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A versatile computational tool for model-based design, control and diagnosis of a generic Solid Oxide Fuel Cell Integrated Stack Module

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ABSTRACT

This work focuses on the development of a control and diagnosis-oriented model of a Solid Oxide Fuel Cell (SOFC) integrated system module (ISM). Fuel cell researchers and developers are currently investing significant resources on such fuel cell-based energy conversion systems, as a consequence of their adaptability to a variety of applications and power size. In this configuration, heat exchanges among components are difficult to manage and, consequently, reliable model-based tools are required to enhance the design phase. Therefore, the main heat exchange mechanisms (including radiation, here modeled via view-factors-based approach) are evaluated by simplifying 3-D geometries, as well as assuming the outlet temperature from each component as its state variable. The resulting lumped parameters model was proven effective in achieving the required compromise between accuracy and computational time, particularly in view of its real-world deployment for advanced balance of plant (BoP) analyses, as well as within control and diagnostic model-based tasks. Moreover, the entire SOFC ISM model is generic and can be suitably applied to different layouts, through the characterization of main model parameters. Simulation results are in agreement with experimental data collected on a non-conventional micro-CHP system, named HoTBox™, tested under nominal operating conditions within the EU funded project DIAMOND.

1. Introduction

Power generation systems based on Fuel Cells (FC) are among the most promising technologies to guarantee the achievement of medium-term decarbonization targets in Europe, North America, Japan and Korea. China, whose energy consumption has grown with high rates in the last decade, is also investing in FC [1]. FC have notable potential for power generation in stationary, portable and transport applications and may support the increasing need for sustainable energy resources. FC technology allows combining high efficiency with minimum (or completely null when fueled by pure hydrogen) harmful emissions (sulphur, nitrogen and carbon oxides, hydrocarbon pollutants and particulate), as well as significantly reducing CO_2 emissions. It is worth remarking that all FC technologies are the cleanest among those converting fossil energy [2]. Moreover, noise emission is not a concern, thus enhancing their use in any practical use. High temperature SOFCs are particularly well suited for stationary applications, generating electricity and heat for cogeneration.

The high temperatures, reached by the SOFC during its nominal operation, make necessary paying significant attention to the thermal management of the stack and its ancillaries. For years, the layout has been designed around an adiabatic stack, fed with anodic and cathodic gases processed in pre-reformer and heat exchangers. The main objective was to supply gases at the desired inlet temperature, while guaranteeing stack stability over time and minimizing the temperature gradient across its channels, in such a way as to improve durability. That layout is the technical evolution of prototypes derived from laboratory arrangements and has the advantage of easily controlling the stack input temperatures by adjusting gases flow rates. Medium/high power system configurations are not mature yet for market deployment; thus, most of the research has been directed towards multi-stacks arrangements, whose main management problem is the balancing among the generation units [3]. On the other hand, low power SOFC for cogeneration applications have received a strong impulse in the last decade and the research has led to new configurations, where all components are fitted within a single compartment to improve their thermal performance [4]. In such a system (see Figs. 1 and 2), the stack and hot ancillaries (i.e. pre-reformer, heat exchangers and afterburner) are not adiabatic and exchange heat among them. Therefore, the proper design of the system requires a complex optimization exercise, whereas

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Nomenclature

Acronyms

APU	auxiliary power unit
BoP	balance of plant
CHP	combined heat and power
CPOx	catalytic partial oxidation
GT	gas turbine
HE	heat exchanger
MSE	mean squared error
O/C	oxygen to carbon ratio
PB	afterburner
PR	pre-reformer
S/R	steam to carbon ratio
SOFC	solid oxide fuel cell
SR	steam reformer

