Computation of Thermal Conductivity of Gas Diffusion Layers of PEM Fuel Cells

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Abstract

Polymer electrolyte membrane (PEM) fuel cells are promising candidates for automotive applications due to the low operating temperature which allows for relatively short start-up times and the high flexibility of the delivered power. In PEM fuel cells, gas diffusion layers (GDL) – in combination with bipolar plates – are usually employed to distribute the reactants over the electrode surfaces. The GDL has not only the function to provide gas access to the catalyst layer, but also to allow the removal of the product water, to mechanically stabilize the membrane-electrode assembly and to provide electronic and finally also thermal conductivity between catalyst layer and bipolar plate.

The thermal conductivity of the GDL plays an important role in the management of the heat transfer in PEM fuel cells and therefore is important for simulation of fuel cell performance and for fuel cell design. While the measurement of thermal conductivity by experimental means is possible, it remains challenging due to the anisotropy and the high porosity and the available experimental data is rather limited. In the following, the numerical computation of effective thermal conductivity of GDLs based on 3D structure data – with spatial resolution on the μ m-scale – will be discussed. The 3D structure data is derived using two different approaches: 1) the 3D GDL structure is measured experimentally applying x-ray computed tomography [1, 2]; 2) the 3D GDL structure is simulated by a randomly generated fiber geometry [3]. The computation of thermal conductivity requires the solution of the steady state, purely diffusive three-dimensional heat transfer equation. In the present approach, the convection and radiation transport, as well as thermal contact resistance and phase changes were not taken into account.

Usually porous carbon fiber papers or cloths are used as gas diffusion layers and they are infiltrated with polytetrafluoroethylene (PTFE) to improve the GDL's ability to remove product water. Typical carbon fiber diameters are between 5 and 10 μ m, typical porosities of GDLs are between 70 and 90 %. The GDL can contain a microporous layer (MPL) to improve the water management within the PEM fuel cell.

Commercially available gas diffusion layers were investigated by x-ray computed tomography (CT). This lab-based technique allows for a non-destructive determination of 3D structure with a resolution well below 1 μ m. The sample is placed between x-ray source and 2D detector and a projection image of the sample is acquired. This is repeated for different orientations of the sample with respect to the x-ray/detector setup and based on this series of projection images, the 3D structure of the sample is reconstructed. Each voxel has now to be assigned to a certain material in the sample or to air, based on the gray level of the voxel in combination with morphological information.

On the left of the figure, the 3D structure of SGL GDL 35 BC acquired by X-ray computed tomography is shown. In this carbon paper based GDL, the fibers run approximately straight and are parallel to the plane defined by the carbon paper. The carbon fibers and the 3D structure of the gas diffusion layer were clearly resolved. As an alternative approach, fiber structures were randomly generated (see right) using the Geodict software [4].



3D structure and cross-section of a GDL as determined by x-ray computed tomography (left) and randomly generated (right). The micro porous layer (MPL) is clearly visible in the CT cross section. In the cross section of the randomly generated structure, the fibers (red) are clearly separated from PTFE (grey).

Because of the numerical generation of the structures, the influence of different parameters such as fiber orientation, fiber diameter and PTFE fraction could easily be investigated. Additionally, the carbon fibers are clearly separated from the PTFE – due to the numerical generation of the structure – while carbon fibers and PTFE show similar contrast in x-ray computed tomography.

As expected, the computed average in-plane thermal conductivity for all data – based on computed tomography or numerical generation – is larger than the average through-plane thermal conductivity due to the anisotropy of the fiber orientation. Furthermore, a clear dependence of thermal conductivity on the porosity and - especially for the carbon cloth - also on the local orientation of

the fibers was observed. The calculated thermal conductivities were validated through a comparison with existing experimental data.

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