Applied Thermal Engineering 31 (2011) 2740–2748

Contents lists available at ScienceDirect

Applied Thermal Engineering

journal homepage: www.elsevier.com/locate/apthermeng

Design improvement of circular molten carbonate fuel cell stack through CFD Analysis

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ARTICLE INFO

Article history:
Received 13 September 2010
Accepted 28 April 2011
Available online 8 May 2011

Keywords:
Molten Carbonate Fuel Cells
CFD model
Stack model
Design improvement

ABSTRACT

Molten carbonate fuel cell (MCFC) is a promising technology for distributed power generation. The core of an MCFC power generation unit is the stack, where various fuel cells are connected together in series and parallel in order to obtain the desired voltage and power. Stack geometry and configuration are major engineering topics, as inhomogeneous temperature or mass fractions cause inefficient performances of the fuel cells, as efficiency and power smaller than the expected and shorter lifetime. A detailed model is a useful tool to improve stack performances, through design improvements.

In this paper, a 3D model of a stack composed of 15 circular MCFC, considering heat, mass and current transfer as well as chemical and electrochemical reactions is presented. The model validation is conducted using some preliminary experimental data obtained for an MCFC stack developed in the Fabbricazioni Nucleari laboratories. These results are examined in order to improve the stack configuration. It is shown that power density may be increased of about 20% through double side feeding. In addition, the average temperature gradients in the axial direction are reduced of more than 70%. Significant reductions in the temperature gradients, especially in transversal direction, can be achieved by adjusting the mass flow rate of cathodic gas supplied to the various cells.

1. Introduction

Molten Carbonate Fuel Cell (MCFC) is a fuel cell which electrolyte is a ceramic matrix filled of sodium and potassium carbonates, in molten form. The operating temperature is usually between 600 °C and 700 °C in order to allow effective ion conduction and prevent from rapid voltage degradation. Carbonate ions are produced on the cathodic side, by the electrochemical reaction

$$1/2O_2 + CO_2 + 2e^- = CO_3^- \quad (1)$$

and migrate through the electrolyte to the anodic side, where the following reaction occurs

$$H_2 + CO_3^- = H_2O + CO_2 + 2e^- \quad (2)$$

One of the main advantages of MCFCs is the potential high efficiency that can be achieved with hybrid cycles, where the fuel cell is integrated with a microturbine. This kind of plants is still not commercial, but several installations are now operating. Some of the issues are related with plant lifetime and discrepancies between theoretical and real performances. Detailed models of MCFC can be used to understand the phenomenological behavior [1], evaluate the effects of possible changes in the design [2], examine the operating conditions for diagnosis [3] or control purposes [4], predict the performances of a cell within a complex plant, such as a hybrid plant [5]. Various single cell and stack models have been proposed in the last 30 years. A comprehensive review of the models proposed in the eighties and nineties is available in [6]. Because of the computational limitations, associated to both hardware and software, significant hypotheses had to be formulated which nowadays may be overcome. A hypothesis which is still popular, especially in the case of transient simulation [7], is that of plug flow. This allows one to reduce the number of computational cells, as discussed in [8]. The full 3D analysis is usually adopted for planar structures [9], sometimes using a coarse mesh.

Other possible approaches in the case of stack modeling are based on repeated cells with proper boundary conditions to account for the position within the stack [11], on model reduction (2D) [10] and on quasi-3D models obtained through 1D [3], 2D [12] or network models [13] with proper inputs from parallel layers.

This paper aims to investigate possible improvements that can be achieved by introducing design changes at stack level. A

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doi:10.1016/j.applthermaleng.2011.04.046

Nomenclature

$D_{i,\text{eff}}$	Effective diffusion coefficient ($m^2\ s^{-1}$)
D_{ij}	Mass diffusion coefficient ($m^2\ s^{-1}$)
E_k	Apparent activation energy (K^{-1})
F	Faraday constant (mol^{-1})
h	Specific enthalpy ($J\ kg^{-1}$)
$\vec{i}$	Current density vector (A m-2)
$\vec{J}_i$	Diffusive flux of species i ($kg\ m^{-2}\ s^{-1}$)
J_o	Exchange current density ($A\ m^{-2}$)
K	Permeability (m^2)
k	Thermal conductivity ($W\ m^{-1}\ K^{-1}$)
k_{eff}	Effective thermal conductivity ($W\ m^{-1}\ K^{-1}$)
M	Molecular weight ($kg\ mol^{-1}$)
n_e	Number of electrons
p	Pressure (Pa)
R	Universal gas constant ($W\ mol^{-1}\ K^{-1}$)
s	Specific entropy ($J\ kg^{-1}\ K^{-1}$)
S_i	Species source term ($kg\ m^{-3}\ s^{-1}$)
S_h	Heat source term ($W\ m^{-3}\ s^{-1}$)
T	Temperature (K)
v	Specific volume ($m^3\ kg^{-1}$)
V	Velocity ($m\ s^{-1}$)
$\vec{V}$	Velocity vector ($m\ s^{-1}$)

Greek symbols

ϕ	Potential (V)
β	Transfer coefficient
ε	Porosity
η_{act}	Activation overpotential (V)
μ	Viscosity ($m\ s^{-2}$)
ρ	Density ($kg\ m^{-3}$)
σ	Electric conductivity ($\Omega^{-1}\ m^{-1}$)
τ	Tortuosity
ω_i	Mass fraction of species i

prototype composed by 15 circular molten carbonate fuel cells, manufactured by the Italian company Fabbricazioni Nucleari [14], is considered.

