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Impact of compression on gas transport in non-woven gas diffusion layers of high temperature polymer electrolyte fuel cells

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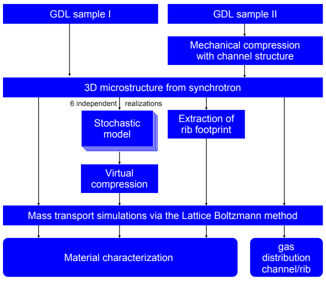
HIGHLIGHTS

- Detection of microstructure with synchrotron X-ray tomography.
- Mechanical compression of the microstructure.
- Virtual compression of a stochastic geometry model.
- Transport simulation with the Lattice Boltzmann method.

GRAPHICAL ABSTRACT



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ABSTRACT

Gas transport in non-woven gas diffusion layers of a high-temperature polymer electrolyte fuel cell was calculated with the Lattice Boltzmann method. The underlying micro structure was taken from two sources. A real micro structure was analyzed in the synchrotron under the impact of a compression mask mimicking the channel/rib structure of a flow field. Furthermore a stochastic geometry model based on synchrotron X-ray tomography studies was applied. The effect of compression is included in the stochastic model. Gas transport in these micro structures was simulated and the impact of compression was analyzed. Fiber bundles overlaying the micro structure were identified which affect the homogeneity of the gas flow. There are significant deviations between the impact of compression on effective material properties for this type of gas diffusion layers and the Kozeny-Carman equation.

1. Introduction

The knowledge of the characteristics of polymer electrolyte fuel cell (PEFC) components is essential for the efficient operation of fuel cells and stacks. It can be supported by mass transport simulations at different spatial scales. The gas flow is often affected by material properties of the components. Gas diffusion layers (GDL) are used in low temperature PEFCs as well as in high temperature PEFCs (HT-PEFC) in order to distribute gases from the channels under the ribs of the flow field and collect the product gas on the cathode side. The transport characteristics of the GDL depend highly on the micro structure of the material which is of stochastic nature and can furthermore change under mechanical

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compression. In former times, the effect of GDL was typically neglected in three dimensional (3D) cell and stack simulations [1]. But with increasing computational power the effect of GDL properties is often included [2]. Research groups are working on several fields covering the micro structure of the material and its characterization regarding mass transport and its impact on fuel cell applications. Experimental work and modeling of GDL complement one another in the development of PEFC and HT-PEFC. At this point, modeling of the micro structure [3–5] is often complemented by transport simulations. The micro structure of the material needs to be detected and transformed into geometry information to be used by the simulation software. The impact of transport characteristics on the fuel cell operation is of considerable evidence for the design of improved materials.

Experimental studies can follow various approaches. The permeability of GDLs was measured by Feser et al. [6] and also by Hussaini and Wang [7]. Taira and Liu [8] measured the effective permeability of GDL under the land region of a flow field. The general agreement of commonly used equations for permeability and tortuosity with visualizations of the micro structure of GDL was shown by Fishman and Bazylak [9]. The permeability of porous materials can be related to geometric properties for certain materials as shown by Tamayol et al. [10] and Hooman et al. [11] in their investigations on single phase gas transport in GDL. Several groups investigated liquid water distribution in operating PEFCs with neutron [12–14] and synchrotron X-ray imaging [15,16]. Experimental studies on the effect of compression on the performance of a PEFC were presented by Lee et al. [17]. Another kind of experiments was presented by Ye et al. [18] who investigated the bypass of water under the rib between two parallel gas flow channels. The GDL in their experiments was compressed by applying a defined tension to the flow field. A link between the micro structure of porous materials and its transport properties was presented by Koponen et al. [19]. Effective properties as permeability and tortuosity can be calculated from the flow fields resulting from Lattice Boltzmann (LB) simulations. This work bridges experimental work and simulations on both micro structures and cell level.

