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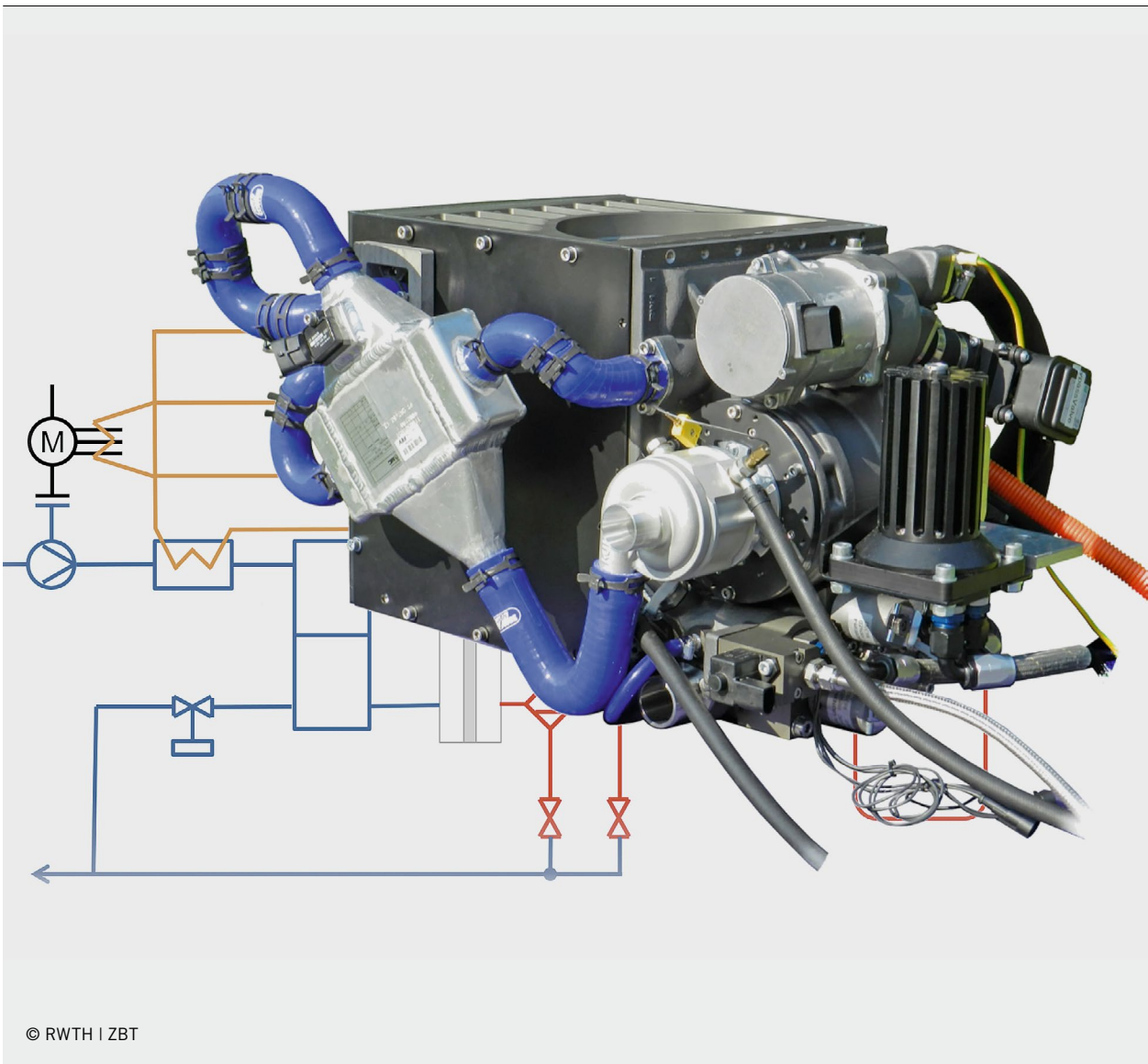
Modular Fuel Cell System Simulation Environment with Focus on Membrane Water Management

The water balance of a fuel cell decisively influences its performance. For examination, within an FVV research project a stack/system model was developed at the Chair of Thermodynamics of Mobile Energy Conversion Systems (TME) at RWTH Aachen University and the Hydrogen and Fuel Cell Center ZBT in Duisburg. In the follow-up project (FVV no. 1411), the model is being extended in order to particularly illuminate the influence of liquid water.



