Mass transport simulations in EC/HPC films using the Lattice Boltzmann method

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ABSTRACT:

Using the Lattice Boltzmann method, we have performed simulations of diffusion and flow in geometries obtained from 3D confocal laser scanning microscopy (CLSM) data of ethyl cellulose (EC)/hydroxypropyl cellulose (HPC) films, with the purpose of understanding the relationship between the film structure and mass transport for coated formulations applications. Simulations were made possible through development of novel types of boundary conditions for the Lattice Boltzmann equation, suitable for the very complicated geometry in the film. The results of the simulations were compared to the experimentally determined effective diffusion coefficients of water and metoprolol succinate in the films, and some general but not perfect agreements were obtained. The discrepancies suggest, with additional input from scanning electron microscopy (SEM) data, that some parts of the structure with small pore size were not visible in the CLSM images. With estimates of pore size and volume fraction from SEM images, we have taken some steps towards modeling those parts of the structure in order to achieve a better understanding and agreement with the experimental results. We will discuss the treatment of microscopy data necessary for performing simulations as well as the limits of microscopy data and how to get past those limitations.