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Seminar

Complex Nonlinear Processes in Chemistry and Biology

Honorary Chairman: **G. Ertl**
Organizers: **M. Bär, C. Beta, H. Engel, M. Falcke, M. J. B. Hauser, A. S. Mikhailov, P. Plath, L. Schimansky-Geier, H. Stark**

Friday, 22 October 2010, 16:00 s.t.

Prof. Raymond Kapral

Chemical Physics Theory Group, Department of Chemistry, University of Toronto

Diffusion-Influenced Enzyme Kinetics

Abstract

A particle-based mesoscopic model for enzyme kinetics will be described and used to investigate the influence of diffusion on the reactive dynamics. Both the nonreactive and reactive dynamics are constructed to satisfy mass, momentum and energy conservation laws, and reversible reaction steps satisfy detailed balance. Hydrodynamic interactions among the enzymes and complexes are automatically accounted for in the dynamics. Diffusion manifests itself in various ways, notably in power-law behavior in the evolution of the species concentrations. Regimes where the product production rate exhibits either monotonic or non-monotonic behavior as a function of time are found. In addition, for long times the species concentrations display both $t^{-1/2}$ and $t^{-3/2}$ power-law behavior, depending on the dynamical regime under investigation. For high enzyme volume fractions cooperative effects influence the enzyme kinetics. The time dependent rate coefficient is computed and shown to depend on the enzyme concentration. Lifetime distributions of substrate molecules newly-released in complex dissociation events are determined and shown to have either a power-law form for rebinding to the same enzyme from which they were released, or an exponential form for rebinding to different enzymes. The model can be extended to incorporate a more detailed description of enzymes and can be used to explore a variety of issues related cooperative effects and diffusion on enzyme kinetics.

Reference:
Jiang-Xing Chen and Raymond Kapral, Mesoscopic Model for Diffusion-Influenced Enzyme Kinetics, submitted (2010)

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