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Voltage-driven translocation through a nanopore: How can we define the capture radius? (G)*

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In most polyelectrolyte translocation studies, regardless of the shape of the pore and the strength of the driving force, the polymer chain has to go through three basic steps: (i) diffusion; (ii) capture; (iii) threading. The capture process remains rather ill-understood because it cannot easily be visualized or inferred from the blockage current measured across the nanopore. To estimate the size of the so-called capture zone, a capture radius R_C is generally defined as the radial distance from the pore center where diffusion-dominated polymer dynamics (at large distance) cross over to drift-dominated dynamics (closer to the pore). However, some of the definitions for R_C are ambiguous and over-simplified. In this talk, we propose several different approaches to define and estimate the value of R_C for the case of a charged particle diffusing in a liquid and attracted to the entrance of the nanopore by the presence of an electric field. The inhomogeneous electric field outside the nanopore is calculated by analytically solving the Laplace equation in Elliptical Coordinate, instead of using a point-charge approximation. We present a theoretical analysis of the Péclet number (Pe) as well as 2D Lattice Monte Carlo (LMC) simulations with different simulation protocols, including (i) dynamic simulations of the capture of a single particle by a nanopore situated on a reflecting wall and, (ii) the evolution of the concentration of particles in the presence of reservoir-like boundary conditions. Moreover, we study the effects of particle-wall hydrodynamic interactions on the capture radius by modifying the diffusivity of the particle near the wall.

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