Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2021-0101

Vol. **31**, No. 3, pp. 707-738
March 2022

# Anomalous Sorption Kinetics of Self-Interacting Particles by a Spherical Trap

Antonio Raudino[1], Antonio Grassi[1], Giuseppe Lombardo[1], Giovanni Russo[2], Clarissa Astuto[3,*] and Mario Corti[4]

[1] *Department of Chemical Sciences, University of Catania, Viale A. Doria 6-95125, Catania, Italy.*
[2] *Department of Mathematics, University of Catania, Viale A. Doria 6-95125 Catania, Italy.*
[3] *Applied Mathematics and Computational Science, King Abdullah University of Science and Technology (KAUST), 4700, Thuwal, Saudi Arabia.*
[4] *CNR-IPCF Viale F. Stagno d'Alcontres, 37, 98158 Messina, Italy.*

Received 12 May 2021; Accepted (in revised version) 7 October 2021

**Abstract.** In this paper we propose a computational framework for the investigation of the correlated motion between positive and negative ions exposed to the attraction of a bubble surface that mimics the (oscillating) cell membrane. Specifically we aim to investigate the role of surface traps with substances freely diffusing around the cell. The physical system we want to model is an anchored gas drop submitted to a diffusive flow of charged surfactants (ions). When the diffusing surfactants meet the surface of the bubble, they are reversibly adsorbed and their local concentration is accurately measured. The correlated diffusion of surfactants is described by a Poisson-Nernst-Planck (PNP) system, in which the drift term is given by the gradient of a potential which includes both the effect of the bubble and the Coulomb interaction between the carriers. The latter term is obtained from the solution of a self-consistent Poisson equation. For very short Debye lengths one can adopt the so called Quasi-Neutral limit which drastically simplifies the system, thus allowing for much faster numerical simulations. The paper has four main objectives. The first one is to present a PNP model that describes ion charges in presence of a trap. The second one is to provide benchmark tests for the validation of simplified multiscale models under current development [1]. The third one is to explore the relevance of the term describing the interaction among the apolar tails of the anions. The last one is to quantitatively explore the validity of the Quasi-Neutral limit by comparison with detailed numerical simulation for smaller and smaller Debye lengths. In order to reach these goals, we propose a simple and efficient Alternate Direction Implicit method for the numerical solution of the non-linear PNP system, which guarantees second order accuracy both

*Corresponding author. *Email addresses:* `clarissa.astuto@kaust.edu.sa` (C. Astuto), `araudino@unict.it` (A. Raudino), `agrassi@unict.it` (A. Grassi), `glombard@unict.it` (G. Lombardo), `russo@dmi.unict.it` (G. Russo), `mario.corti@unimi.it` (M. Corti)

 

in space and time, without requiring solution of nonlinear equation at each time step. New semi-implicit scheme for a simplified PNP system near quasi neutrality is also proposed.

**AMS subject classifications**: 26Bxx, 65Mxx, 35Qxx, 65M06

**Key words**: Spherycal trap, quasi-neutrality, finite differences, Coulomb potential, Poisson-Nernst-Planck system, ADI discretization, semi-implicit scheme.

## 1 Introduction

The dynamical trapping of diffusing particles by either a single or a distribution of moving traps is an interesting topic that has been employed to model a variety of real problems in chemistry, physics and biology. Different ideal models have been proposed in the literature over the years. Most of the papers consider ideal traps where the diffusing particles impinging on its surface are irreversibly adsorbed (or chemically transformed).

The broad field of biochemical reactions is grounded on the notion of stochastic encounters among diffusing particles. Although encounters do not guarantee chemical reactions among the colliding particles, they represent a key prerequisite for the reaction to occur. These concepts have been widely developed in the chemical-physics literature decades ago [2]. Since then, they have been extended to complex supra-molecular biochemical assemblies (like the protein searching for target sequences on DNA strands [3]), to the prey-predator ecological models [3–6] or to the trapping phenomena in presence of static [7] or oscillating fields [8,9]. Trapping effects on the diffusive motion of particles are particularly relevant, introducing substantial deviations from the ideal behavior. Indeed, in normal diffusion the mean square displacement $\langle \mathbf{r}^2 \rangle$ of the diffusing particle is proportional to time, while the trap modified behavior scales as: $\mathbf{r}^2 \approx Dt^{\alpha}$, where $D$ is the diffusion coefficient and $\alpha < 1$ is the anomalous diffusion exponent (for a recent review see, e.g., [10]).

In the previous examples, traps and preys have a comparable size, or, in other words, model focus on the very first event of catching a single pray (the so-called Mean First-Passage Time (MFPT) problems). There exists another broad class of traps (extended or multi-traps for short) and their dimension are much larger than that of a single prey. Large multi-traps act as scavengers for the impinging particles, adsorbing (reversibly or irreversibly) every particle reaching the interface. Typical examples are the growing crystals in a super-saturated solution, the chemical reactivity of a solid catalyst particle immersed in a sea of reactants, the nutrients diffusing toward the receptors-covered cell surface and so on. An important phenomenon occurring when considering large traps is that the catching history modifies the late catching efficiency through saturation of the available binding sites. Among the plethora of models describing trapping dynamics in presence of saturation effects, we would like to mention the classical Ward-Tordai model [11, 12, 14] explaining the diffusion-controlled coverage kinetics of a surface by