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Coupling of a continuum fuel cell model with a discrete liquid water percolation model

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ABSTRACT

An iterative algorithm is developed to directly integrate a discrete liquid water percolation model into a 3D continuum fuel cell model. In the continuum model the thermodynamic processes, most relevant for the water management and fuel cell performance, are calculated. For the discrete liquid water distribution in the porous transport layer (PTL), a water path network model is used, calculating the discrete, injection pressure and condensation scenario dependent saturation distribution.

The saturation in the PTL is compared to synchrotron visualization data and a good comparison is found. Using the model, the influence of PTFE content, the application of a microporous layer, PTL perforation and ionomer desorption rate on the water configuration and fuel cell performance are analyzed. The interfacial liquid water is identified as an important parameter for the liquid water transport and the oxygen diffusivity to the active areas.

Introduction

Water management is important for the performance and stability of low temperature polymer electrolyte membrane (PEM) fuel cells. To avoid losses due to blocked reactant transport paths by liquid water in the porous electrode structures, the product water of the electrochemical reaction has to be transported to the gas channels efficiently. To minimize flooding, operating the cell with dry inlet gases is an option to shift the water transport mechanisms towards water vapor diffusion. However, dehydration of the polymer membrane leads to losses in proton conductivity due to the strong dependency of the proton conducting mechanisms on the ionomer humidification. Optimization strategies therefore aim on changing the liquid water transport properties of the porous components to avoid flooding on the one hand while preventing drying on the other hand.

For the water management, the liquid water transport properties of the porous transport layer (PTL) is a key issue. On the one hand, owing to its position between the place of the water generation in the catalyst layer and water expel in the channel water, liquid water accumulations are very likely to occur in the PTL. On the other hand, these liquid water accumulations directly block the oxygen diffusivity between the catalyst layer and the channel.

Due to the requirements for thermal and electric conduction, cost and porosity, porous transport layers (PTLs) commonly consist of a fibrous substrate (FS) which is a layer of carbon fibers fixed together using a binder. In recent time, different approaches have been developed to improve the water management of the materials [1]. Treatment with PTFE

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is used to increase the hydrophobic effect of the PTL. Experimental studies showed that up to PTFE in the FS increase the cell performance and stability [1–7]. However, by adding PTFE also the porosity and thermal/electric conductivity of the materials is changed which can lead to changed water management in the fragile thermodynamics of the fuel cell.

Adding a microporous layer (MPL) to the FS is another approach that has shown the capability to improve the water management properties of the PTL. The MPL mainly consists of micro carbon particles and PTFE, leading to a high porosity and highly hydrophobic wetting. However, the reasons behind the improved performance are still subject of ongoing investigations. Possible positive impacts can be the reduced contact resistance between the CCL and the PTL, a better water back-diffusion from the cathode to the anode [8–10] or a reduced saturation in the FS due to a smaller number of breakthrough paths [11–14].

To determine the influence of the PTL design on the fuel cell performance, modeling has to capture the sensitive and highly coupled 2-phase water management and the coupling with the cell performance. The transport of liquid water, water vapor and dissolved water in the electrolyte as well as phase change has to be considered. Thermal effects also play a significant role due to the high influence on the phase change processes. Furthermore, oxygen and proton transport are both strongly influenced by the liquid water in the porous media and the dissolved water in the polymer electrolyte. To calculate these transport processes commonly continuum modeling is used applying Fick's or Maxwell–Stefan diffusion for the gas phase. For the liquid water transport a Darcy approach [15] is often applied which was originally developed for modeling liquid transport in porous sands. However, the application to the highly porous and hydrophobic PTL with the low flow rates in fuel cells remains questionable [16]. Discrete pore-network models have shown to model the characteristics of the liquid water transport in these media more adequately than the continuum models [15–23]. The fingering effect, experimentally observed for highly hydrophobic and porous materials [24,25], is captured using these models. Furthermore, inhomogeneous wettability distributions can be included in the discrete models which can have a significant effect on liquid water transport [16].

To investigate the influence of design parameters on the fuel cell thermodynamics, to date the discrete models have only been applied to estimate effective PTL properties like capillary pressure- saturation curves and oxygen diffusion characteristics which are used in continuum models. To improve the transfer of the liquid water transport characteristics to the fuel cell thermodynamics, a direct integration of the two modeling approaches would be of high value.

In the presented paper, an approach is developed to combine the advantages of a discrete liquid water modeling approach with a continuum fuel cell model for the first time. An iterative algorithm is used which allows to directly integrate a discrete liquid water percolation model into a 3D continuum fuel cell model. The model incorporates the thermodynamic processes relevant for determining the influence of the 2-phase water management on the fuel cell performance (heat, charge, water vapor, oxygen, dissolved water and liquid water transport). As a discrete model, a water path network model [26] is used which models the liquid water distribution in the porous media for defined liquid water injection pressures and a phase change situation. The presented approach concentrates on the coupling algorithm between a state-of-the-art continuum model and the discrete water path percolation model. However, also other discrete models like pore network models can be coupled with the continuum model using the described algorithm. The advantage of the water path network model compared to state-of-the-art pore network models is that the PTL design parameters can be directly addressed to analyze its influence on the cell performance [26].

Model description

Discrete PTL network model

The discrete percolation model is based on a water path network and is described in our previous publication [26]. The 2D solid structure of the FS is generated using the porosity and the stochastic distribution of contact angle, object orientation and objects dimension as an input. Based on the FS structure, the model calculates a network of stable water paths between all object pairs in the domain. The saturation distribution is then determined based on the network for a defined injection pressure and the condensation/evaporation source.

For the MPL, different groups found that the water transport takes place mainly through the MPL cracks leaving the saturation in the MPL low [12–14,27–30]. These cracks form during the production process of the MPL and have a width in the range of [12,20] compared to a main pore size of 17 nm of the bulk material [31]. Considering this, we neglect the saturation in the MPL but the number of injection points into the FS is reduced to the places of the MPL cracks.

Continuum fuel cell model

The focus of the model is to analyze the influence of the water management on the fuel cell performance. Therefore, the continuum model captures the major influencing physics which are identified as the distribution of temperature (T, defined in CCM, PTL, GDP), oxygen and water vapor concentration (c_{O2},c_{H2O}, defined in PTL), membrane water content (λ, defined in CCM), protonic potential (ϕ, defined in CCM) and the capillary pressure (p_{cp}, defined in PTL). The continuum model is described in the following section. The governing equations, boundary conditions, general equations and used constants are summarized in Tables 2–5.

The 3D model geometry consists of half a channel, half a rib, the CCM and the cathode PTL (Fig. 1). The catalyst layers are implemented as interfaces between the CCM and PTL domain. The anode components and processes are neglected except for the H_2O ad-/desorption in the anode catalyst layer (ACL).

Since the discrete model is a 2D model, five models are placed along the channel with a distance of 40 μm. In-between, the continuum model interpolates both the distribution of material *mat* and liquid water *s* using a nearest neighbor interpolation.