

A numerically highly efficient dynamic quasi-2D PEMFC model including non-isothermal and phase change processes

Florian Altmann^{1,2,3}, Dominik Kuzdas³, Dominik Murschenhofer⁴, Johanna Bartlechner²,
Christoph Hametner², Stefan Jakubek², Stefan Braun³

¹Institute of Applied Physics, TU Wien, Wiedner Hauptstraße 8-10, 1040 Wien, Austria

²Institute of Mechanics and Mechatronics, TU Wien, Getreidemarkt 9, 1060 Wien, Austria

³Institute of Fluid Mechanics and Heat Transfer, TU Wien, Getreidemarkt 9, 1060 Wien, Austria

⁴Institute of Engineering Thermodynamics, DLR, Pfaffenwaldring 38-40, 70569 Stuttgart, Germany
florian.altmann@tuwien.ac.at

Current PEMFC simulation environments are complex and computationally demanding, limiting their applicability for dynamic simulations. To address these challenges, this work presents a highly efficient non-isothermal PEMFC model with multiphase flow, tailored for dynamic simulations. The model extends the isothermal approach by Murschenhofer et al. [1], bridging the gap between numerically expensive 3D models and fast 0D/1D models that lack spatial resolution by using a quasi-2D approach, see Figure 1(a).

The proposed model captures key phenomena, including two-phase transport by convection, multi-component diffusion and capillary fluxes in the gas channels (GCs) and gas diffusion layers (GDLs), and membrane water transport by electro-osmotic drag and diffusion as well as nitrogen crossover through the membrane. It also accounts for finite-rate mass transfer during sorption and desorption processes between the membrane and the electrodes, as well as heat generation from chemical reactions, finite proton conductivity, and phase changes. A numerical scheme employing linearisation in time (LIT) of the governing equations and a Chebyshev collocation method for spatial discretisation ensures low computational effort. By further utilizing a particle swarm optimization algorithm, it is easily possible to extract otherwise inaccessible model parameters by fitting the model's polarization curve to a desired reference case, e.g. to data from an experimental setup.

Validation of the model is conducted against steady-state computational fluid dynamics (CFD) simulations of a 3D fuel cell geometry performed using AVL Fire™. The results of the LIT model, in terms of polarization curves and the distributions of gaseous species, temperature, liquid water, and PEM water content, show fairly good agreement with the CFD simulations, while reducing the computational effort from hours to minutes. The latter two comparisons are illustrated in Figures 1(b,c). Furthermore, the transient behaviour of temperature and liquid water accumulation in the electrodes qualitatively aligns with data from existing literature [2, 3].

The model's capabilities offer a valuable tool for fuel cell control engineering, facilitating efficient control unit optimization and state-observer predictions. Its computational efficiency makes the presented model particularly suitable for widespread parameter studies and performance analyses.

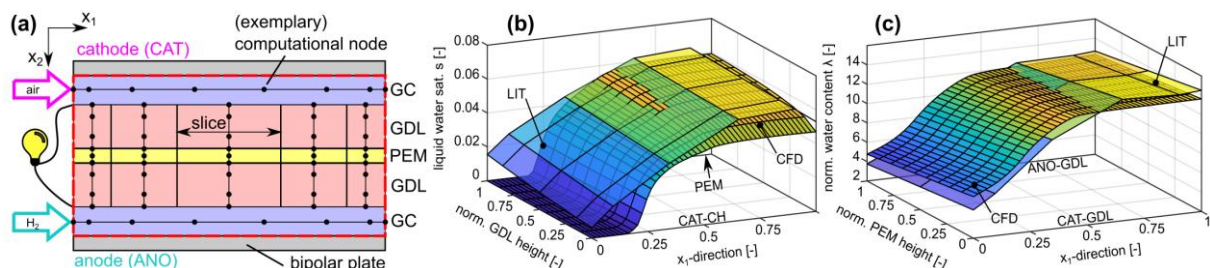


Figure 1: (a) Quasi-2D computational domain. Comparison of steady-state results from the LIT model and CFD simulations: (b) liquid water saturation in the cathode GDL, (c) PEM water content.

References:

1. D. Murschenhofer et al., *Energ. Convers. Manage.* **162** (2018), 159-175
2. H. Wu et al., *J. Electrochem. Soc.* **157** (2010), B1-B12
3. A. Goshtasbi et al., *J. Electrochem. Soc.* **166** (2019), F3154-F3179