Rapid Characterization of Mass Transfer in Fiber Composites Using a Commercial Volumetric Adsorption Instrument

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MOF/fiber composites have shown much promise as protective equipment for the capture and remediation of chemical warfare agents. However, the practical application of these composites requires an understanding of their mass transport properties, as both mass transfer resistance as the surface and diffusion within the materials can impact the efficacy of these materials. Experimental characterization of molecular transport typically requires specialized and expensive facilities, such as confocal Raman microscopy or infrared Raman microscopy, which – although they provide beneficial insights – suffer from limited accessibility, inhibiting the development of new applications of porous materials.

In this talk, we present a new Fickian diffusion model to quantitatively characterize the surface permeation and in-pore diffusion of molecules in MOF/fiber composites having cylindrical shapes. The new diffusion model takes input data from a commercial volumetric adsorption instrument, which is readily accessible in most laboratories compared to other specialized facilities for studying molecular diffusion. Using this newly developed method, we were able to study the mass transport of *n*-hexane and 2-chloroethyl ethyl sulfide (CEES) in composite fibers of MOF-808 and functionalized polymers of intrinsic microporosity. We found that transport in these materials is dominated by surface barriers, and diffusion within the bulk of the composite materials is fast in comparison. These preliminary insights and the model introduced in this work lay the groundwork for the design of next-generation composite materials for practical applications.

References:

1. F.A. Son[†], K. Shi[†], R.Q. Snurr, O.K. Farha, Mass Transport of n-Hexane and 2-Chloroethyl Ethyl Sulfide in Fiber Composites of MOF-808 and Amidoxime-Functionalized Polymers of Intrinsic Microporosity, in preparation.

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