

1-D+1-D PEM Fuel Cell Stack Model for Advanced Hardware-in-the-Loop Applications

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ABSTRACT

As part of a system model, a PEM fuel cell stack model is presented for functional tests and pre-calibration of control units on hardware-in-the-loop (*HiL*) test benches. From the basic idea to couple a 1-D membrane model with a spatially distributed abstraction of the gas channel, a real-time capable 1-D+1-D PEM FC stack model is constructed. Fundament for the *HiL* usage is an explicit formulation of the commonly implicit model equations. With that, not only calculation time can be reduced, but also model accuracy is preserved. A validation using test bench data emphasizes the accuracy of the model. Finally, a runtime and eigenvalue analysis of the stack model proves the real-time capability.

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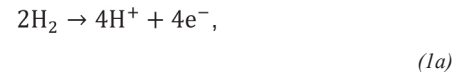
INTRODUCTION

The development of modern drive concepts is strongly influenced by the challenge to meet legal emission regulations and customer demands for powerful but also comfortable and reliable propulsion. By significant improvements in costs, efficiency, and durability, fuel cells get more and more attractive for commercial automotive usage [1]. Their ability to convert hydrogen into electrical energy in a clean way in conjunction with large driving ranges and short refueling times, resolves central problems in present electrical vehicle concepts. However, competitiveness of fuel cell systems requires ongoing progresses. This comprises constructive as well as functional improvements in control, diagnosis, and operation functionalities to exploit given technological potentials. As helpful development tools, hardware-in-the-loop methods have proven themselves in practice by their suitability to improve the functional development process while reducing costs. With the aim to test control unit software as realistic as possible, *HiL* setups offer the option to substitute the physical test bench with a mathematical abstraction. According analog or digital sensor and actuator signals are reproduced to communicate directly with the control unit. Making the assessment and test of functional software possible, regardless of the availability of test benches, is a significant contribution to decrease costs and speed-up functional development for fuel cell control units (*FCCU*). Moreover, automation and reproducibility of the results are additional key benefits as well as the replacement of safety critical, costly, and time intense investigations. But the mandatory modelling of the physical

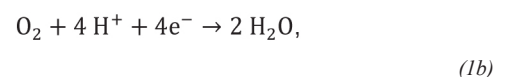
system is restricted by the required real-time capability of the resulting equations. With that, runtime limitations but also stability of the used solver method have to be taken into account explicitly. Despite this, due to the influence of fluid, thermal, and electrochemical phenomena on efficiency as well as life cycle [2], modern *FCCU* development demands highly sophisticated multi-domain PEM FCS models.

Basis of the energy conversion within a fuel cell is a spatially separated redox-reaction of hydrogen H_2 and oxygen O_2 according to

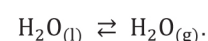
Anode:



Cathode:



Water:



With water and wasted heat, only non-polluting emissions are released. In detail, hydrogen H_2 is oxidized to H^+ at the positive electrode (anode). By an exclusively proton conducting membrane, the released electrons are forced to pass an external load where they perform work while protons can diffuse directly through the membrane. At the cathode side, protons as well as electrons reduce oxygen to water. The generated amount of water cannot be neglected for a correct description of the thermodynamic state. Thus, phase transition within the stack has to be considered. Fig. 1 depicts the schematic structure of a PEM fuel cell. Central part is the conjunction of gas diffusion layer (GDL), catalyst layer (CL) and membrane also denoted as membrane electrode assembly (MEA). These layers determine the electrochemical characteristic of the overall fuel cell stack. The outer bipolar plates including the reactant and coolant channels specify the mass and heat transport within the cell.

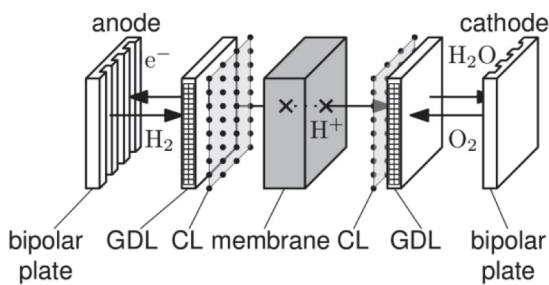


Fig. 1. Functional layers of a PEM fuel cell.