1 LIQUID WATER INFLUENCE IN THE FUEL CELL

The model, which emerged from the FVV predecessor project "FC System Simulation – Membrane Water Management" (FVV project no. 1298) [1], can be used for cell, stack, component and system design as well as for operating strategy development, among other things. The stack model is based on a fuel cell model developed at the ZBT, which, in addition to the general current and voltage dependencies, also represents spatially resolved processes within a Polymer Electrolyte Membrane Fuel Cell (PEM-FC) [2, 3]. Besides, the cold start capability of fuel cells is also being investigated in the FVV follow-up project. At operating temperatures of 20 °C or below, the air can absorb orders of magnitude less water in gaseous form than at nominal operating temperature. Therefore, considering liquid water and the associated interactions is mandatory.

The first step is to calculate the amount of liquid water and the opposing saturation of the Gas Diffusion Layer (GDL). The approaches used are based on the work of Ferreira [4]. On the one hand – similar to Fick's diffusion law – the liquid water is the driving force for water transport in this process. On the other hand, it is the liquid water itself to form the transport channels for the water. The water transport can be described by Eq. 1, with s being the saturation, N the molar flow of liquid water, ρ the density of liquid water, M the molar mass, K the absolute permeability, μ the dynamic viscosity, σ the surface tension, θ the contact angle, ε the porosity, J the Leverett J-function, dz the water transport path length, and ds the difference in saturation between the electrode and the channel:

Eq. 1 $$N_{H_2O,l} = \frac{\rho_{H_2O(l)}}{M_{H_2O}} \frac{K s^3}{\mu_{H_2O}} \frac{\sigma \cos\theta_c}{\sqrt{K/\varepsilon}} J(s) \frac{ds}{dz}$$

Since the conductivity and the saturation by liquid water are coupled by the third power, small amounts of liquid water lead to significant saturations of the GDL. In the literature various models can be found for the influence of water on the effective diffusion coefficient D_{eff} [5, 6]. However, basically all these models have in common that the reduced free diffusion space has an overproportionally large influence on D_{eff}. Compared to the free gas space and the space filled with porous material, **FIGURE 1** (a and b), additionaly the average length of the diffusion paths is increased in the space with pores blocked by liquid water, **FIGURE 1** (c). Eq. 2 is used for the calculation, where D_{eff} refers to the dry state and $D_{eff,l}$ refers to the state filled with liquid water:

Eq. 2 $$D_{\mathrm{eff},l}(s) = D_{\mathrm{eff}} (1 - s)^3$$

The diffusion within the catalyst layer is calculated analogously.

FIGURE 2 shows exemplary calculation results of the extended model. Along the entire cathode channel, a higher saturation is calculated under the channel, **FIGURE 2** (left), which can be explained by the longer diffusion path from the electrode below the landing to the channel. The higher saturation of the GDL under the landing results in the current density under the channel being higher than the corresponding current density under the landing,