The analysis is conducted through a full 3D model of the stack. The model accounts for heat, mass and charge transfer; chemical and electrochemical reactions are considered through proper boundary conditions and source terms in the partial differential equations. The results show that non-homogeneous distributions of temperature and reactant mass fractions occur both at cell level and stack level. This means that there are significant differences in temperatures and concentrations between zones in a cell and also between the various cells. This behavior, already shown in previous studies conducted on different cell and stack geometries [4,12,15,16] and confirmed by the experimental analysis, is responsible for undesired behaviors: efficiencies or power densities lower than expected, due to larger resistances, and reduced lifetime, due to high temperatures and large temperature gradients. Possible design changes that allow one to reduce gradients at cell level have been examined in [17]. Here possible design changes at stack level are proposed. These changes are basically conducted by intervening on the oxidant mass flow rate supplied to the various cells. The stack configuration analyzed in this paper allows one to increase the mass flow rate to the cells at higher temperature, obtaining a more homogeneous distribution. This subject is not widely treated in the literature. In [18] a mixed experimental-numerical approach is used to improve the performance of an MCFC stack. A simple numerical model is used to adjust some orifices and homogenize the flow distribution. No thermal analysis is conducted. In [19] two stack configurations, co-flow and counter-flow, are compared using experimental analysis. In [20] the reverse problem is considered, i.e. the effects of bad flow distribution are simulated for a SOFC stack.

2. MCFC stack geometry and Model

The stack is composed of an external supporting structure in stainless steel, where distribution channels are located, and an internal portion, which includes the electrodes, the electrolyte and the porous distribution layers.

Fig. 1 shows the mesh of the computational domain, which corresponds to a quarter of the entire stack. This shows the 15 cells, together with the axial inlet and outlet ducts for fuel and cathodic gas. Fuel flows from the bottom to the top and air from the top to the bottom. These gases enter each single cell through radial ducts also represented in the figure. In total there are 4 inlet anodic channels, 4 inlet cathodic channels, 4 outlet anodic channels and 4 outlet cathodic channels.

Fig. 2 shows a schematic of a single fuel cell, together with the external structure, the 16 axial ducts (A–D are the inlet anodic ducts, E–H the inlet cathodic ducts, I–L the outlet anodic ducts and M–P the outlet cathodic ducts) and the radial ducts. To show the various layers of the cells and the main flow paths, two cross sections are drawn in Fig. 3.

The fuel cell consists of a total of 11 layers: 2 external supporting layers in stainless steel, 2 porous inlet channels (for fuel and cathodic gas), 2 stainless steel plate with small axial orifices in the center, 2 outlet channels, anode, electrolyte and cathode. In the inlet channels, the fluid enters from the four radial channels: those connected with ducts A–D distribute the fuel to the inlet anodic channel (in Fig. 3, the axial duct A and the corresponding radial duct is represented), and those connected with ducts E–H

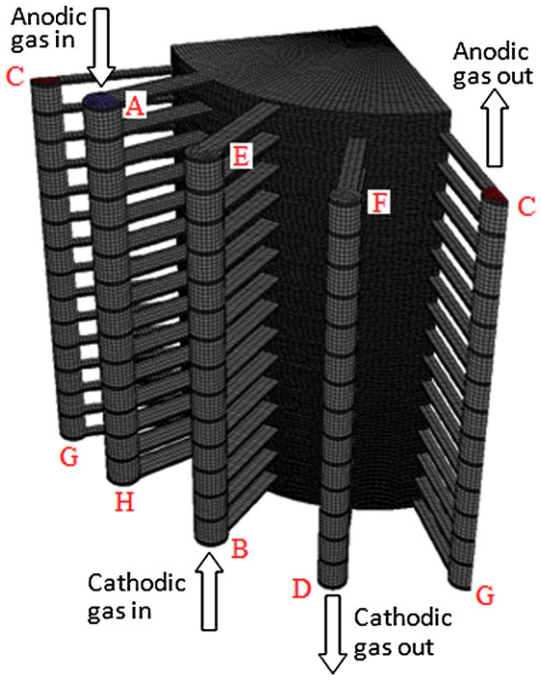

Fig. 1. Mesh of the computational domain.