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3.7 Diffusion of Proteins in Nanochannels - A Many-Scale Simulation Approach

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Transport and surface interactions of macromolecules in nanopore membranes play a key role in many processes of technological importance. Although the use of porous materials provides a large surface-to-volume ratio, the efficiency of the operations is often determined by transport behavior, and this is complicated by the fact that transport paths (i.e., the pores) are frequently of molecular dimensions. Under these conditions, wall effects become significant, with the mobility of molecules being affected by hydrodynamic interactions between protein molecules and the wall. The nature and range of these interactions depend on the characteristics of the protein, the surface, and the intervening medium, and they can become especially pronounced when energetic interactions lead to adsorption on pore walls.

Modeling of transport in pores is normally carried out at the continuum level, making use of such parameters as hindrance coefficients; these in turn are typically estimated using continuum methods applied at the level of individual diffusing particles. Although particle-wall interactions can be incorporated in such models, the application of continuum models, and the appropriate parameter values to use, is open to question when interactions become so strong as to result in adsorption in pores of molecular (i.e., nano) dimensions. For such systems there are also qualitative issues that have not yet been addressed thoroughly, including pore constriction due to adsorbed molecules, and conditions leading to, and mechanism of, pore blockage by adsorbed molecules.

Understanding the mechanism of diffusion through nanochannels is important not only from a theoretical perspective, but also in view of the potential application of nanopore silicon membranes in drug delivery systems. Indeed, it has been shown that the release rate of proteins from such devices is constant for a long period, under suitable choice of the experimental parameters, such as initial concentration and channel/solute size. This property can be exploited in clinical medicine for prolonged and constant (i.e., ideal) administration of active principles. In this view, it is of outmost importance to have a quantitative method for device tuning and for the prediction of the amount of drug released in the patient body with a given amount of time.

In this work we propose, for the first time, an integrated, many-scale modeling approach based on the application of atomistic molecular simulations and macroscopic mathematical modeling to the analysis and the physical description of anomalous diffusion of some model proteins from microfabricated silicon membranes, having pores of nanometric size in only one dimension. The molecular modeling procedures were applied with a twofold purpose: i) to elucidate the specific mechanisms of interaction between each biopolymer and the silicon surface at the nanolevel, and ii) to derive molecular energetic and structural parameters to be employed in the formulation of the mathematical model of diffusion, thus filling the gap between the nano- and the macroscale.