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Boundary effects for diffusion of particles in finite arrays of traps: Does the classical mean field theory really work?

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Abstract

The problem of diffusion of small particles among static ideally absorbing traps randomly located in 3D domains serves as a common framework for the theoretical description of a wide range of different applications throughout chemistry, physics, and biology. After a long hiatus, interest in this problem was rekindled mostly in biological applications like enzyme catalysis, nutrient consumption due to diffusion including oxygen consumption by human tissue cells, calcium uptake by intestinal cells, bacterial absorption of various sugars etc. [1].

For many years it was commonly accepted that the theoretical description based on the well-known classical mean field approximation with respect to so-called coarse-grained concentration field inside the given array of traps is the best suited to the posed problem [1-3]. It is expedient to recall here the famous saying by S. Lec: “To get to the source, we must swim against the flow”. Therefore, in this presentation will include a critical review of a great quantity of existing studies on the problem. My recent work has shown that the widely used mean-field equation for the coarse-grained particle concentration works only deep inside the spherical array of randomly distributed traps.

To describe the coarse-grained concentration behavior within the diffusion layer near the array’s boundary, I developed a new approach based on the renormalization group. The diffusive interaction between sinks are taken into account by employing the monopole approximation, which proved to be good for spherical traps. A new equation with respect to the coarse-grained concentration nearby the boundary was derived. Our theory predicts that the characteristic penetration length is longer than what follows from the standard mean-field approximation. To elucidate the physical basis of this problem, a dimensional analysis of appropriate control parameters was performed. It was found that the criterion numbers for the strength of the diffusion interaction and for the smallness of the penetration length have simple and, at the same time, fundamental meanings. With the aid of the proposed new equation, the time-dependent concentration of particles outside the spherical ensemble of traps and the total flux of particles on the boundary of this array were calculated. This is contrasted with both the analytical and numerical results of the recent paper [4]. The future extension of this study may include the diffusion and absorption of particles to arrays of traps randomly distributed in domains other than spherical [5, 6].

References

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Profile

Prof. Traytak graduated from Mathematics & Mechanics Department of Moscow State University. He completed his PhD in the mechanics of liquids, gases and plasma at Moscow Aviation Institute. Prof. Traytak primary research interests are in the following areas: Boundary-value problems of the diffusion equation, Application of singular perturbation methods, Addition theorems and their use in diffusion theory, Theory of diffusion-influenced reactions, Mechanics of aerosols and Stokes hydrodynamics, and Phoretic propulsion.

Staff and students at all levels are welcome to attend.

Venue and Time:

This talk will be held on Thursday 2 May at 11 am at the Campbelltown Campus in Lecture Theatre 5 (CA-21.G.03). Also via **Zoom** https://uws.zoom.us/j/963276314

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