Geometric reconstruction and numerical analysis for characterization of transport properties at various levels of water saturation in micro/nano structure of catalyst layers

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To develop a self-humidifying membrane with good water uptake characteristics, it is highly desirable to understand the transport properties and microstructure of catalyst layer in PEMFC. In this work, two real samples (a. self-humidifying layer with High tortuosity humidifying catalyst layer), and b. standard catalyst layer) are three dimensionally reconstructed by Focused Ion Beam Scanning Electron Microscopy tomography. From the developed 3D models, we derive the transport properties – permeability, capillary pressure and diffusivity followed by structural properties such as porosity and surface area. By coupling the effective structural and transport properties to COMSOL, we develop a two-dimensional model to predict the performance of the two CLs, at relative humidity levels of 20 % and 100 %. Further to demonstrate the completeness and accuracy of the proposed models, the results of the numerical study are also validated experimentally.