Exploring Process-Structure Linkages for Slot Die Extruded Composite Membranes Using Data Science Techniques

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Slot die extrusion offers the possibility of cheaper composite membrane materials for applications such as water filtration membranes due to its scalable and continuous nature. However, within the coating window there exist an infinite number of process parameter combinations that will produce a composite membrane of desired thickness and material properties. Understanding how these different combinations of parameters affect the structure of the membrane can result in improved filtration performance and better pore and particle distributions. The challenge is to identify the critical combination of process parameters that results in the ideal microstructure for optimum performance, a task in which data science techniques from the emerging materials informatics field are well-suited.

Material informatics techniques were utilized to identify process-structure linkages in composite membranes, by coupling microcomputed tomography (µCT), image segmentation, spatial statistics, and regression analysis. The materials used to form the composite membranes for detailed analysis include: cellulose acetate (CA) with an average M_n ~ 30,000, 1-Methyl-2-pyrrolidone (NMP) with an analytical purity of 99.0+%, and glass microparticles (4-22 µm), with deionized (DI) water was used as the non-solvent agent. Composite membranes composed of 20% CA to NMP by mass with a 0.5% volume fraction of glass particles were manufactured using slot die extrusion with thicknesses varying from 404 to 448 µm and the ratio of the film thickness to standoff height of the die from the substrate varied between 0.8 to 4.0.

The steps of a characterized membrane are shown in Figure 1, using the succeeding method. The three dimensional microstructure of the composite membranes was captured using µCT, as depicted in Figure 1a. The µCT images were then segmented into discrete phases representing the glass particles, polymer matrix, and pore structure, as shown in Figure 1b. Lastly, spatial statistics of the membranes were computed using digital signal processing, as illustrated in Figure 1c.

A dimensionality reduction and correlation routine was applied to identify the process-structure linkages, based on the results from the spatial statistics and the process parameters. It has been found that the ratio of the film thickness to the gap height has an influence on the distribution of the microparticles relative to the membrane surfaces.

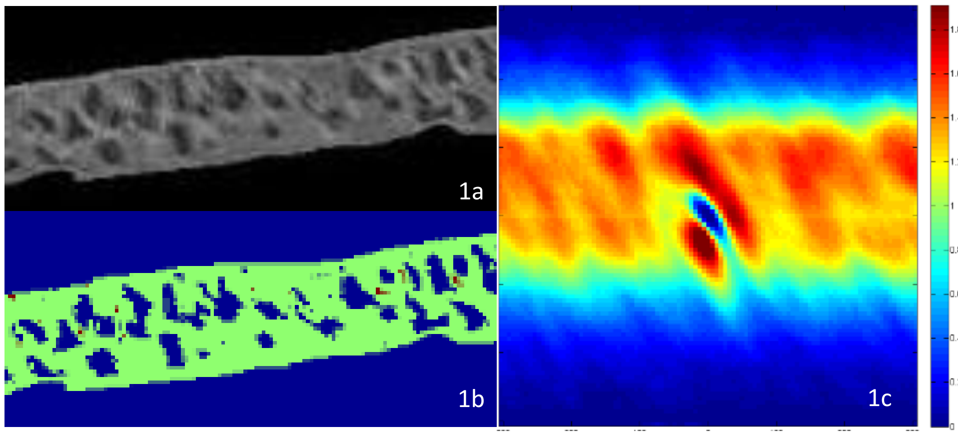

Figure 1: a) Three-dimensional image of a composite membrane slice by microcomputed tomography. b) Discrete phases glass particles (red dots), polymer matrix (green), and pore structure (blue). c) Location of phases relative to each other, with an example of the particle location relative to the pores shown.