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Machine Learning for the Characterization of Fibrous Gas Diffusion Layers for Polymer Electrolyte Fuel Cells

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The permeability of gas diffusion layers (GDLs) depends on their micro-structure, and is relevant for transport simulations at higher scales, e.g., fuel cells and stacks. Given the micro-structure, the permeability can be obtained from transport simulations [1], which typically requires large computing resources. Such GDLs are used in polymer electrolyte fuel cells (PEFCs), as well as in some electrolysers.

Drawing on previous published simulations [1] of gas flow through fibrous GDLs, a convolutional neural network (CNN) was trained [2, 3]. The underlying data were based on a stochastic geometry model that also featured different binder models and compression levels. A small number of micro-structures –541 –was sufficient for not only achieving good accuracy in the predicted permeability but also for reproducing the binder type as a hidden feature that was not explicitly trained.

The training data for the CNN are micro-structures generated by means of a stochastic geometry model [1]. The fibers with a diameter of 7.5 µm were created layer-wise. The fiber orientation is stochastically-equivalent to the real structure of Toray 090 material, which was validated using X-ray synchrotron imaging [1]. An additional binder was added using four kinds of binder sub-models. The resulting micro-structures were provided in both uncompressed and compressed forms. The output feature –label data for the CNN –was the through-plane permeability of the GDL, calculated by means of Lattice–Boltzmann simulations of single-phase flow through the micro-structure. Because the LB simulations required large computational resources, it was intended to take a limited number of these to train a CNN that can predict permeability with sufficient accuracy. This was achieved using historical data from previous investigations [1]. Validated with five-fold cross validation, the CNN was able to predict the permeability with an accuracy greater than 5% for uncompressed micro-structures, as well as relevant compression levels [3]. Although the binder type was not provided for training the CNN, this hidden feature was reproduced by the predictions using the trained CNN.

The calculation of the permeability of the micro-structures required high-performance computers (HPCs); the training of the CNN also requires large computational resources, preferably GPU-based ones. With a trained CNN, the prediction of permeability can be run on a standard computer.

Transport simulations were run on the hardware of the Jülich Supercomputing Centre, grant: CJIEK30. The neural network was trained on GPU nodes of the CLAIX system at RWTH Aachen University, using grants jara0070 and p0020317.

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Participation

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References

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