Applied Thermal Engineering 82 (2015) 98–109

Contents lists available at ScienceDirect

Applied Thermal Engineering

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

Research paper

Dynamic behaviors of a molten carbonate fuel cell under a sudden shut-down scenario: The effects on temperature gradients

M.C. Law [a, *], V.C.-C. Lee [a], C.L. Tay [b]

[a] Department of Mechanical Engineering, School of Engineering and Science, Curtin University, CDT 250, 98009 Miri, Sarawak, Malaysia
[b] Department of Chemical Engineering, School of Engineering and Science, Curtin University, CDT 250, 98009 Miri, Sarawak, Malaysia

HIGHLIGHTS

- MCFC electrode thermal gradients under steady, pulsating co-flow and counter-flow conditions are analysed.
- Counter-flow MCFC has lower thermal gradients compared to those of co-flow.
- Pulsating flow causes higher maximum temperature gradients compared to steady-flow.
- In some cases, pulsating flow causes lower average thermal gradients than steady-flow.

ARTICLE INFO

Article history:
Received 11 October 2012
Accepted 8 November 2014
Available online 3 March 2015

Keywords:
Molten carbonate fuel cell
Co-flow
Counter-flow
Pulsating flow
Simulation
Temperature gradient

ABSTRACT

A three-dimensional (3-D), dynamic model of a molten carbonate fuel cell (MCFC) is developed in the current work. The model takes into account the heat and mass transfers of various reacting gas species. Yuh and Selman's model is implemented to solve the voltage–current relationship. In addition, water-gas shift (WGS) reaction is also included in the model. The simulation result is validated with published experimental data. The model is used to study the effects of steady and pulsating flows on the temperature gradients of MCFC electrodes in a shut-down event. Co-flow and counter-flow of MCFC are included in this study. The results show that higher thermal conductivity and smaller gas temperature difference before and after shut down event ensure better structural integrity of the fuel cell. In addition, under the simulated condition, the counter-flow operating condition is better for MCFC due to its overall lower temperature and also temperature gradients. In the case of the pulsating flow, the change of electrode temperature gradient is greater in co-flow MCFC compared to that of counter-flow MCFC. The sinusoidal profile of an electrode temperature gradient is more visible when both anode and cathode gas channels are subject to pulsation. A steady gas flow ensures a lower maximum temperature gradient in an electrode. Nevertheless, the simulation result also shows that under certain pulsating flow conditions, the cathode electrode will have a lower average temperature magnitude compared to that of steady-flow.

1. Introduction

The pressure of increasing price and pollutant emission of conventional fuels has encouraged the advancement of green energy technologies. One of the most promising candidates for stationary power sources is molten carbonate fuel cells (MCFC). Apart from being a clean energy source which does not emit greenhouse gas, an MCFC is able to produce high power output (of the order of Megawatt) with an electrical efficiency of around 45–65% [1]. An MCFC is also suitable to be used as part of a hybrid system due to its modularity and high operating temperature (600–1000 °C) [1]. Successful commercialization of an MCFC requires a minimum lifespan of at least 5 years [2]. Nevertheless, due to the high operating temperature and thermal cycling, the lifespan of an MCFC can be reduced as a result of the cracking of electrolyte matrix and the thermal creep of porous structures [1,2]. The operation of an MCFC is a multi-physics process which couples fluid dynamics, heat transfer and electrochemical reactions. Thus, the control of temperature field of an MCFC requires a good understanding of the afore-mentioned processes. This can be achieved by mathematical modelling of an MCFC instead of experimental investigations which are expensive and time-consuming.

* Corresponding author. Tel.: +60 85443824; fax: +60 85443837.
E-mail address: m.c.law@curtin.edu.my (M.C. Law).