Various research groups are working on transport simulations in the micro structure of GDLs. Matyka et al. [20] calculated the tortuosity from streamlines which were obtained from two-dimensional LB simulations in randomly constructed porous structures. Thomas et al. [21] determined the accuracy of such results in relationship to the spatial discretization of the micro structure. Espinoza et al. [22] investigated the effect of compressed GDL on the permeability and tortuosity of a GDL with two-dimensional LB simulations. Gao et al. [23] focused on liquid water transport in GDL micro structures using three-dimensional LB simulations. Paper-type GDLs were reconstructed by Daino and Kandlikar [24] under consideration of the distribution of polytetrafluorethylene (PTFE) in the micro structure. Another stochastic geometry model [25] was taken by Froning et al. [26] to determine permeability and tortuosity of paper-type GDL represented by evaluating transport simulations in the micro structure. Through-plane and in-plane transport simulations using the Lattice Boltzmann method (LBM) were performed in micro structures under different levels of compression up to 50%. Nabovati et al. [27] calculated through-plane and in-plane permeability and tortuosity of reconstructed paper-type GDL using LB simulations. Under different conditions regarding homogeneous and heterogeneous porosity distributions they found higher in-plane permeabilities and lower in-plane tortuosities than the through-plane counterparts. Another kind of GDLs uses non-woven fleece, also made of carbon fibers. Su et al. [28,29] use this type of GDL in their investigations on polymer binder and platinum distribution in catalyst layers. Non-woven fiber based materials can have a more complex micro structure which is also available for stochastic modeling. Gaiselmann et al. [30,31] investigated non-woven GDL from Freudenberg. They identified fiber bundles as superposed structures and incorporated them as a feature of their stochastic geometry model. Rama et al. [32] simulated gas transport in GDLs with the LBM in three-dimensional micro structures of woven carbon-cloth GDL from reconstructed X-ray micro-tomography which were compressed by applying dedicated weights to the GDL structure. They calculated pore sizes, porosity, permeability and tortuosity of woven GDLs under varying grades of compression. The anisotropy of the GDL as a function of compression was also presented.

Effective transport properties obtained from measurements or micro scale simulations can be used as model parameters in higher spatial scales. The presence of liquid water at low temperatures leads to different dominating effects for PEFC and HT-PEFC. In particular, Chippar et al. [33] studied the effect of GDL compression in PEFCs. They considered the impact of compression on effective transport properties of the GDL and the water saturation. Ju [34] studied the effect of anisotropy of the GDL on heat and water transport in a fuel cell. He investigated the anisotropy of the current density under the channel and under the rib crossways to the flow direction of a 0.5 mm wide channel. Hossain et al. [35] investigated the effect of GDL permeabilities on the efficiency of PEFC using a two-phase model. They observed high deterioration of the performance of a PEFC at low in-plane permeability of the GDL. Qi et al. [36] calculated the deformation of the GDL of a PEFC under mechanical compression. Bosomoiu et al. [37] investigated effective transport properties of fresh and aged GDL also under the land and channel regions of a flow field of a HT-PEFC. Chippar and Ju [38,39] modelled the gas crossover through the MEA of a HT-PEFC between a pair of fuel and gas channels of 1 mm width. The relevance of their investigations is affirmed by HT-PEFC stacks when they are assembled with meander type flow fields. Lüke et al. [40] measured the inhomogeneity of the current density distribution in a HT-PEFC stack with meander flow fields operated under several conditions.

In our paper we simulated gas transport in the micro structure of a GDL. The investigation was motivated by the research of Lüke et al. [40] and Kvesić et al. [41]. Their experiments on HT-PEFC stacks and corresponding Computational Fluid Dynamics (CFD) simulations showed the evidence of in-plane gas transport under the ribs of meander type flow fields. Liu et al. [42] presented a HT-PEFC with spiral flow fields which also benefits from in-plane gas transport under the ribs. To get insight into the underlying processes the micro structure of a Freudenberg GDL of type H2315 was investigated in the BESSY synchrotron by Tötzke et al. [43]. From this micro structure a stochastic geometry model of the GDL was developed [44]. The geometry model can generate stochastic equivalent geometries of the uncompressed and compressed micro structure. Furthermore, the real micro structure was investigated in the BESSY synchrotron under the impact of compression by the ribs of the flow field on the micro structure. Transport simulations in these geometries were performed using the LBM. The effective transport properties permeability and tortuosity calculated from the results were analyzed. This numbers can be used for investigations of transport processes on cell and stack level [2,34,41]. Furthermore the inhomogeneous transport of gases under the ribs of the flow field was evaluated.

2. Methods

The micro structure of Freudenberg GDL (type H2315) was investigated in the BESSY synchrotron. The material was compressed virtually and also by a mechanical device according to Fig. 1 which depicts the processes of our investigations. Combining