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Entropy generation approach to cell systems

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HIGHLIGHTS

- The entropy generation describes the irreversibility of the open systems.
- Entropy generation is introduced in the analysis of cancer growth.
- Cancer growth depends on thermodynamic quantities.
- Thermalisation is proven to be a future engineering anticancer therapy.

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ABSTRACT

Cells can be regarded as engines that execute a series of chemical reactions. A malignant cell, that is, a cancerous cell, can be described as an open complex dynamic and self-organising system. The entropy generation approach has been used to evaluate the stationary states for cells in relation to the global results of the cell biophysical and biochemical processes. Then, an entropy generation approach can been used to evaluate malignant behaviour in terms of thermal, chemical and transport processes. A numerical evaluation of the mean value of the entropy generation for cancer is developed. A possible therapy against cancer has been suggested by using molecular thermalisation.

1. Introduction

Biological systems convert energy in one form to another by coupling metabolic and chemical reactions with transport processes [1–12]. This behaviour can be modelled as an adaptive thermal and chemical engine. In such systems, the thermal and chemical processes, such as the transport of matter, energy and electricity, consume free energy and hence occur irreversibly [10,13–15]. When some of these phenomena occur simultaneously, new effects can be generated by their connections [1,16–19].

An analysis of the open dissipative systems can be developed using the concept of irreversibility when described mathematically in terms of entropy generation [20–34]. The formalism can also be related to Keenan's availability [35–40].

The entropy generation extrema theorem has been proven [40,41] as a global approach to analyse the stationary states of open systems. It has been improved in order to evaluate the condition of the stability of the stationary states of linear and non-linear complex systems [19]. In this approach, the free energy, i.e., exergy, gradients are the motive forces of the thermal and chemical processes of any complex system. The system will evolve to assume the configuration that maximises the dissipation [9,11,19,42–45], evaluated by the outside of the system, and minimises the dissipation if evaluated by the inside of the system [19,45].

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Cancer is a set of malignant cells that have lost their control over normal growth [46] and have the following characteristics:

1. precursors, often present in cancers, underlining the relationship between cancer cells and their stroma,
2. blood vessel formation [47], even if there exist avascular tumour growth conditions [46], and
3. a high mitosis-to-apoptosis ratio [47].

Moreover, it was experimentally highlighted [48] that normal samples may contain foci of partially transformed tissue, quiescent only until they are in contact with fibroblasts, which send out normal growth signals [47]: this indicates the fundamental role between the cancer system and its environment. As a consequence of all of these considerations, cancer is easily represented as a non-linear system in non-equilibrium thermodynamic states, characterised by complexity [49] and adaptability [50] and self-organisation in space and time [46].

Consequently, the thermodynamic analysis [51] of cancer is fundamental [52] to understanding the malignant system and eventually to anticancer therapy. To apply any engineering approach, a numerical evaluation of the theoretical results is necessary; indeed, entropy generation is a well-known approach in engineering [27–31,40,41,45,52–66], with many consequences on the fundamentals of thermodynamics [19,67–80] and of the life sciences [9,10,81–86]. Here, it is introduced in the analysis of the cell behaviour. Finally, it was demonstrated that thermodynamics, together with kinetics, allows us to obtain more information than other approaches [87].

To list the foundation of the approach proposed and of some engineering approaches to anticancer treatment, it is fundamental to develop a numerical evaluation of the results theoretically obtained. To do so, in this paper, the physical bases of the method used will be discussed in Section 2, the entropy generation approach to cells will be developed in Section 3, and its numerical evaluation will be introduced in Section 4 with comments followed by thermodynamic discussions in Section 5.

2. Preliminary considerations on open systems and entropy generation

Cells are living systems. They grow and, at a characteristic time, each of them divides into two different cells. At the time of division, the sizes of the single cells vary and, consequently, the sizes of the daughter cells also vary in a particular range [87–89]. A cell's life is a cyclic process. It begins when the cell emerges from cell separation, and it ends with the separation of the daughter cell itself.

The cell as a system is composed of the following parts as shown in Refs. [87,90]:

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

Within the cells, some chemical species undergo chemical reactions with the production of energy and macromolecules, with a consequent increase of the cell volume. Moreover, a part of the energy is lost as heat outflow. Only the final products of the cell processes are known, whereas it is impossible to know any individual step [87].

Consequently, the cell results in an open and complex system. The cell spontaneously exchanges heat, and this heat is related to the behaviour of the cell itself. It represents the interaction between the cell and its environment, a sort of ''spontaneous communication'' of the cell if an observer watches it to analyse its behaviour. This interaction is fundamental to developing a thermodynamic study of the cell. Indeed, cells are too complex to understand the contribution of each process to the global result, and the study of cells as black boxes allows us to simplify the analysis by considering only the inflow and outflow balances. Moreover, it is easier to have access to the cell environment than to the living cell itself.

These considerations allow us to introduce the entropy generation approach to the study of the cells. This approach assumes that [19]:

1. an open irreversible real linear or non-linear system is considered;
2. each process has a finite lifetime τ;
3. what happens in each instant in the range $[0, \tau]$ cannot be known, but what has happened after time τ (the result of the process) is well-known (at least it is sufficient to wait and observe): local equilibrium is not necessarily required;
4. the entropy balance equation is a balance of fluxes of entropy and exergy.

Moreover, the entropy generation approach allows us to analyse the non-equilibrium stationary states by studying the irreversibility of the systems. As it will be highlighted in the next section, the entropy generation approach, using the Gouy–Stodola theorem, considers only the work lost for irreversibility and the temperature of the system environment, which is always considered constant during any process. This approach is theoretically interesting because [19]:

1. it allows to obtain the range in which an open system persists in its stationary states;
2. this is a good description of natural phenomena because it considers the global effects of the chaotic behaviour of the system and its fluctuations around the stationary states;