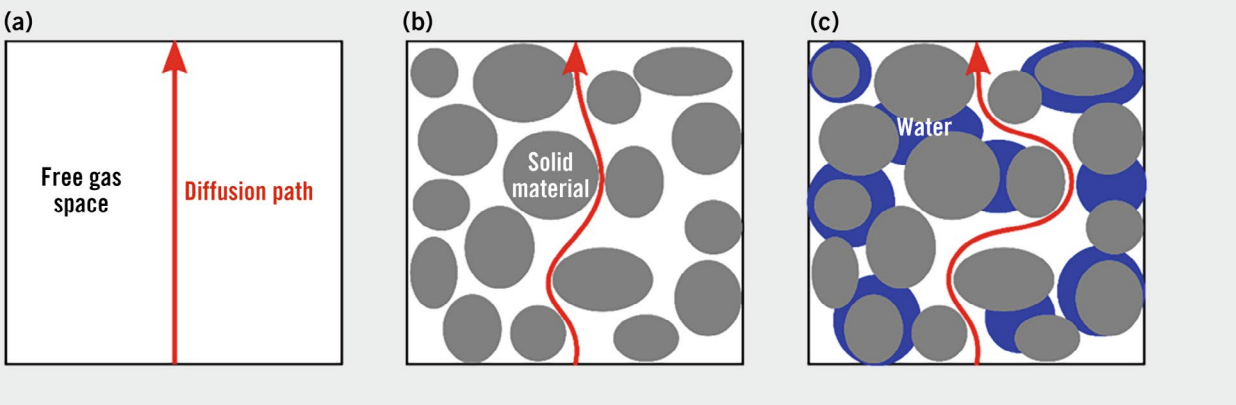


FIGURE 1 Change in the free diffusion path through the free gas space (a), through porous material (b) and through porous material with liquid water (c) (© RWTH I ZBT)

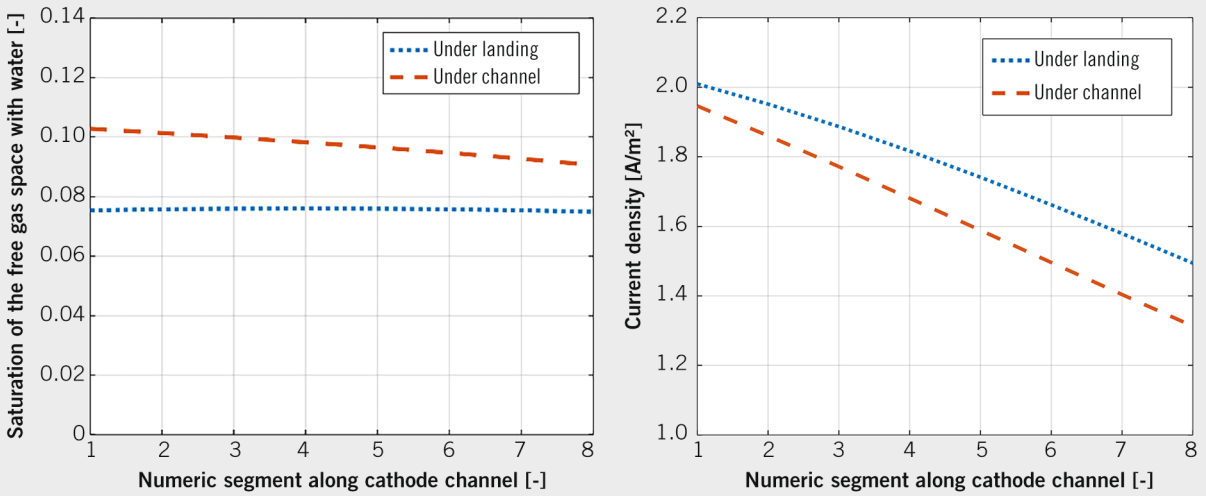


FIGURE 2 Exemplary results for a fully saturated media supply with a stoichiometry of 2, a cell temperature of 70 °C, an operating pressure of 2 bar_{abs} and an average current density of 1.7 A/cm²; calculated saturation in the GDL under the channel and under the landing respectively (left), corresponding calculated current density (right) (© RWTH I ZBT)

FIGURE 2 (right). The higher saturation at the inlet of the cathode compared to the outlet is caused by the higher current density in this region, which leads to increased water production and thus increased water transport.

