Predicting porosity of fibrous fuel cell transport layers with synthetic data and convolutional neural networks

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The rise in interest for fuel cell vehicles has renewed the push for sustainable, efficient, polymer electrolyte membrane fuel cells (PEMFCs). Recent advances in the construction of PEMFC oxygen reduction catalysts and proton exchange membranes have been significant with regard to PEMFC performance; however, water management in the gas diffusion layer (GDL) continues to be an essential avenue for increasing overall cell efficiency (1, 2). Efforts have been made to better understand how the structure of the GDL impacts water management through advanced microstructure characterization techniques such as synchrotron x-ray and laboratory-based computed tomography imaging (3, 4).

These lab-based techniques can often be access limited, time-consuming, and costly. Alternatively, deep learning tools such as convolutional neural networks (CNNs) are openly available resources and have been employed for image analysis since the late 1990s (5). Using CNNs to analyze lower quality data sources (like standard 2D x-ray images) presents a unique opportunity to gain insight into the GDL microstructure from more accessible resources. Recently deep learning has been implemented in geological porous media applications to predict morphological, hydraulic, and mechanical properties with promising results. Since these are properties of interest for the fuel cell community CNNs should be further investigated for analysis of the porous media used in renewable energy devices (6).

We stochastically generated nearly 3000 synthetic porous fibrous materials in this study, exhibiting porosities that ranged from 0.45 to 0.95, similar to commercial GDL materials. The materials were used to create 2D images (density maps) which could be used to train various CNNs to predict the porosity of the original synthetic material. Three CNNs were evaluated; a conventional shallow CNN, and two models based off of ResNet50 and Xception network architectures. All three architectures were able to successfully predict the porosity of the synthetic materials with R^2s of 0.976, 0.98, and 0.98 for the conventional, ResNet, and Xception models, respectively. We then investigated the ability of the models to generalize on real GDL materials; the segmented images of three commercial GDLs were sampled 90 times at varying crop sizes (50 to 600 pixels) with the best performing crop size (200 pixels) yielding a mean absolute error of 0.03. Additionally, it was found that subsampling larger real image crop sizes to the optimal crop size significantly reduced model error and allowed for the more accurate prediction material porosities from larger image segments. This study illustrates the usefulness of CNNs for the image analysis of fibrous GDLs and highlights the potential for CNNs to be further applied to analyze new materials for electrochemical energy conversion.

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