

Effect of crowding and confinement on first passage processes

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How does crowding affect the encounter rate of a particle with a target? The answer to this question has great significance, particularly in biophysics. An important example is the cell cytoplasm where crowding agents typically occupy 20-30% of the total volume and strongly influence the kinetics and thermodynamics of cellular reactions. We examine a model system consisting of hard disks confined in an annulus, as well as some complementary results for the corresponding 3D system, using molecular dynamics simulation, to investigate the effects of crowding and confinement on mean first passage times (MFPTs) and reaction rate. The steady state rate of a color reaction displays a maximum for a packing fraction between 0.2 and 0.3 depending on the system geometry. In the ballistic regime at low density the MFPTs and reaction rate are well described by a kinetic theory model. At higher densities we observe the onset of a diffusive regime that is only qualitatively described by a Smoluchowski-like theory with a constant coefficient of diffusion. The discrepancy is due, in part, to a layering phenomenon that becomes more and more pronounced with increasing density and confinement. We also study the angular distribution of the hitting point on the target sphere and compare with that obtained by solving the diffusion equation with mixed boundary conditions.