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Data Science Approaches for Microstructure Quantification and Feature Identification in Porous Membranes

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Abstract

Rigorous quantification of porous microstructures exhibiting a wide variety of pore shapes, sizes, and their spatial distributions presents a significant challenge. In this work, novel data science approaches are used to characterize the complex microstructures in porous membranes, and to extract the salient features at the pore-scale. Towards this goal, a microstructure generator is developed and utilized to create a large ensemble of porous structures covering a substantial range in measures of features such as the stretched pore shapes (geometrical anisotropy), porosity, specific surface, and pore sizes. Additionally, the morphology of real porous membranes are obtained experimentally by high resolution X-ray tomography. The statistical representations for the simulated and real membrane microstructures are calculated and compared rigorously using novel data science approaches that are based on principal component analyses of the 2-point spatial correlations. This approach allows an objective measure of the difference between any two selected microstructures. The versatility and benefits of this approach for the quantification of microstructures in porous membranes are demonstrated in this paper.

Keywords: Porous membranes, Nano-computed tomography, Voronoi-based algorithm, Two-point statistics, Principal component analysis, Data classification, Pore-scale characterization

1. Introduction

Porous media are most frequently characterized indirectly by conducting macroscopic measurements (e.g., mercury-intrusion porometry, BET measurements, bubble point) [1]. However, these measurements are inherently limited in capturing the real physical characteristics of the microstructure at the pore-scale. With the increasing complexity of the microstructural morphology of modern porous media, macroscopic investigations provide a useful, but highly simplified, measure of the microstructure. For optimum selection of the porous membranes for industrial or medical applications, information such as pore sizes, pore shapes, pore orientations, and their spatial distributions need to be considered. Moreover, with a rigorous quantification of the pore-scale structure, the underlying theoretical models for the performance related macroscopic properties can be improved significantly. For all these reasons, it is beneficial to develop robust and reliable methods for identifying and extracting the salient morphological features of porous media at the pore scale.

There are only a few main methodogical pathways reported for the characterization of porous media in literature [2, 3]. As mentioned earlier, the simplest approaches focus on obtaining estimates of the surface area per unit volume, averaged porosity, and averaged pore size using macroscopic measurements. These approaches are founded in the general principles of capillarity, diffusion, and fluid