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# Thermodynamic analysis of biogas fed solid oxide fuel cell power plants

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# ABSTRACT

The present research study presents the optimization of Solid Oxide Fuel Cell (SOFC) power plants directly fed by biogas. By considering energy and exergy balances for such a system, a detailed thermodynamic model (THERMAS) was designed and implemented. A specific SOFC-based system was selected as case study, equipped with three heat exchangers (preheaters), a reformer, a SOFC-stack system and an afterburner. The use of the simulation tool THERMAS give us the opportunity to investigate all the appropriate parameters that affect system's efficiency based on exergy analysis while incorporating a detailed parametric analysis regarding the whole system. The optimization process relies on the difference between the energy and exergy efficiency by considering an innovative Optimization Factor (OPF) for each simulated system, which is dynamically affected by operational parameters, such as fuel composition, extension of chemical reactions and temperatures. It is found that the use of a pure fuels seems to be meaningless without optimization.

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### 1. Introduction

During the last decades, overpopulation and the consequent excessive overconsumption, characterizes the global existing situation, thus producing a huge amount of wastes (agriculture, animal, food, domestic wastes etc.). These billions tons of wastes can be properly managed and treated to avoid environment pollution and simultaneously to be produced enough electrical energy to cover the human needs despite the limitation of the fossil fuels deposits [1].

Under these considerations, biogas a multi-gas mixture, seems to be an important source of renewable energy as it can be produced by the degradation of biodegradable materials, such as organic wastes under the eco-friendly way of anaerobic digestion [2]. Biogas is primarily composed by methane (CH<sub>4</sub>) and carbon dioxide (CO<sub>2</sub>), while it is saturated with water vapor. By considering the initial organic materials and the time-period for the finalization of the biological process during biogas production, its composition varies. Statistically speaking, it has been shown that the typical values for methane per unit mass of biogas production vary between 50% and 73%, usually attained after a 14 week anaerobic digestion process, while after a 10 week process corresponds to a 40% [1,3]. By concerning carbon dioxide, its values vary from 15% up to 45% and the water vapor from 5% up to 12%, respectively [1,4–6].

Fuel cells are devices that directly convert chemical energy of the feeding fuel to electricity without Carnot limitations [7-9]. As far as biogas is a methane-rich fuel, it stimulates a reliable alternative to fuel options. The increased flexibility on fuel choice that Solid Oxide Fuel Cells (SOFC) advantageously present [10,11], strengthen further biogas utilization in such devices.

Experimental results on SOFC based projects fed with pure methane or ethanol to produce electric energy reveals theoretical energy efficiencies up to 80%–90%, under a totally eco-friendly way [12–14]. Also such a project can achieve satisfactory performance using biogas even with low methane content [15]. Several studies throughout the literature have already examined the economic performance of SOFC systems under different aspects (i.e. the levelized cost of electricity (COE), the biogas cost, the objective function of interest, the power normalized capital cost or the internal rate of return on investment as a function of several operational parameters [16,17]). Also several studies use thermodynamics to perform analysis on SOFC systems combined with heat production [12–14,18] while special effort has been put to investigate the effects of biogas feeding under several assumptions [19].

The basic aim of the presented study is to present a detailed model for the optimization of the operation of SOFC-based power





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plants by using thermodynamics. The optimization is based on fundamental thermodynamics, energy and exergy balances and the corresponding cost analysis. This model has been named THERMAS (THERmodynamic MAthematical Simulation model). In this context, each individual process incorporated in the power production system has been extensively mathematically simulated for different cases that represent real life operational conditions. Therefore, several dynamical parameters as well as several mixture compositions have been taken into account, to cover all the possible incidents. Also THERMAS offers the opportunity to choose a great variety of different values for each operational parameter individually, thus allowing for studies within unexplored and experimentally impossible operational ranges. Finally, THERMAS innovatively introduces exergy efficiency to identify the optimal scenario per system.

#### 2. Theory

The initial fundamental phenomenon which is widely used in engineering and environmental analyses and is required for thorough design and analysis of several physical systems' processes, is based on mass balances. Mathematically, the general mass flow rate balance can be described through the expression [20]:

$$\dot{m}_{in} + \dot{m}_{gen} = \dot{m}_{out} + \dot{m}_{cons} + \dot{m}_{accu} \tag{1}$$

This can be described as the initial criterion to control the proper operation of each device and simultaneously of the whole system during its simulation. Eq. (1) has to be satisfied in each time step of the process, mainly due to the chemical reactions take place that are characterized by different extensions, accordingly to the limitations being put by the materials used and the conditions applied. Obviously,  $\dot{m}_{gen}$ ,  $\dot{m}_{cons}$  and  $\dot{m}_{accu}$  might be zero, dependent on the simulated case.

