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Thermodynamic approach to nano-properties of cell membrane

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HIGHLIGHTS

- Irreversibility is the fundamental quantity for the analysis of biosystems.
- The entropy generation describes irreversibility.
- Cell nanomechanics is useful in biological and medical use.
- A thermodynamic approach to cell nanomechanics is suggested.

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ABSTRACT

Biomechanical analyses of DNA have pointed out the connections among forces, thermodynamics and kinetics. The entropy generation approach has been suggested as a thermodynamic approach to evaluate the accessible states for cancer systems, in relation to their specific thermodynamic quantities, including mechanical properties. In this paper, a theoretical approach for the thermodynamic evaluation of the nano-behaviour of the cell wall is suggested. The aim is to provide theoretical bases to the analysis of cells and their properties by applying the thermodynamic approach to irreversibility.

1. Introduction

Many processes in biological systems are related to nanomechanical properties of cellular structures and membranes [1]. Cell surfaces modifications were highlighted to enhance the therapeutic potential of cell products in medical therapy. For example, a new drug carrier can be designed to be more efficient in relation to drug delivery barriers which exist at every level of drug distribution, including systemic, tissue and cellular levels, as no drug can be effective against cancer until it is successfully delivered within the cancer cells [2].

Moreover, the study of cell surfaces has recently been improved by using images of protein nano-clusters from near-field scanning optical microscopy performed on cells, as well as atomic force microscopy which localizes force-probes of single molecules in living cells. The increasing interest in the analysis of the nanomechanical properties of cell membrane is a fundamental support to theoretical analysis and designing application [3,4].

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The cell as a system is composed of:

1. the cell wall, which represents the outside border of the cell: through the wall the cell can exchange energy and mass flows with its environment;
2. the membrane, which controls the mass flows into and out of the cytoplasm;
3. the cytoplasm, which is an aqueous solution of many chemical species;
4. the organelles, which are specialized subunits that perform specific functions useful to the cell life: the organelles are suspended in the cytoplasm.

The elastic behaviour of cells must be considered as regards mechanical perturbation. Only the membrane and cytoplasm, due to their structures, play a fundamental role because they can be considered as the continuum components of the cell.

Still, although physical, chemical, engineering and biological sciences have achieved fundamental goals in understanding complex systems, many properties of biological structures continue to be unknown [5]. In particular, some biological properties represent the bases for a new approach to disease diagnosis and therapy, as for example in the case of cancer.

In cells many processes as replication, transcription and translation need to convert molecular binding energy, chemical bond hydrolysis and electromagnetic gradient into mechanical work. This mechanical work is related to conformational changes and displacements [2]. The origin of this mechanical conversion of energy is not completely clear. Here, we guess that the mechanical conversion relates to the action of molecular machines which may be operating inside the cell and to the spontaneous electromagnetic coupling among biochemical molecules within the cells. However, it has been experimentally highlighted that these chemical–physical processes, for example cyclic chemical reactions in their natural range greater than 50 kHz, can produce the emission of mechanical waves of typical frequency band, i.e. in the 0–100 kHz range [6]. In cells these emissions have been connected to molecular motors, more specifically to kinesins, dyneins and myosins [7]. Mechanical vibrations in the cell walls have been experimentally studied *in vivo* by evaluating the chemical–physical effects within the same resonance range (0–100 kHz) [1,8,9].

Finally, the implications of the mechanical analysis of DNA have been analyzed in relation both to biological motors and to the design of synthetic nano-scale machines [10]. The biomechanical analysis of DNA has pointed out the connections among forces, thermodynamics, nanomechanical and electromagnetic behaviour of biological structures and kinetics [10,11].

The entropy generation approach [12–20] has recently been used in order to evaluate the accessible states for cancer systems, in relation to their specific thermodynamic quantities. Indeed, the entropy generation approach is a very interesting approach for the analysis of irreversible and complex systems because:

1. it does not need the local equilibrium hypothesis, which allows us to obtain a general and global analysis of the system;
2. it introduces the lifetime of the process, i.e. the time of occurrence of a process;
3. it analyzes systems in a time greater than or equal to the lifetime of the entire process occurred in the system; consequently, it allows studying the full developed process which provides greater information on process results.

This approach should be distinguished from the entropy production approach, because the latter needs the local equilibrium hypothesis and it does not consider process times. They are two different approaches which allow us to analyze systems in two complementary ways.

In this paper, a theoretical approach for the thermodynamic evaluation of nano-properties of cell walls is suggested. Section 2 contains a summary of thermodynamic bases. In Section 3, the numerical evaluation is developed and compared with the experimental results known in literature for which there are not theoretical fundamentals and Section 4 contains some final considerations.

2. The thermodynamics approach to cell membrane

Considering the second law of thermodynamics, the total entropy is defined as [21]:

$$S = \int \left(\frac{\delta Q}{T}\right)_{rev} = \Delta S_e + S_g \tag{1}$$

where ΔS_e is the entropy variation that can be obtained by reversibly exchanging the same energy fluxes throughout the system borders, while S_g is the entropy variation due to irreversibility, the so-called entropy generation. Entropy variation due to irreversibility then measures how far the system is from the state that will be attained in a reversible way [12]: it is always non-negative. Entropy generation is defined as [12]:

$$S_g = \int_0^{\tau} \dot{S}_g d\tau \tag{2}$$

with [21]:

$$\dot{S}_g = \frac{dS}{d\tau} - \sum_{i=1}^{n} \frac{\dot{Q}_i}{T_i} - \sum_{in} \dot{m}_{in} s_{in} - \sum_{out} \dot{m}_{out} s_{out} \tag{3}$$