2 STACK MODEL

For the stack influence, the two most significant cells are considered to represent the most relevant limitations: the central

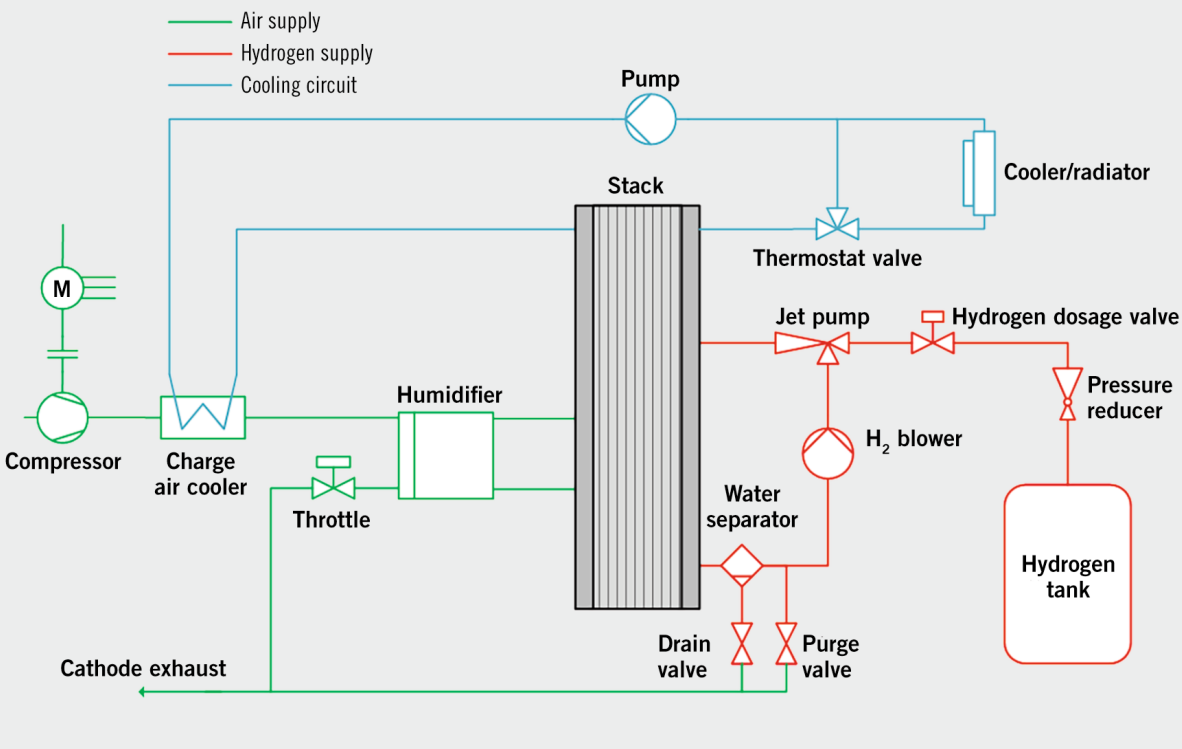


FIGURE 3 Exemplary fuel cell system topology (© RWTH I ZBT)

