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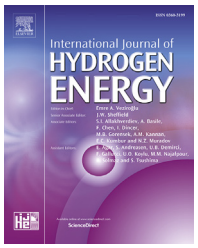

Theoretical and experimental investigation of syngas-fueled molten carbonate fuel cell for assessment of its performance

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ARTICLE INFO

Article history:
Received 5 April 2017
Received in revised form
18 July 2017
Accepted 1 October 2017
Available online 28 October 2017

Keywords:
Syngas
Molten carbonate fuel cell
Numerical simulation model
Experimental validation

ABSTRACT

Electrochemical, thermal, electrical and flow parameters of a Molten Carbonate Fuel Cell (MCFC) are organized in a reduced order model, which is a 0-D mathematical model. The aim was to simulate different fuel cell working conditions taking into consideration a reduced number of parameters.

The reduced order model for an MCFC fed by syngas is formulated and implemented in Matlab.

A validation process for experimental data of the MCFC was made for some fuel and oxidant mixtures and adequate results are shown. The maximum percentage error ranges between 3.7% and 5.4% in the various considered cases.

At the anode, the direct internal water gas shift chemical reaction and the electrochemical consumption of carbon monoxide in addition to electrochemical consumption of hydrogen are considered. The ratio between the molar flows of carbon monoxide and hydrogen electrochemically consumed is a function of average rates of the electrochemical reactions and influences fuel cell performance. Furthermore, the simulation model is used to estimate the fuel cell performance varying the above-mentioned ratio. Acting on this ratio the performances of and MCFC fed by syngas and hydrogen could become comparable.

Introduction

Molten Carbonate Fuel Cells (MCFCs) have already reached a high electrical conversion efficiency of conventional primary fuel used (hydrogen or natural gas), but can also use non-conventional fuels such as the gas produced by the gasification of coal or woody biomass (syngas) and this enhances their eco-environmental compatibility.

The gas produced by the gasification of coal with technical oxygen (syngas), when properly purified, consists primarily of hydrogen (H_2) and carbon monoxide (CO). It can be mixed with

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https://doi.org/10.1016/j.ijhydene.2017.10.006
0360-3199/

Nomenclature

Symbols Units

i	current density A cm^{-2}
r	area specific resistance Ω cm^2
E	voltage V
R	gas constant J mol^{-1} K^{-1}
T	temperature K
Fa	Faraday constant C eq^{-1}
p	pressure atm
K	equilibrium constant $atm^{-0.5}$
U	utilization factor
F	molar flow mol s^{-1}
A	active surface cm^2
n	number
δ	thickness cm
σ	conductivity Ω^{-1} cm^{-1}
α	reaction degree
q	ratio between the CO and H_2 molar flows at the anode
v	rate of reaction mol l^{-1} s^{-1}
k	reaction rate constant l mol^{-1} s^{-1} or $l^{0.75}$ $mol^{-0.75}$ s^{-1}
C	concentration mol l^{-1}
ν	stoichiometric coefficient
ε	sufficiently small value
SC	Steam to Carbon

Subscripts

1,2,3	indices
max	maximum
out	at the outlet
ca	cathode
an	anode
H_2cr	hydrogen chemical reaction
COcr	carbon monoxide chemical reaction
H_2O, H_2, CO, CO_2, N_2,O_2	steam, hydrogen, carbon monoxide, carbon dioxide, nitrogen, oxygen
f	fuel
eq	equivalent
l	layer
e	electrolyte
OC	open circuit
in	at the inlet
b	consumed at the anode
fc	fuel cell
calc	calculated
hyp	hypothesized
s	specific

Superscripts

—	mean value
→	vector

steam to feed directly the anode of the fuel cell (Direct Internal Water Gas Shift, DIWGS). In the DIWGS case, CO and steam are converted into carbon dioxide (CO_2) and H_2 by the WGS chemical reaction, and the hydrogen produced with that initially contained in syngas are consumed electrochemically directly at the anode for the electrical energy production. In the anode, the electrochemical consumption of CO in addition to the electrochemical consumption of H_2, influences the fuel cell electrical performance. Furthermore, an increase of the CO electrochemical consumption leads to a reduction of the amount of CO converted into additional H_2 by WGS chemical reaction and to a reduction of the thermal energy required to produce the steam inside an energy system with MCFC.

Numerical modeling is a very useful tool for the study of this problem.

In the literature, a number of simulation models of an MCFC [1–25] have been presented. Some of these simulation models [1,2,4–8,11–17,19,25] are stationary while others [3,9,10,18,20–24] are dynamic. The stationary MCFC simulation models consider as an anode feeding gas a gas rich in H_2 without CO [11–16], reformed gas from a gas mixture of methane and steam [5], a gas mixture of methane and steam [8] a gas mixture consists mainly of CO and H_2 [1,2,4,6,7,17] and they are zero-dimensional [15–17], mono-dimensional [6], two-dimensional [1,2,4,5,8,11,14,19] and three-dimensional [7,12,13,24,25].

Only some of these simulation models consider CO electrochemical consumption at the anode [8,20].

Some authors have been working for years on numerical modeling of high temperature fuel cells fed by syngas or natural gas in stand-alone configuration or coupled to a gas turbine to produce electric and thermal energies [26,27], with particular attention to the CO_2 separation problem [28–30].

Detailed simulation models require the knowledge of many parameters, related to the internal resistance, the activation and concentration voltage losses at the anode and at the cathode. More detailed simulation models also require the knowledge of other parameters such as the tortuosity, porosity and diffusion coefficients, which are difficult to determine and which are related to the microscopic properties of the fuel cell components. In most cases, these parameters are determined for few polarization curves considering dry hydrogen as fuel and they cannot be applicable to other operating conditions and for other fuels of the fuel cell. A detailed simulation model requires longer calculation time for its numerical solution, because of its greater complexity, and it is less suitable to have feedback on the performance and on outlet gases composition of an MCFC in real time, when MCFC is only a device inside a more complex energy system. The reduced order simulation models require knowledge of only few parameters, they are more easily manageable from the numerical and analytical points of view with respect to detailed physical models and they describe the behavior of the MCFC fed by different feeding gases and in different operating conditions with a reasonable accuracy.

In this article, a reduced order simulation model formulated by an author of this article [15,16] for an MCFC fed at the anode only by a rich H_2 gas without CO, has been further developed to consider also syngas as the anode feeding gas.

In particular, this simulation model considers also the anode WGS chemical reaction and the electrochemical reaction of CO consumption in addition to the electrochemical reaction of the H_2 consumption. It was implemented in Matlab environment and it is able to estimate the polarization curve