8th EBSA European Biophysics Congress,
August 23rd–27th 2011, Budapest, Hungary

P-295

Monte Carlo simulation study of diffusion controlled reactions in three dimensional crowded media

Laura Pitulice[1,2*], Eudald Vilaseca[3], Adriana Isvoran[1, 2],Josep Lluís Garces[4] and Francesc Mas[3]

[1]Department of Chemistry, West University of Timisoara, Timisoara, Romania
[2]Nicholas Georgescu-Roegen Interdisciplinary Research and Formation Platform, Laboratory of Advanced Researches in Environmental Protection, Timisoara, Romania
[3]Physical Chemistry Department and Research Institute of Teoretical and Computational Chemistry of Barcelona University (IQTCUB), Barcelona, Catalonia, Spain
[4]Chemistry Department, Lleida University (UdL), Lleida, Catalonia, Spain

E-mail: pituliceii@yahoo.com

Published data reveal that the rate coefficients of diffusion controlled reactions taking place in crowded media are time dependent. Within this study we have performed on lattice 3D Monte Carlo simulations concerning Michaelis-Menten enzymatic reactions in crowded media, such as the cytoplasmatic region of the cells. We have considered the same size and mobility of the reactant particles and different crowding conditions using distinct concentrations and sizes of the immobile obstacles. The results we have obtained indicate a fractal like kinetics with the degree of fractality that changes with the concentration and dimension of the obstacles. The simulation data also reflect that, depending on the temporal scale, molecular crowding can bring positive or negative effects on reaction kinetics. Comparing the cases studied, for short periods of time the value of the initial rate constant generally increases with the degree of crowding. For longer periods of time and larger distances, molecular crowding slows down the reaction kinetics in every case, due to smaller diffusion coefficients of the reactants, having a more intense effect for the cases with higher degree of crowding.