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ORIGINAL ARTICLE

Phenomenology and energetics of diffusion across cell phase states

Md. Ashrafuzzaman

Department of Biochemistry, King Saud University, Riyadh, Saudi Arabia

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Abstract Cell based transport properties have been mathematically addressed. Cell contained cross boundary diffusion of materials has been explained using valid formalisms and related analytical expressions have been developed. Various distinguishable physical structures and their properties raise different general structure specific diffusion mechanisms and controlled transport related parameters. Some of these parameters play phenomenological roles and some cause regulatory effects. The cell based compartments may be divided into three major physical phase states namely liquid, plasma and solid phase states. Transport of ions, nutrients, small molecules like proteins, etc. across inter phase states and intraphase states follows general transport related formalisms. Creation of some localized permanent and/or temporary structures e.g., ion channels, clustering of constituents, etc. and the transitions between such structures appear as regulators of the transport mechanisms. In this article, I have developed mainly a theoretical analysis of the commonly observed cell transport phenomena. I have attempted to develop formalisms on general cell based diffusion followed by a few numerical computations to address the analytical expression phenomenologically. I have then extended the analysis to adopting with the local structure originated energetics. Independent or correlated molecular transport naturally relies on some general parameters that define the nature of local cell environment as well as on some occasionally raised or transiently active stochastic resonance due to localized interactions. Short and long range interaction energies play crucial roles in this regard. Physical classification of cellular compartments has led us developing analytical expressions on both biologically observed diffusion mechanisms and the diffusions's occasional stochasticity causing energetics. These analytical expressions help us address the diffusion phenomena generally considering the physical properties of the biostructures across the diffusion pathways. A specific example case of single molecule transport and localized interaction energetics in a specific cell phase has been utilized to address the diffusion quite clearly. This article helps to address the mechanisms of cell based diffusion and nutrient movements and thus helps develop strategic templates to manipulate the diffusion mechanisms. Application of the

E-mail address: mashrafuzzaman@ksu.edu.sa
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theoretical knowledge into designing or discovering drugs or small molecule inhibitors targeting cell based structures may open up new avenues in biomedical sciences.

1. Introduction

Cell has various structural compartments. The compartments are divided into three major physical phase states namely liquid, plasma and solid states. Cell based transport of nutrients, small molecules, ions, etc. across inter-phase and intra-phase states follows general transport formalisms. Recently, we have published a paper to address this issue quite in detail (Ashrafuzzaman, 2015). We shall brief some of the aspects here. Some localized permanent and/or temporary structures and time dependent structural transitions also appear as regulators of the transport mechanisms. The minimum energy conformation (energy minimization) and stability (often refers to lifetime) of such structural complexes are found to contribute heavily into determining their transport properties and thus regulating the diffusion across them. In this article, I have developed mainly a theoretical analysis of the cell transport phenomena (Ashrafuzzaman and Tuszynski, 2012a) from cell component structural and localized interaction energetic points of view. To do so we need to present a clear analysis on the cell based various structural phase states (Ashrafuzzaman, 2015). I have then attempted to develop formalisms on general cell based diffusion followed by a special example case of ion channel (Ashrafuzzaman et al., 2006, 2012, 2014; Ashrafuzzaman and Tuszynski, 2012b,c; Huang, 1986; Andersen et al., 1999; Greisen et al., 2011). Ion channels are well known to help a cell establish communication between different distinguished cell phase states creating compartments. Ion channels are also known to help bypass certain phase states that sometimes may act as a barrier. Ion channels therefore participate directly in cell based general diffusion. Besides addressing the phenomenological aspects of general transport formalisms, I have also attempted to address the issue energetically.

As a specific example case we can try to address the cell membrane transport. Physical properties of lipid bilayers regulate integral membrane protein functions in a manner that depends on the hydrophobic coupling between the bilayer and the membrane proteins. Fig. 1 demonstrates such cases for special types of ion channels. Thus the membrane which is a plasma state may be bypassed by nutrients through some membrane residing temporary structures. The channels residing across membrane make passages for ions and various nutrients (Fig. 1). To address this issue we have theoretically developed a method to calculate the coupling energy between a lipid bilayer membrane and an integral transbilayer β-helical gramicidin A (gA) ion channel immersed in an aqueous phase using the screened Coulomb interaction often used in solving interactions between particles in a many-body condensed matter system (Ashrafuzzaman and Tuszynski, 2012b). This analysis proves that the localized structural changes as observed near the transport events play a crucial role to determine the transport phenomena. But it is also true that such structural changes appear due to mainly various physical processes like intercomponent charge based interactions, elastic coupling of the participating agents, localized aqueous dielectric condition, etc. Our theoretical calculation indicates that any change in the localized energetics of such an ion channel type structure is due to perturbations in the physical properties of the bilayer or/and gA channels should reflect through changes in the structural stability. In laboratory we can detect such structural changes in terms of lifetime of the structure, e.g., see the channel stability addressed in Ref. (Ashrafuzzaman and Tuszynski, 2012b).

2. Cell based structures and classified physical states

Biological cell has various components. Those can be classified into various physical structural classes. A detailed structural analysis may help them to be grouped among solid, liquid and plasma phase states. Fig. 2 shows model representation of a cell's various components. The general cell structure is quite known for sometime but analysis on the physical states of these structural components is yet to be made or known poorly. Here we shall make a biophysical analysis of this biological issue.

2.1. Cell's general structures

All cells are enclosed by cell envelopes which consist of cell walls covering plasma membranes. Both of the prokaryotic and eukaryotic cells have membranes. A membrane primarily separates the interior of a cell from the exterior, it regulates the selective movements of particles across it, and most importantly maintains an electric potential of the cell. The inside world is a combination of various structures as schematized in Fig. 2.

2.2. States of the general cell structures and related interactions

Biological cells are generally considered as soft matter. When we see a cell we in fact see its outside look that means we see the cell membrane. Beyond the membrane, in the cell's dissected state, there found to exist various things as shown in Fig. 2. These cellular constituents fall in different physical structure categories. Solid, liquid, and gas are the major physical states. Between solid and liquid there exists another state called plasma state. All these states appear with certain physical properties, certain kinds of inter particle interactions, certain types of shapes and sizes, etc. The mechanical and electrical properties of various states are also different. In a cell we find all of these states but gas. Some of these mentioned cellular structures permanently fall within a state while others temporarily or to be more specific many structures experience transitions between states. Sometimes some of the building blocks of any structure fall in a physical state class but the collective structure may not necessarily fall in the same class rather they are often found to be falling in a different state.