Roman symbols

A	area/m^2
ASR	area specific resistance/Ω cm^2
AU	air utilization/%
$\dot{C}$	flow heat capacity/W K^{-1}
c_p	specific heat capacity at constant pressure/J Kg^{-1} K^{-1}
$\dot{E}$	enthalpic power flow/W
E_a	activation energy/J
F	Faraday constant/C mol^{-1}
F_{ij}	view factor
FU	fuel utilization/%
G	Gibbs free energy/J
h	specific enthalpy/J mol^{-1}
H	enthalpy/J
h_{conv}	heat convective coefficient/W m^{-2} K^{-1}
I	current/A
j	current density/mA cm^{-2}
k	chemical equilibrium constant
K	heat capacity/J K^{-1}
$\dot{m}$	mass flow/g s^{-1}
$\dot{n}$	molar flow/mol s^{-1}
n_{cell}	number of cells
n_{el}	number of electrons
N	number of data
P	pressure/Pa
p_{H_2}	hydrogen partial pressure /Pa/Pa
p_{H_2O}	water partial pressure //Pa
p_{O_2}	oxygen partial pressure /Pa/Pa
$\dot{Q}$	heat flow/W
R	universal gas constant/J mol^{-1} K^{-1}
R_i	thermal resistance/K W^{-1}
$\dot{r}$	reaction rate/mol s^{-1}
T	time/s
T	temperature/K
V	voltage/V
V_{Nernst}	Nernst ideal potential/V
X	molar fraction/%

Greek symbols

Δ	change
ε	emissivity
H	efficiency/%
Λ	thermal conductivity/W m^{-1} K^{-1}
P	mass density/Kg m^{-3}
Σ	Stefan-Boltzmann constant

Footers

A	air
An	anode
Av	average
C	cold
Ca	cathode
F	fuel
H	hot
Max	maximum
Min	minimum
In	inlet
Off	offset
out	outlet
ox	electro-oxidation
ref	reforming
shift	water gas shift

the thermal management entails advanced control strategies. Moreover, the diagnostic activity to perform, while the system runs on-field, is even more cumbersome, due to thermo-fluid dynamic interaction and because of the difficulties in placing extra sensors within the high temperature box. In such a context, model-based approaches for thermal analysis are crucial and advanced mathematical tools need to be exploited for either off-line (i.e. design and optimization) or on-line (i.e. monitoring, control and diagnosis) uses [5,6].

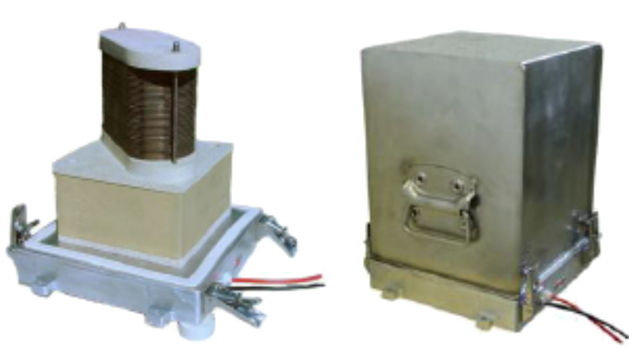

Fig. 1. An example of HotBox™ SOFC system. The system here modeled consists of two stacks [26]

Numerical simulation is fundamental to support the development of SOFC prototypes in a wide range of operating points and nominal conditions, instead of performing time-consuming and costly experimental campaigns [7]. Thus, the research field on models for simulation of SOFC systems is extremely dynamic. Al Moussawi et al. [8] developed an electrochemical model to simulate a trigeneration system for residential applications; Xenos [9] et al. presented a flexible mathematical model for planar SOFCs to simulate the dynamic conditions, particularly in critical operating points, such as start-up, load change or in the occurrence of drastic changes in the inlet temperatures of the gas streams. Likewise, Bae et al. [10] studied, via a physical 3-D model, the transient response of thermodynamic variables after electrical load change, in order to provide useful guidelines to develop new design concepts that can soften degradation processes arising from dynamic operating conditions. Moreover, they stressed the need of a real-time model-based control system to improve the reliability of cell micro-structure and stack configuration. Barelli et al. [11] developed a dynamic model of a hybrid SOFC coupled with a gas turbine system (SOFC/GT); Ferrari et al. [12] analyzed pressurized hybrid SOFC/GT