Contribution ID: **795** Type: **Oral 20 Minutes**

Exploring the limits of macro-homogeneous models of carbon-fiber papers

Thursday, 17 May 2018 09:44 (15 minutes)

Carbon-fiber papers (CFPs) are an integral component of many energy-conversion and energy-storage technologies, including gas diffusion layers (GDLs) in polymer electrolyte membrane fuel cells (PEM fuel cells), cathode GDL in PEM electrolyzers and metal-air batteries, and as electrodes in redox flow batteries (RFBs). CFPs must fulfill several functions such as providing adequate mechanical support to the membrane electrode assembly, a transport pathway for reactants/products through its pore volume, and electrical and thermal conductivity through its solid fibrous structure. In RFBs, they have the added functionality of providing an active catalytic surface area. Understanding of the transport processes that occur in CFPs is necessary to help predict cell performance and durability, optimize materials and diagnose problems. The most common technique used to model these thin porous media is the macro-homogeneous approximation based upon the existence of a representative elementary volume (REV). However, the applicability of the continuum approach to CFPs has been questioned many times, and the error introduced in the predictions is certainly unclear.

In this work, the limitations of macro-homogeneous descriptions of CFPs are explored for various single-phase transport processes: diffusion, convection and electrical/thermal conduction. Multiple sub-domains with different widths and thicknesses are examined by combining the lattice Boltzmann method with X-ray tomography images of uncompressed CFPs. The results show that a REV cannot be defined due to the lack of a well-defined separation between pore and volume-averaged scales in these inherently thin heterogeneous materials. The representative size in the material plane is in the order of 1 mm, which is comparable to the rib/channel width used in the above-mentioned devices. As for the through-plane direction, no representative length scale smaller than the thickness can be identified. In particular, it is found that the highly porous surface region (amounting up to 20% of the material) can significantly reduce the through-plane electrical/thermal conductivity.

In the second step, fuel cell performance predictions using a pore-scale model are compared to a traditional macro-homogeneous model. The results show that the overall mass, heat and charge fluxes predicted by both models are similar, provided that the macro-homogeneous model is equipped with suitable effective properties. However, the spatial distributions can be significantly different due to the lack of separation of scales. Specifically, the pore-scale simulations reveal the presence of inhomogeneities in the transport of species and heat that are not accounted for by the macro-homogeneous model. These deviations could have a substantial impact when modeling degradation phenomena, which are sensitive to local conditions.

References

Acceptance of Terms and Conditions

Click here to agree

Primary authors: GARCÍA-SALABERRI, Pablo Ángel (Universidad Carlos III de Madrid); Dr GOSTICK, Jeff Thomas (University of Waterloo)

Presenter: GARCÍA-SALABERRI, Pablo Ángel (Universidad Carlos III de Madrid)

Session Classification: Parallel 9-B

Track Classification: MS 4.16: Two-Phase Flow and Reactive Transport through Thin Porous Layers