

Understanding Protein Diffusion in Polymer Solutions:

A Hydration with Depletion Model

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Understanding the diffusion of proteins in polymer solutions is of ubiquitous importance for modeling processes in vivo. Here, we present a theoretical framework to analyze the decoupling of translational and rotational diffusion of globular proteins in semidilute polymer solutions. The protein is modeled as a spherical particle with an effective hydrodynamic radius, enveloped by a depletion layer. Based on the scaling formula of macroscopic viscosity for polymer solutions as well as the mean-field theory for the depletion effect, we specify the space-dependent viscosity profile in the depletion zone. Following the scheme of classical fluid mechanics, the hydrodynamic drag force as well as torque exerted to the protein can be numerically evaluated, which then allows us to obtain the translational and rotational diffusion coefficients. We have applied our model to study the diffusion of proteins in two particular polymer solution systems, i.e., poly(ethylene glycol) PEG and dextran. Strikingly, our theoretical results can reproduce the experimental results quantitatively very well, and fully reproduce the decoupling between translational and rotational diffusion observed in the experiments. In addition, our model facilitates insights into how the effective hydrodynamic radius of the protein changes with polymer systems. We found that the effective hydrodynamic radius of proteins in PEG solutions is nearly the same as that in pure water indicating PEG induces preferential hydration, while in dextran solutions, it is generally enhanced due to the stronger attractive interaction between protein and dextran molecules.