In the presented work, a transient 1-D+1-D PEM FC stack model is proposed. Embedded in a system model and coupled to a real control unit, sophisticated closed-loop *HiL* test and development applications are addressed. Initially, basic model requirements are determined by reviewing the hardware in the loop use-case. The 1-D+1-D FCS modelling is outlined afterwards, to introduce the detailed abstraction of the stack. Here, the 1-D membrane water content and water flux modelling as well as the 1-D abstraction of the gas channel and bipolar plate is discussed. The coupling of the spatially distributed models is performed using fluid, thermal and electric boundary conditions. Finally, the resulting stack model is evaluated using test bench data in combination with a simulation study. Periphery like hydrogen recirculation and air conditioning is out of the scope of this work. On the example of the air supply system, the modelling of the overall system as well as the coupling with the stack is discussed in [3].

FCS MODEL

Advanced *HiL* applications conduct functional development and pre-calibration of control units. Regardless of the specific test cases, a flawless closed-loop operation of control unit and the emulated stack has to be ensured. Therefore, a qualitatively correct model behavior is necessary. This comprises accurate stationary and dynamic behavior over the complete operating range from idle to full load of the stack. While a complex periphery is needed for the optimal conditioning of cell reaction (1), a suitable multi-domain fuel cell stack model is mandatory to reproduce the interactions with the supply system precisely. Beyond that, the *HiL* application comprises a variety of additional requirements:

- R1. The model complexity is restricted by the demand for real-time capability. Hence, the balance between *FCCU* test requirements and accuracy of the model comes to the fore. In addition, not only the choice of the solver algorithm is restricted, also the stability must be investigated in detail.
- R2. PEM fuel cells are such compact devices, including proprietary materials, that the identification of model parameters can be a critical task. The parameterization of such a model should be possible using common test-bench data. Non-measurable parameters are obtained by data sheet specifications and literature values. Dedicated fitting parameters ξ are introduced to ensure accurate behavior.
- R3. The sampling rates of the *FCCU* are usually in a range of $\tau_{\text{ecu}} = 1 - 10\text{ms}$. According to Shannon's Law [4], only transients with a time constant τ larger than twice of the sampling rate can be unambiguously reconstructed from the control unit according to

$$\tau \geq 2 \cdot \tau_{\text{ecu}} \quad (2)$$

In the modelling process, faster transients shall be neglected.

- R4. The applicability of the model is strictly associated with the considered phenomena. Typical operations like (cold) start-up, extended idle and hydrogen purge shall be possible. From that, application-related effects like water transport through the membrane as well as temperature dependent stack and fluid characteristics have to be considered.
- R5. The cell design is a key aspect of intense system optimization and influences the operation strategy significantly. This is emphasized by the difference of co-/counter-flow architectures [5]. The non-linear characteristics of the fuel cell make it necessary to consider the spatial distribution of the cells.

The presented requirements R1-R5 influence the overall modelling of the fuel cell stack. Furthermore, a clear concept is crucial to provide exchangeability and ensure a suitable handling of such a complex model.

In literature, a variety of PEM fuel cell stack models are proposed for real-time applications. Most approaches focus on a single cell model with a detailed consideration of the functional layers, but neglecting the spatial distribution of the cell [6], [7]. In contrast, a multi-cell model is presented in [8]. However, the handling of such models in daily practice is usually inconvenient, because a detailed parameterization of *GDL* and *CL* is necessary. Nevertheless, a real-time proved spatially distributed fuel cell stack model is not known to the best of the author's knowledge which covers the requirements R1-R5. Referring to the work of [9] and [10], a detailed 1-D+1-D multi-domain fuel cell stack model for real-time applications is presented. This includes a transient membrane water content model, non-linear current distribution as well as application-related cold start effects to enable advanced *HiL* operations with a *FCCU*.

Preliminaries

An essential property of fuel cell systems is, that the condition for the cell reaction changes considerably across the stack. The mass conversion according to reaction (1) influences the local availability of the reactants. The production and phase transition of water impacts the state of the membrane and with that the electric behavior of the cell. But the occurring non-linear current, humidity, and temperature distribution along the gas channel geometry cannot be taken into account with a lumped-parameter model. Nevertheless, advanced operation strategies like internal humidification address the spatially distributed characteristics on purpose.

Initial point of the modelling is the consideration of the flow-field layout. Hereby, the cell is separated into single segments along the channels according to fig.2. While the z -coordinate follows the gas flow, the x/y -coordinate is arranged perpendicular on the membrane/gas channel. Each cell segment conducts all functional layers of a fuel cell including electrodes and *MEA*. As basis for the stack modelling, the following general assumptions can be made.

