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Optimum performance for energy transfer in a chemical reaction system

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HIGHLIGHTS

- Optimal performance of an isothermal engine driven by the chemical energy transfer is presented.
- Efficient power and Omega criterion are applied as objective functions.
- Optimal efficiency shows a similarity for the isothermal engine analyzed.

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ABSTRACT

This paper presents an optimal performance analysis for an isothermal model which performs work at a steady state via the energy transfer from a chemical reaction, using the methodology of the so-called Finite Time Thermodynamics (FTT). Furthermore, three optimal operation modes namely, Maximum Power, Maximum Omega function and Efficient Power are presented for the model. Results show analogies in the optimal performance between thermal and isothermal engine models.

1. Introduction

Molecular motors are machines that operate in cycles and convert chemical energy into useful work, mainly from the hydrolysis of the ATP molecule, to perform a variety of cellular functions such as DNA replication, repair and transcription of RNA, protein synthesis and transport between cell and other elements [1]. Such machines operate in a constant temperature environment unlike heat engines which are limited by the Carnot (η_C) efficiency. The limit value of efficiency for molecular motors is one and can be reached only in the limit when the output power is zero.

Biochemical processes of living cells occur at ambient or near-ambient temperatures [2,3] at which the rates of spontaneous leak processes are limited, but, cells selectively improve the kinetics of their energy-coupling reactions with enzymes, which effectively create alternative reaction paths with lower activation energies. Enzymes lower activation energies by 30 to 100 kJ/mol, which, at $T = 298.15$ K, corresponds to increases in reaction rates of 5 to 17 orders of magnitude [4]. Indeed, the survival of living systems often depends heavily on their reproduction rate and, thereby, on the rate of energy conversion in the cells. On the other hand, thermodynamic efficiency is an important factor in the yield of reproduction processes, so that, energy conversion in living cells is expected to occur where a trade-off between both performance aspects is considered.

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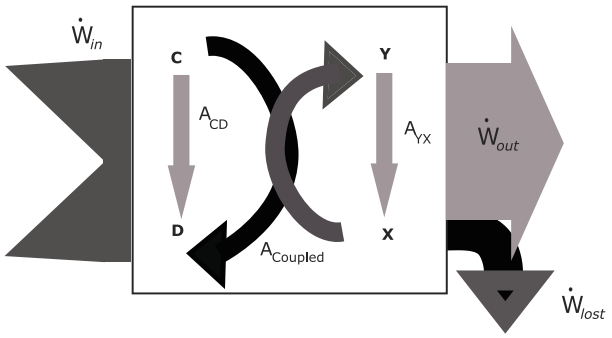

Fig. 1. Scheme of a (bio)chemical reaction model, sketched by Lems [21].

In 1975 Curzon and Ahlborn [5] presented an expression for Efficiency at Maximum Power (EMP) modeling a thermal machine which executes a Carnot-type cycle, a new branch of thermodynamics emerged in the last decades, known as Finite Time Thermodynamics (FTT). The model proposed by Curzon and Ahlborn operates between two heat sources with high and low temperatures, T_h and $T_c (< T_h)$, respectively, and the expression for the EMP obtained was $\eta_{CA} = 1 - \sqrt{T_c/T_h}$, a result that in principle is independent of the model parameters and only depends on the temperatures of the heat reservoirs; analogously this is what happens with the efficiency for a reversible Carnot cycle ($\eta_C = 1 - T_c/T_h$). Although to obtain the efficiency of Curzon and Ahlborn, it is necessary to consider that the heat transfer involved obeys a linear law. Notice that previously other authors [6,7] have found the same expression for similar models. An important advantage observed in the results obtained in FTT is that optimal efficiency values are closer to those observed in real machines [8]. Within the context of the FTT several objective functions to be optimized under rich criteria have been introduced and, many models of heat engines have been proposed and analyzed which perform as motors, heat pumps or refrigerators [9,10].

It has recently been reported [11–13] that thermal engines show some kind of universality in the behavior of the efficiency at maximum power [13], although the analyzed models are different in nature and scale, for instance, macroscopic, stochastic or quantum [14–16].

Traditionally most of energy-transfer devices discussed by the FTT were heat engines although, some optimal performance analyses were also conducted where biochemical reaction models were analyzed [17–19]. In recent years, isothermal engines with kinetic [20–22] and mesoscopic [23,24] description have been published, as those which convert non-thermal energy (mainly chemistry) into useful work. The importance of these models is that the energy production processes that are observed in the molecular biological level machines obey similar principles.

In this paper, an optimal performance of a system that produces work via chemical energy transfer by the coupling of two chemical reactions using the methodology of FTT is presented. The performed analysis takes into account three operating regimes namely: Maximum Power, Omega Function and Efficient Power criterion, respectively. Two special cases for the (bio)chemical device efficiency are presented: (i) The general numerical case and (ii) A limit case where analytic results are found.

2. Model for chemical energy transfer

The model that would be analyzed was performed by Lems et al. in 2007 [21]. In his model, Lems studied a system of biochemical reactions shown in Fig. 1, the chemical energy is transferred at 298.15 K, in a coupled chemical reaction in which the favorable reaction $C \rightarrow D$ is used to manage the unfavorable reaction $X \rightarrow Y$, a well known procedure in bioenergetics where the biological tasks are managed by the energetic coupling of the reactions [4]. The system considers two leak reactions, which dissipate chemical energy without contributing to production of work output.

To describe the system operation, initially the potential of each individual reaction to deliver work is considered. The ability to perform work of a chemical reaction is determined by its affinity (A) of the reaction [21], representing the degree of non-equilibrium between reactants and products, and is determined by the chemical potential μ_i, and the stoichiometric coefficients ν_i.

From the work proposed by Donder [25] it is known that the affinity can be written as the negative of the change in Gibbs free energy of reaction ($-\Delta_r G$),

$$A = -\Delta_r G = -\sum_i \nu_i \mu_i. \tag{1}$$

Each of the reactions involved in the system gives (see Table 1).

When $A > 0$, the products of the reaction are at a lower energy level than the reactants, the reaction is possible until thermodynamic equilibrium is reached, when $A = 0$ (see Fig. 3). At equilibrium, there are no reaction forces that handle the reaction and therefore the production no longer has the potential to generate work.