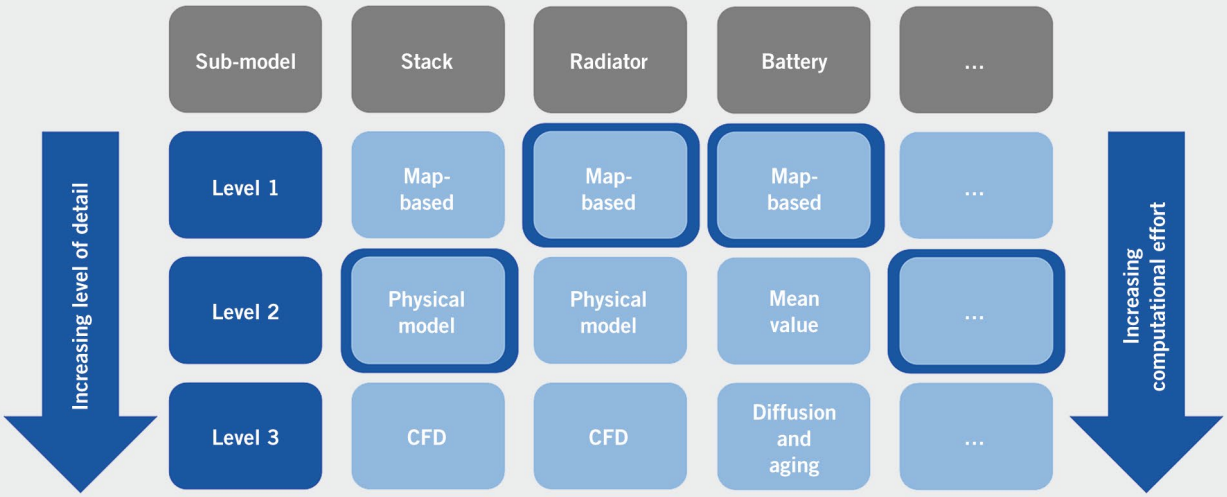


FIGURE 4 Modular model concept (© RWTH I ZBT)

middle cell and a border cell. The border cell is coupled to the inert thermal mass of the end plates and represents the coldest cell in the warm-up process and thus the cell with the largest amount of liquid water. The central cell, however, can lead to limitations under particularly dry conditions. The model can be adapted to individual stacks by means of various electrochemical and geometric parameters, thermal masses as well as conductivity values.

3 SYSTEM MODEL

Apart from the stack, several auxiliary units are required to operate a fuel cell system. These can be classified into the air and hydrogen supply systems and the cooling circuit. An exemplary setup of a fuel cell system is shown in **FIGURE 3**. The interaction of the components of the fuel cell system is discussed, for example, in [7].

With the modular approach pursued in the research projects, individual requirements can be addressed during development. Not only can the developed platform be used to obtain a basic understanding of the interactions in a fuel cell system with a detailed physical model or to create a reduced model for controller development. The modular structure of the system modeling environment with defined universal interfaces provides the ability to replace any component model of the system by an alternative with a different level of model fidelity and complexity. Thus, the overall model can be designed user-specifically with different levels of detail and complexity. The general approach of the system model environment is visualized in **FIGURE 4**.

To represent cold start conditions, the existing generic fuel cell system model is supplemented with the simulative representation of liquid water. For this purpose, an additional liquid water path is included in every relevant component model, which directly interacts with the transported gaseous water. The liquid water is formed as soon as the partial pressure of the gaseous water exceeds the temperature-dependent saturation vapor pressure. It is then fed to the liquid water path. Furthermore, the liquid water phase is taken into account in the energy balance.

4 USE CASES

For the simulation environment described, an exemplary model was built based on the Breeze fuel cell system [8] – a range extender for an electric vehicle. Validation was performed using corresponding test bench and vehicle measurement data [9]. In the model, a membrane humidifier was added to the system, which uses the water content of the cathode exhaust gas to humidify the dry cathode supply air. The possibility to bypass the humidifier was also implemented in order to control the humidity of the cathode supply air, **FIGURE 3**. In addition to the operating parameter optimization, also the use cases of system design, component sizing, and controller development were demonstrated.

Among other applications, the system model can be used to evaluate the system behavior for numerous operating parameter variations in order to determine combinations that lead to optimal system efficiencies. The system efficiency results from the hydrogen consumption and the net system power, with the latter being composed of the electrical stack power minus the power consumption of the compressor, the hydrogen recirculation blower and the coolant pump.

