Abstract:
The functionalization of polyolefin fibers is a complex multiphase reaction-diffusion process. Depending on the application, the extent of functionalization ranges from fiber surface treatment to complete fiber stabilization. The objective of this effort is to design a process to achieve a fully stabilized polyolefin fiber in which each filament is sulfonated uniformly from the surface to the core. During this process, the reactant diffuses from the bulk liquid phase through a bundle of hundreds to thousands of filaments to the polymer surface. Subsequently, the reactant diffuses into and reacts with the polymer. This paper presents the development and application of a reaction-diffusion model for the liquid phase sulfonation of a single polyethylene filament. The model computes the radial distribution of sulfonated polyethylene, unreacted polyethylene, and diffusing $\text{SO}_3$. Experimental data from elemental analysis (CHSN/O) and SEM-EDS enable quantification of the extent of sulfonation as a function of radial position in partially sulfonated filaments produced in a continuous, multistage sulfonation reactor. These data provide the basis for estimates of diffusion coefficients and reaction rate parameters. Experiments conducted under conditions of partial conversion combined with this reaction-diffusion model of the polyolefin sulfonation process identified the key rate controlling steps, providing insights into key factors for developing a robust process that can achieve the objective of uniform functionalization.

Biography:
Dan Hickman is a Fellow in the Reaction Engineering group in the Engineering and Process Science department of The Dow Chemical Company's Core Research & Development organization. He received his B.S. in chemical engineering from Iowa State University (1988) and his Ph.D. in chemical engineering from the University of Minnesota (1992) in the field of short contact time catalytic monolith reactors. In his 24 years with Dow, Dan has been a subject matter expert and technical leader in reaction engineering and process development for numerous reaction systems across a variety of Dow businesses and technologies. Dan has led the development of kinetic and reactor models for many developmental and commercial reactor systems, including stirred tank reactors, trickle bed reactors, and fluidized bed reactors. His contributions at Dow include designing reactors for three commercial processes. Dan holds 16 U.S. patents and is an author of 19 journal articles and more than 175 internal Dow reports.