distribution shows that the cell temperature is kept almost constant as no local hot spots are present which benefits the lifetime of a MEA
- No significant degradation was seen during operation
- It appears that the polarization curve is well reproduced by the model

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