How to find a small target on a surface? Surface-assisted search dynamics

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***Short Abstract* — The process of a reactant search for a target located on a surface is ubiquitous in Nature. We study the dynamics of a reactant search for a small target on a two-dimensional surface from the bulk using both a continuum and discrete model. We find that depending on the scanning length λ of the reactant on the surface, which is determined by the reactant-surface interactions, the search dynamics are different and the combination of 3D and 2D diffusion can minimize the search time T. We discuss the relevance of our results with some recent experiments.**

***Keywords* — search dynamics, intermittent search.**

I. Extended Abstract

In many natural and technological systems, participating particles switch between spatial regions that are characterized by different geometries and dimensionalities. Examples include heterogeneous chemical catalysis when reacting molecules have to be absorbed to the solid catalysts before the reaction can take place [1]; transcription proteins finding the specific target sequences on DNA at the start of most major biological processes [2]. Such complex processes with intermittent search dynamics have been intensively studied in recent years, but molecular mechanism of underlying phenomena still remain not well understood.

We present a comprehensive theoretical approach to describe the search process for the target, which is localized on two-dimensional (2D) surface, while the reacting species start in the bulk solution around the surface segment. Both continuum and discrete-state stochastic methods are developed and compared with each other. We identified three major search regimes, which are characterized by comparing the surface scanning length of the reacting molecules with the size of the surface segment. A full analytical description of the search dynamics is obtained for all ranges of parameters, which is also tested by extensive Monte Carlo computer simulations. In addition, the role of the surface segment size and the location of the target are evaluated. It is found that the application of the continuum model provides only qualitative but not quantitative description of the process. The mean search times calculated in the continuum model are significantly underestimated, and the largest difference is observed in the realistically most significant 2D+3D search regime. These arguments suggest that it is not reasonable to apply the continuum model framework for understanding the molecular mechanisms of the surface-assisted search phenomena, especially for the quantitative analysis.

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