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"Simulation of transport and reaction processes in porous membranes"

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Abstract

Aided by modern hardware and software advances, state-of-the-art computational techniques and virtual reconstructions have emerged recently as essential tools for the design of novel or improved materials, and for the discovery of innovated or enhanced properties of existing ones, successively corroborated by experimentation. Candidates for components with enhanced properties and processes with elevated performances are often suggested, designed and screened through simulations, even ahead or in place of usually strenuous and costly synthesis and characterization experiments. Extensive knowledge of key aspects and mechanisms of the flow, transport, sorption and separation phenomena in the interior of membranes on micro- and nanoscales is able to provide valuable insights on a significant number of processes related to porous membranes, and facilitate membrane design and optimization.

Recent studies have shown that the efficiency of modern hemodialysis processes is controlled by module geometry, membrane properties, and operating conditions. Optimization of membrane performance usually requires extensive and laborious experimentation. Detailed mathematical models are often necessary to predict the performance of hemodialysis operation under various operational conditions at more affordable accuracy and time scales. The primary purpose of this line of work is to develop detailed models that will predict the removal of blood toxins during hemodialysis using multi-layered mixed matrix membranes. The modeling and simulation background of relevant membrane separation processes will be presented, and focus will be placed on the computer-aided reconstruction of porous membranes for controlled transport and separation of biological fluids, along with the development of models and algorithms for the simulation of protein-bound toxin dissociation, transport, and sorption phenomena in digitized porous membranes either impregnated with sorbents or coupled with living cells for blood purification.