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Design of structure of sodium alginate membranes filled with iron oxide nanoparticles based on experimental results and simulation of diffusion process

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For each material, it is possible to individually select the optimal parameters that most accurately describe its unique nature and that influence the features that interest the user. We investigate the morphology of cross-sections of the sodium alginate membranes filled with various amount of magnetite and crosslinked using different agents. We expect that different amount of magnetite particles in alginate matrix cross-linked by different agents influence on structure and morphology properties and also affects the diffusion and transport properties. Therefore, we try to explore the ways of showing this relationship by simulating the motion of a particle in the membrane environment. In our case, it is a simulation of random walk on the structures of hybrid alginate membranes. Also, for a better understanding of the problem, we model structures of two-dimensional heterogenic membranes which resemble real hybrid alginate structures and then simulate random walk on them. The generated structures of polymeric membranes are created with the desired quantity, size and distribution of obstacles, which corresponds to the given amount of magnetite in the hybrid alginate membrane. Generated membranes possessing specific parameters that are comparable to the real hybrid alginate membranes filled with magnetite. Simulations of the particle motion support understanding of the mass transport through polymer materials and give a real chance to find the relation between diffusion and structure properties.

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