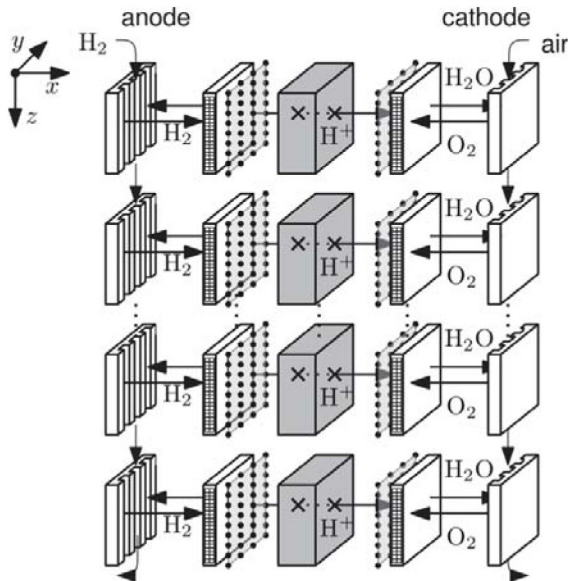


Fig.2. Cell discretization using straight flow field and coolant channel design for simplicity.

- A1. All gases are considered as ideal gases. In addition to hydrogen H_2 at the anode, respectively oxygen O_2 at the cathode, water vapor H_2O and nitrogen N_2 are distinguished.
- A2. Reactant pressure losses occur exclusively in the gas channel. Pressure drops in the catalyst and gas diffusion layer are neglected.
- A3. The large thermal capacity of the coolant causes a linear temperature increase in the cooling channel. Contrary to this, a non-linear temperature profile for the reactants can be assumed by their small thermal capacities.
- A4. Compared to the bipolar plate, the mass of the *MAE* is neglectable. A homogenous temperature distribution along the x -axis can be assumed and heat transfer processes between adjacent *MAEs* are not regarded.

- A5. The expansion of the membrane in direction of the x - axis is smaller by magnitudes as in z/y - direction. Thus, spatial pressure and concentration gradients as well as the transport of protons and water through the membrane take place exclusively in x -direction.

A1-A3 describe basic assumptions for the physical modelling and are recalled when applied. For the overall model structure, A4 and A5 are of major importance. Here, heat and mass exchanged between adjacent *MEAs* is excluded. In consequence, the boundary conditions given by gas channel and bipolar plate model determine the state of the *MEA*. On the one hand, the electric cell behavior is decoupled from the thermal and fluid modelling, and on the other hand, stack design affects solely the outer cell parts simplifying the model handling. Finally, the separate discussion of *MEA* and bipolar plate modelling is motivated.

MEA Modelling

Electric Subsystem

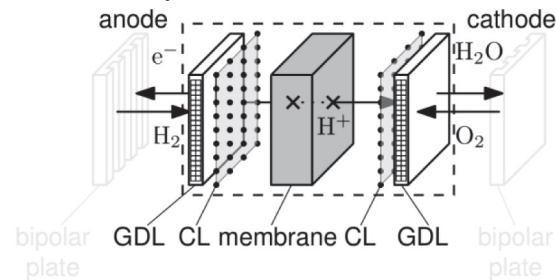


Fig.3. Fuel cell membrane electrode assembly.

The electrical behavior of a fuel cell system is mainly determined by the membrane electrode assembly according to fig. 3. Here, the overall cell voltage V_{cell} is expressed by a sum of different terms related to various physical phenomena

$$V_{\text{cell}} = V_{\text{rev}} - V_{\text{ohm}} - \eta_{\text{act}} - \eta_{\text{lim}} \quad (2)$$

The reversible cell voltage V_{rev} , also denoted as Nernst voltage, marks the upper theoretical limit of the cell voltage V_{cell} . The charge transfer resistance at the catalyst layers is considered via the activation loss η_{act} . Losses due to the transport of H^+ through the membrane and electrons through the *GDL* are summarized in V_{ohm} . Finally, the limited gas transport in the gas diffusion layer is considered by the concentration loss term η_{lim} [11].

While the steady state assumption regarding R3 holds for reversible and ohmic cell voltages, the transients of activation and limitation losses are taken into account. The corresponding differential equation for the so called double layer effect at the electrode surface [11] reads as

$$\dot{\eta}_{\text{act}} = \frac{j}{c_{\text{DL}}} \left(1 - \frac{\eta_{\text{act}}}{V_{\text{act}}} \right), \quad (3)$$

with the current density J , the double layer capacity C_{DL} , and the steady state activation loss V_{act} . In a simplified way, the limitation losses η_{lim} are defined by

$$\dot{\eta}_{lim} = \frac{J}{c_{lim}} (V_{lim} - \eta_{lim}). \quad (4)$$

Both phenomena in eq. (3) and (4) are based on the aggregation of charge/concentration at the catalyst/gas diffusion layer.

