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Diffusive Interaction in the Clusters of Sinks: Theory and some Applications

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1. Introduction

Bulk diffusion-controlled reactions play an important role in many physical and chemical processes that occur in solutions [1]. We investigate the diffusion-controlled reactions for so-called trapping model: $A+B\rightarrow A$, where particles of kind A (sinks) are static and have infinite capacity. For the sake of simplicity we assume also that sinks are of the same radii R and located in a spherical region of radius L with a number concentration n_A. As quickly as the diffusing reactants B encounter a sink surface, they react immediately. The primary task for the theory is the derivation of the total flux of B particles into the i th sink

$$\Phi_i^{(N)} = -Dn_0 \int_{\partial\Omega_i} \left(\mathbf{n}_i \cdot \nabla u\right)\big|_{\partial\Omega_i} dS , \qquad (1)$$

where $u = 1 - n_B/n_0$, $n_0 = \lim_{r_i\to\infty} n_B$, n_B and D are the local concentration and diffusion coefficient of particles B, $\partial\Omega_i$ is the surface of i th sink. Particularly for the simplest case of one sink formula (1) leads to the well-known Smoluchowski expression [1]

$$\Phi_1^{(1)} = 4\pi R D n_0 . \qquad (2)$$

One can see that in many-sink arrays the concentration field n_B around any test sink is changed by the presence of other sinks. This effect we called "the diffusive interaction" (DI) with analogy to the hydrodynamics interaction for many particle systems in Stokes flow. So the main goal of this paper is twofold: (a) to solve the diffusion equation in the spherical cluster of sinks taking into account the DI and (b) using this solution estimate the characteristic lengths for diffusing reactants B.

2. Characteristic numbers of spherical cluster of sinks

Solving the diffusion equation with the aid of renormalization group approach we have found the concentration field inside the cluster with N sinks and determined that the characteristic penetration length $l_p = R/3\phi$, where $\phi = 4\pi R^3 n_A/3$ is the volume fraction of the sinks. Thus the thickness of the boundary layer where reaction occurs depends on the "outer characteristic number" $\chi_{\text{out}} = l_p/L$. One can see that this important number may be rewritten as follows:

$$\chi_{\text{out}} \propto \frac{4\pi L^2}{N \cdot 4\pi R^2} . \qquad (3)$$

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Therefore the outer characteristic number is just the ratio of the whole cluster surface area to the total surface areas of sinks which compose this cluster. It is worth noting that we showed that for large values of "inner characteristic number" $\chi_{\text{in}} = \lambda/L$ (where $\lambda = R/(3\phi)^{1/2}$ is the characteristic screening length inside the infinite array of sinks) one can treat the cluster of sinks as an effective sink of radius L. In its turn this number one can write in the form

$$(\chi_{\text{in}})^2 \propto \begin{cases} \dfrac{4\pi L D n_0}{N \cdot 4\pi R D n_0} \\ t_r / t_D^L = 1/4\pi R n_A L^2 \end{cases}, \qquad (4)$$

where $t_r = \lambda^2/D$ is the time of depletion for B particles inside the infinite array and $t_D^L = L^2/D$ is the time for diffusion passing of the whole cluster of sinks. So the inner number χ_{in} depends on ratio of total flux into the effective sink to the sum of unperturbed by DI total fluxes into sinks (see formula (2)).

Obtained results may be applied to describe various real physical and chemical systems. As an important example we present here only results on diffusion combustion of a spherical cloud of fuel droplets. Experimentalists qualitatively distinguish four regimes of combustion of droplet clouds: (a), (b), (c), and (d) (see section 15.1 of the book [2]). It follows from our theory that these regimes one can quantitatively arrange as:

$$\frac{R}{L} >> \frac{1}{\sqrt{N}} >> \frac{1}{N} \qquad \text{(a)}$$

$$\frac{1}{\sqrt{N}} >> \frac{R}{L} >> \frac{1}{N} \qquad \text{(b)}$$

$$\frac{R}{L} \sim \frac{1}{N} \qquad \text{(c)}$$

$$\frac{R}{L} << \frac{1}{N}. \qquad \text{(d)}$$

3. Conclusion

We presented here the theory of diffusive interaction of static sinks arranged in a spherical region and absorbing particles diffusing towards this region. Due to the fact that death processes are of great importance in physics and chemistry our theory and particular obtained criterion numbers may be widely used to describe numerous applications.

References

[1] S.A. Rice, Diffusion-limited Reactions, Elsevier, Amsterdam, 1985.

[2] J. Warnatz, U. Maas, R.W. Dibble, Combustion: physical and chemical fundamentals, modeling and simulation, experiments, pollutant formation, Springer, Berlin; New York, 2001.