http://dx.doi.org/10.1016/j.applthermaleng.2014.11.083
1359-4311/

Notation

B–V	Butler–Volmer equation -
C	fluid capacitance Pa/m^3
c_p	specific heat capacity at constant pressure J/(kgK)
D_i^m	mixture-averaged diffusion coefficient for gas species i m^2/s
$D_{i,eff}^m$	effective diffusion coefficient of gas species, i in porous media m^2/s
F	Faraday's constant C/mol
E^0	maximum possible reversible cell voltage V
E_{eq}	reversible cell voltage V
ΔH_f	enthalpy of formation J/mol
i_{ct}	charge transfer current density A/m^2
k	thermal conductivity W/(mK)
$k_{WGS,f}$	rate of reaction of water-gas shift reaction mol/(m^{3}Pa^{2}s)
$K_{p,f}$	partial pressure equilibrium constant for formation process -
$K_{p,WGS}$	partial pressure equilibrium constant of water-gas shift reaction -
L	fluid inertia Pas^2/m^3
M_i	molecular weight of a gas species i kg/mol
p	pressure Pa
q	fluid flow rate m^3/s
$\dot{Q}$	heat source J/mol
R	fluid resistance Pa/(m^{3}s)
R_u	universal gas constant J/(molK)
$\dot{R}_i$	reaction rate of a gas species i mol/(m^{3}s)
$_t$	time s
T	temperature K
V_{cell}	voltage of a cell V
v_i	diffusion volume of a gas species, i -
x_i	mole fraction of a gas species, i -
z	non-dimensional quantity defined in (15) -

Vector Quantities

I	identity matrix -
J$_i$	mass flux relative to mass average velocity kg/(m^{2}s)
u	velocity vector m/s

Greek Symbols

ε_m	emissivity of a material -
ε_p	porosity -
η	overpotential V
$_\kappa$	permeability m^2
δ_k	thickness of a material, k m
μ	dynamic viscosity Pas
ρ	density kg/m^3
ω_i	mass fraction of gas species, i -

Subscripts

a	anode
c	cathode
eff	effective
g	gas
Ohm	ohmic
p	porous
r	reaction
s	solid
WGS	water-gas shift

Superscripts

T	transpose

Currently, there are four levels of MCFC models, i.e. electrode, cell, stack and system levels. Electrode models simulate the generation of current/voltage as a function of operating temperature, pressure and gas species [3,4]. Cell models [5] usually include detailed multi-physics modelling of gas channels, electrodes and electrolyte of a single fuel cell. This model assumes that the simulation results are similar to other fuel cells in a stack. On the other hand, stack models simulate the temperature and flow fields of a group of fuel cells. This enables the study of the effects of flow inhomogeneity on the fuel cell stack [6,7]. The drawback of the stack models is due to its high computational cost. Lastly, for the system level, a MCFC is also integrated with other components such as micro-turbines and compressors. This type of model is used for assessing system performance and control strategies [8,9]. Literature survey shows that there are only a few models which presented the transient behaviour of a MCFC. For instance, Brouwer et al. [10] developed a two-dimensional (2-D) model for a MCFC stack. The model consisted of conservations of gas species and energy. The authors did not solve for Navier–Stokes equations and thus avoided the high computational cost. Simplified Butler–Volmer (B–V) and agglomerate models were used to model the voltage–current relationship of a MCFC. Both models were used to study the transient response of a MCFC whereby the load resistance was varied. Power and voltage responses were validated with experimental data. The authors found that the agglomerate model produced better predictions than the simplified B–V model. Liu and Weng [11] applied simplified one-dimensional (1-D), transient equations for fluid pressure drop, gas species, heat transfer and electrochemical reactions to simulate a MCFC. The model showed that when the fuel cell was subjected to 2% step decrease of fuel molar rate, it took 100 s for the fuel cell temperature and voltage to reach new steady state values. Lee et al. [12] developed a 2-D dynamic MCFC model to study the effects of molar flow rates of various gas species and utilization of fuel on the fuel cell performance. The authors reported a short settling time for the fuel cell due to high flow rate (0.44 mol/hr of anode gas flow rate) and small size of the fuel cell (10 cm $\times$ 10 cm). He and Chen [13] used a commercial CFD software to simulate a transient, 3-D MCFC under a cross-flow operating condition. Though the model was not validated with any experimental data, the authors claimed that the simulated results had good comparisons with other theoretical models. Ramandi et al. [14]applied a sinusoidal voltage in their MCFC model to study the time scales of various physical processes that occurred in a fuel cell. These researchers further investigated the dynamic behaviour of an MCFC during a start-up process [15]. They concluded that significant electrochemical reaction occurred in the first 10 s of the fuel cell operation. After that the gas temperature was slowly increased owing to the heat transported from the solid phase.

Another aspect that is often neglected but increasingly receives attention in the fuel cell research is the effects of pulsation on the fuel cell performance. It was shown [16] that pulsations aided the mass transfer of oxygen in the cathode gas channel which in turn increased the maximum power density. The effect of pulsation can also be introduced by using corrugated flow channels. Heidary et al. [17] found that the pulsating flow in a corrugated channel was capable of enhancing the heat transfer rate by 90% in a direct methanol fuel cell.