Engineering processes are also based on the First Law of Thermodynamics, referred as energy balance theory and for the needs of the current modelling will constitute the second criterion which has to be satisfied for each device. The energy balance of a heat exchanger can be expressed as [21]:

$$T_{in}\left[\sum_{i} M_{i}(C_{P})_{i}\right]_{in} = T_{out}\left[\sum_{i} M_{i}(C_{P})_{i}\right]_{out}$$
(2)

where  $C_P$  is the molar specific heat capacity. By assuming ideal gases, this can be calculated through NASA Polynomials with the appropriate specific coefficients for each chemical element [22].

During biogas reforming the total energy balance can be described as [22,23]:

$$T_{in}\left[\sum_{i} M_{i}(C_{P})_{i}\right]_{in} + [Q_{burn}]_{ref} + |\Delta H_{WGS}|$$
$$= T_{out}\left[\sum_{i} M_{i}(C_{P})_{i}\right]_{out} + \Delta H_{ref}$$
(3)

where  $[Q_{burn}]_{ref}$  is the extra thermal energy supplied by the afterburner for the finalization of the reforming process. The enthalpy changes,  $\Delta H_{WGS}$  and  $\Delta H_{ref}$  are characterized by positive or negative values due to the exothermic and endothermic character of each reaction, respectively.

As concern the considered SOFC-stack system modelling, we must underline the absence of an extra thermal energy term and the presence of exothermic reactions, while an extra energy term is derived by the produced electric load, W<sub>el</sub>. Also, regarding the afterburner's operation, it is necessary to consider the environmental

thermal losses,  $[Q_{burn}]_{env}$ , and the supplied thermal energy to the reformer,  $[Q_{burn}]_{ref}$ , as well as the enthalpy changes due to the several exothermic reactions. The above presented energy balance theory is followed as well in both SOFC-stack system and afterburner, as reveal Eq. (4) and Eq. (5) respectively:

$$T_{in}\left[\sum_{i} M_{i}(C_{P})_{i}\right]_{in} + |\Delta H_{H_{2}}| + |\Delta H_{CO}|$$
  
=  $T_{out}\left[\sum_{i} M_{i}(C_{P})_{i}\right]_{out} + W_{el}$  (4)

$$T_{in}\left[\sum_{i} M_{i}(C_{P})_{i}\right]_{in} + |\Delta H_{burn}| = T_{out}\left[\sum_{i} M_{i}(C_{P})_{i}\right]_{out} + [Q_{burn}]_{ref} + [Q_{burn}]_{env}$$
(5)

From the very beginning of the systematic development of electricity generating systems based on fuel cells, research was focused on the approximation of optimal values of the major operational parameters by considering the first law of thermodynamics (energy balance theory). In fact, it was followed until the second law of thermodynamics acquired practical significance in the optimization of energy systems [23]. Since then, the exergy analysis has been accepted as a sound method for the interpretation of the axiomatic role of the second law in the design and optimization of energy conversion systems in terms of efficiency [14]. Also it constitutes a supplementary tool to aim in decision making about the operational parameters and criteria that may lead to optimal system's operation.

Mentioning that exergy is actually a thermodynamic property that describes the maximum useful work provided by a system during to its reversible transition to a thermodynamic state in equilibrium with its environment, it seems to play a crucial role during simulation process [24]. The exergy analysis (availability analysis) determines in general the location, cause and magnitude of energy resource waste and loss [25]. Exergy depends on both the states of the system and its environment while exergy calculation considers processes of thermal, mechanical and chemical character and it is convenient, however, to be separated into two terms. More precisely, physical exergy, e<sub>ph</sub>, expresses the useful work that a chemical component can produce if it is brought reversibly from the state of the system to the "restricted dead state", which is a state in thermal and mechanical equilibrium with the environment and can be generally expressed as [26]:

$$e_{ph} = \int_{T_0}^{T} C_P dT - T_0 \left[ \int_{T_0}^{T} \frac{C_P}{T} dT - Rln \left( \frac{P}{P_0} \right) \right]$$
(6)

On the other hand, chemical exergy  $e_{ch}$ , expresses the useful work that the chemical elements can produce if it is brought reversibly in chemical equilibrium with the environment. It is essential to be used an appropriate "exergy reference environment" in order to be estimated the standard chemical exergy  $e_0$  according to the relation [26]:

$$e_{ch} = M_{tot} \left( \sum_{i} x_i(e_0)_i + RT_0 \sum_{i} x_i \ln x_i \right)$$
(7)

As far as the characteristics of each device are unique, the aforementioned approach has to be mathematically modelled for all the processes in each operational step. The exergy balance of a heat exchanging process in a SOFC based system, during present simulations, can be expressed as [26]:

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