DEVELOPMENT OF DYNAMIC MODEL FOR IIR-SOFC FUELLED BY VARIOUS PRIMARY FUELS

MISS SUREEWAN AREESINPITAK
ID: 52910409

A THESIS SUBMITTED AS A PART OF THE REQUIREMENTS
FOR THE DEGREE OF MASTER OF ENGINEERING
IN ENERGY TECHNOLOGY AND MANAGEMENT

THE JOINT GRADUATE SCHOOL OF ENERGY AND ENVIRONMENT
AT KING MONGKUT'S UNIVERSITY OF TECHNOLOGY THONBURI

2ND SEMESTER 2010

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Abstract

Solid Oxide Fuel Cells (SOFCs) operate at high temperature and generally require the heating step for increasing system temperature from ambient to operating temperature of 1173 K. In the present work, a tubular SOFC was simulated with the aim of predicting the system temperature gradient with time during the starting-up period. Firstly, various gas compounds including nitrogen, hydrogen and synthesis gas (or syngas; the mixture of H_2 and CO) were applied as the heating media. The assumptions made include: initial temperature and pressure of 500 K and 1 bar; SOFC load voltage of 0.7 V; and a fuel utilization of 80%. During heating-up period, the characteristics of this SOFC system were predicted in terms of product gas distribution and temperature gradient (with time) along the length system. It was found that, for the case of SOFC heated by hot nitrogen, it takes around 30 hours for the system to reach its operating temperature of 1173 K. On the other hand, the SOFC fed by hydrogen, the temperature of the system reaches 1173 K after only 2 minutes due to the rapid exothermic electrochemical reaction; this extremely high heating rate (0.93K/s) could result in high thermal stress of material and subsequent damage of the SOFC system (based on the literature, the heating rates should be less than 0.5 K/s). In the case of SOFC fed by syngas, the SOFC temperature reaches 1173 K after 30 minutes. For the calculation, the heating rate of SOFC fed by syngas is 0.37 K/s and this rate is compatible with SOFC material. As the next step, the direct use of hydrocarbon fuels (i.e. methane, methanol and ethanol) as primary fuel and heating-up gas for SOFC with indirect internal reforming operation (IIR-SOFC) were investigated. It was found that the heating rates during the starting-up period for methane, methanol and ethanol were observed to be 0.31 K/s, 0.11 K/s and 0.26 K/s respectively, which is also compatible with the cell material. Among these hydrocarbon fuels, SOFC fueled by methanol was found to obtain the highest power density under steady state conditions. It should also be noted that the effect of inlet steam/carbon (S/C) ratio for IIR-SOFC fueled by these hydrocarbon fuels (i.e. methane, methanol and ethanol) was also studied by varying the S/C ratio from 2.0 to 3.0 and 4.0. It was found that the changing the inlet S/C ratio negligible effects on the heating rate during the starting-up period for all types of hydrocarbon feeds. Nevertheless, it noticeably affected the temperature of the system under steady state condition, from which the use of high S/C molar ratios (S/C ratio of 4.0) resulted in higher system temperature. Therefore, this leads to the lower power density achievement at steady state conditions. Finally, IIR-SOFC with co-flow pattern (co-flow of air and fuel steam though fuel cell) provided smoother temperature gradient along fuel cell and higher power density than that with counter-flow.

Keywords: Indirect internal reforming; heat-up period; Transient; Dynamic model; SOFC

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LIST OF ABBREVIATIONS AND SYMBOLS

Abbreviations

DIR	Direct Internal Reforming
EMF	Electo-Motive-Force
ER	External Reforming
HHV	High Heating Value
IIR	Indirect Internal Reforming
IR	Internal Reforming
MCFC	Molten Carbonate Fuel Cell
MSR	Methane Steam Reforming
OCP	Open-Circuit Potential
PEMFC	Proton Exchange Membrane Fuel Cell
PEN	Positive electrode/Electrolyte/Negative-electrode
POX	Partial Oxidation Reaction
RWGS	Reverse Water-Gas Shift reaction
SOFC	Solid Oxide Fuel Cell
WGS	Water Gas Shift reaction

Symbols

A	Area , m^2
a_i	Activity of component 'i'
C	Total molar concentration, mol/L
C_p	Specific heat of the gas streams, kJ/molK
$D^e_{i,k}$	The effective molecular diffusivity, m^2/s
D^{ks}_i	The Kundsen diffusivity, m^2/s
E	EMF or open circuit voltage, Volts
F	Faraday's constant
F_{12}	Gray-body transfer factor from surface 1 to surface 2
ΔG_f	The change in Gibbs free energy of formation

Δg_f^o	The change in Gibbs fee energy of formation per mole (kJ/mole) at STD
ΔH	The change of heat of reaction , kJ/mol
$(-\Delta H)_{elec}$	Heat of the electrochemical reaction, kJ/mol
j_0	Exchange current density , mA/cm^2
j	Current density, mA/cm^2
j_{H_2}	Current density from hydrogen oxidation reaction , mA/cm^2
k_i	Rate constant for reaction 'i'; unit will be specific to the form of the rate expression
k_{cond}	Thermal conductivity, W/m^{2}K
N_i^D	The bulk molar diffusive flux of gas component , mol/ms
n	Number of electron that pass round the external circuit
P_{SOFC}	The local power density , W/m^2
p^o	Standard partial pressure, atm
p_i	Partial pressure of species i
R	Universal gas constant; 8.414 kJ/ molK
R_{elect}	The hydrogen oxidation reaction rate, mol/m^{2}s
R_{ohm}	Ohmic Polarization, Ω m^2
Q_{rad}	The heat flux (W) from convection
q_{cond}	The heat flux from conduction,W/m^2
q_{conv}	The heat flux from convection, W/m^2
ΔS	The change in Entropy, kJ/mol
T	Temperature, K
U_{eff}	Fuel utilization factor
V_{call}	Voltage drop of the whole cell, Volts
V_{ohmic}	Voltage drop caused by ohmic losses , Volts
V_{act}	Voltage drop cause activation losses , Volts
x_i	The mole fraction of gas

Greek letters

$\alpha_{a,c}$	Charge transfer coefficient of anode and cathode
σ	Stefan-Boltzmann coefficient
ε	Emittance
η_{cell}	Cell efficiency
λ_{air}	Air ratio

Superscripts

$^{\circ}$	Standard condition

Subscripts

i	Component (methanol, water, hydrogen, etc.)
j	Reaction (SRM, WGS, etc.)
Act	Activation losses
$Cell$	Cell stack
Con	Concentration losses
ohm	Ohmic losses
$elec$	Electrochemical reactions