The results of an exemplary pressure variation are shown in **FIGURE 5**. Higher partial pressures of the reactants lead to higher cell efficiencies. In the low partial load range, the higher cell efficiency at higher pressures does not compensate for the additional compression power, whereas at higher loads the higher stack efficiency dominates. For high loads and volume flows, low pressure levels cannot be maintained due to high exhaust back

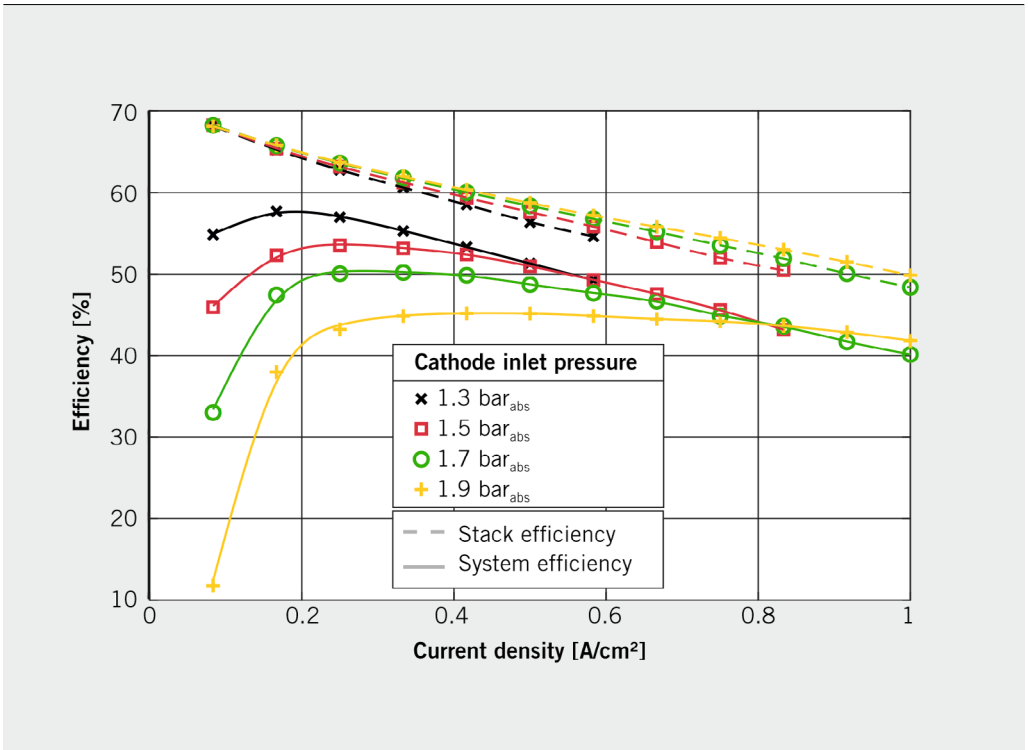


FIGURE 5 Stack and system efficiencies using simulated parameter variation to determine the optimal cathode inlet pressure; boundary conditions: coolant inlet temperature T = 65 °C, coolant temperature spread ΔT = 10 K, cathode stoichiometry λ = 2, relative cathode inlet humidity φ = 65 % (© RWTH I ZBT)

pressures. Therefore, the curves of the considered configuration and shown here in **FIGURE 5** end at medium load points. This parameter variation leads to a load-dependent optimal operating pressure profile.

5 SUMMARY AND OUTLOOK

As a crucial influence factor, the water balance for fuel cell performance should be considered on cell, stack, and system levels. In order to realize a model for a variety of use cases, a combined stack/system model for fuel cells was developed in a first project, focusing on the water transport effects and the resulting membrane humidity. While the stack model can be parameterized for different stack geometries and cell configurations, the system model can be adapted to user needs due to its universal interfaces and modular design. For an exemplary system topology, the applicability as a tool for system design and component dimensioning as well as for the analysis of operation and control strategies was demonstrated. In a second, ongoing project, the allowable operating range of the model is being extended to colder operating conditions. Simulations based on Computational Fluid Dynamics (CFD) – in particular for the stack and membrane humidifier – are used to investigate the influence of liquid water and ice on gas transport.

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