In general, the steady state cell potential according to eq. (2) is a complex term influenced by current density J , cell temperature T_{cell} , reactant pressures and the humidity of the membrane. As an example, the reversible cell potential V_{rev} can be obtained by the equilibrium of the fundamental cell reaction (1) and reads as

$$V_{rev} = V_{rev}^0 + \xi_1 (T_{cell} - T_{ref}) + \xi_2 T_{cell} \ln \left(\frac{p^{H_2} \cdot \sqrt{p^{O_2}}}{p_{ref}^{1.5}} \right), \quad (5)$$

with the hydrogen and oxygen partial pressure p^{H_2} and p^{O_2} as well as the parameters [12]

$$\begin{aligned} \xi_1 &= -8.5E^{-4} \frac{V}{K}, & \xi_2 &= 4.308E^{-5} \frac{V}{K}, \\ p_{ref} &= 101330 \text{ Pa}, & T_{ref} &= 273.15 \text{ K}. \end{aligned}$$

In contrast, a variety of phenomenological and empirical approaches exist for the loss phenomena [12],[13],[14]. Thus, activation and limitation losses are formulated generally

$$V_{act} = f_{act}(T_{cell}, J, p^{O_2}, p^{H_2}, \xi_{act}), \quad (6)$$

respectively

$$V_{lim} = f_{lim}(T_{cell}, J, p^{O_2}, p^{H_2}, \xi_{lim}), \quad (7)$$

including the parameters ξ_{act} and ξ_{lim} . The limited conductivity of membrane and electrode is considered via Ohms law

$$V_{ohm} = J \cdot (R_{mem} + R_{cont}), \quad (8)$$

with the membrane and contact resistance R_{mem} and R_{cont} . While the contact resistance is determined by the material properties of the electrodes and reads as

$$R_{cont} = f_{cont}(T_{cell}), \quad (9)$$

the membrane resistance R_{mem} is defined using the thickness of the membrane l_x , as well as the relative conductivity σ_{mem} and the dimensionless fitting parameter $\xi_{mem,\sigma}$ by

$$R_{mem} = \frac{l_x}{\xi_{mem,\sigma} \cdot \sigma_{mem}}. \quad (10)$$

Beyond this fundamental relation, different phenomenological approaches exist to consider temperature and water content [15], [16]. In common, an approach of the form

$$\sigma_{mem} = \sigma_{30}(\lambda_{mem}) \cdot \sigma_T(T_{cell}), \quad (11)$$

is used. Where σ_{30} is assumed as linear water content characteristics at reference temperature of $T_{cell} = 303 \text{ K}$ according to

$$\sigma_{30} = 0.5139 \cdot \lambda_{mem} - 0.326. \quad (12)$$

Especially for cold start-up of the stack, varying cell temperature can be considered with σ_T , which is realized by an Arrhenius approach [15]. The scaling from cell to stack level via

$$V_{stack} = n_{cell} \cdot V_{cell}, \quad (13)$$

is determined by the number of cells n_{cell} per stack. With that, the electric modelling of the MEA can be finalized.

Thermal Subsystem

A proper and efficient description of the fluid membrane behavior is a central challenge in fuel cell modelling. As results from several transport phenomena, a non-linear membrane water distribution $\lambda(x)$ is determined which influences the electric behavior according to eq. (11). In addition, typical material properties like the membrane water diffusion coefficient $D(\lambda, T)$ cannot be identified trivially and vary in literature [17], [18]. Thus, interchangeability and handling of the membrane model equations must be considered to cover changing requirements regarding R3.

A well-known approach taking diffusion and the electro-osmotic drag into account is proposed in [15]. For that, a non-linear boundary value problem has to be solved to obtain the water flux $\dot{m}_{mem}^{H_2O}$ through membrane as well as the mean-value water content λ_{mem} . However, the required iterative solver methods make a reliable prediction of the calculation time impossible and exclude real-time application. Different approaches are given in literature to circumvent this obstacle. In [19], a linearization is used to attain an explicit formulation of the membrane equations at the cost of accuracy. In [5], a reformulation of the membrane equations leads to a polynomial equation of third order which can be solved.

An attractive way to minimize calculation effort and conserve model accuracy is given by [9]. Basic idea is to solve the complex membrane equations offline and provide membrane data via more-dimensional maps. A normalization of the central water transport equation reduces the order of the maps and makes the solution adjustable to different types of membranes without recalculating the table data.