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Analytical modelling of boiling phase change phenomenon in high-temperature proton exchange membrane fuel cells during warm-up process

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ABSTRACT

This paper investigates the thermal and water balance as well as the electro-kinetics during the warm-up process of a Hydrogen/Oxygen high-temperature proton exchange membrane fuel cell (HT-PEMFC) from room temperature up to the desired temperature of 180 °C. The heating strategy involves the extraction of constant current from the fuel cell, while an external heating source with a constant heat input rate is applied at the end plates of the cell simultaneously. A simple analytical unsteady model is derived addressing the boiling phase changing phenomenon in the cathode catalyst layer (CCL) and cathode gas diffusion layer (CGDL) of the cathode that occurs when the temperature of the fuel cell reaches the boiling temperature of water. Parameters such as the heat input rate, extracted current, cathode pressure and cathode stoichiometric flow ratio are varied and their effects on the temperature, liquid water fraction and most importantly, the voltage profiles with respect to time, are explored. A comparison between other existing heating strategies using the model suggests that there is insignificant improvement in warm-up time when current is extracted from room temperature considering a single cell. However, considering the solution for a typical 1-kW stack suggests that reductions in warm-up time and energy consumption can be expected. In addition, the results show that boiling phase change is found to be a key factor that affects the level of water saturation in the porous media such as the CCL and CGDL during the warm-up process, when current is extracted from the start of the process i.e. room temperature. However, the energy consumption due to boiling phase change is found to be negligible as compared to external heating input rate. The parametric studies show that the variation of heat input rate, extracted current and cathode pressure have significant effect on the cell voltage that is strongly dominated by the liquid water fraction in the porous media. On the other hand, the variation of cathode stoichiometric flow ratio is found to have minimal effect on the output cell voltage. The parametric studies also indicate that boiling phase change is present for a significant period of time under typical operating conditions.

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Nomenclature		v_{liq}	specific volume of liquid water $18.015 \text{ e}^{-6} \text{ m}^3/\text{mol}$
Alphabets		Greek	
a	effective catalyst area per unit volume, $\text{m}^2 \text{ m}^{-3}$	α	charge transfer coefficient, –
A_{MEA}	active electrode area, m^2	β	linear expansion coefficient, –
C	molar concentration, mol m^{-3}	δ	thickness, m
C_p	thermal capacity, $\text{J kg}^{-1} \text{ K}^{-1}$	ϵ	porosity, –
D_i	mass diffusivity of species, $\text{m}^2 \text{ s}^{-1}$	ζ	stoichiometric flow ratio, –
E_{gen}	heat generation in catalyst layer, W or J s^{-1}	η	over potential, V
E_o	open circuit voltage, V	κ	conductivity, S m^{-1}
E_a	activation energy, J mol^{-1}	ρ	density, kg m^{-3}
F	Faraday's constant 96487 C mol^{-1}	Superscripts and subscripts	
h_{lg}	enthalpy change between liquid water and water vapour, J mol^{-1}	0	initial value
h_s	interfacial thermal conductance between domains, $\text{W K}^{-1} \text{ m}^{-2}$	1	domain 1 consisting of end plate, gas diffusion layer and bipolar plates
$h_{s,eff}$	effective interfacial thermal conductance between domains, W K^{-1}	2	domain 2 consisting of the cathode catalyst layer
I	current density, A m^{-2}	a	anode
i_o	reference exchange current density, A m^{-2}	acc	accumulation
i_{oc}	exchange current density, A m^{-2}	ACL	anode catalyst layer
j	transfer current density, A m^{-3}	BP	bipolar plate
L_{lg}	enthalpy change between liquid water and water vapour, J kg^{-1}	c	cathode
M	molar mass, kg mol^{-1}	CCL	cathode catalyst layer
\dot{n}_{H_2O}	water generation/removal rate, mol s^{-1}	CGDL	cathode gas diffusion layer
n_{H_2O}	water storage capacity, mol	eff	effective
p	pressure, atm or bar	EP	end plate
\dot{Q}_{in}	heat input rate, W or J s^{-1}	g	gas
R	universal gas constant $8.314 \text{ J mol}^{-1} \text{ K}^{-1}$	in	inward
R_Ω	cell ohmic resistance, $\Omega \text{ m}^2$	lg	phase change between liquid and gas
S	entropy, $\text{J mol}^{-1} \text{ K}^{-1}$	liq	liquid
t	time, s	MEA	membrane electrode assembly
T	temperature, K	mem	membrane
V	volume, m^3	prod	production
V_{cell}	cell voltage, V	ref	reference value
		sat	saturation
		Ω	ohmic

1. Introduction

Fuel cells are generally perceived to be one of the next promising alternative energy sources considering its potential uses in a variety of applications [1]. One of the major reasons for this direction strongly relates to the bloom of Hydrogen production methods and storage capabilities [2]. As far as fuel cells are concerned, HT-PEMFCs are considered as the next generation of power producing devices due to their superior performance compared to the low-temperature proton exchange membrane fuel cells (LT-PEMFCs) [3,4]. Nevertheless, several obstacles dominate the field of HT-PEMFC, causing a delay of its commercialization. The whole dynamics and directions of these new challenges pertaining to high-temperature operation are different as compared to the ones experienced in LT-PEMFC. Over the past decade, research activities were mainly focussed on the development of fuel cell components that have high temperature degradation

resistance. Producing high-temperature membranes with sufficient proton conductivity are one of the key focuses and numerous efforts have been reported in the literature [5,6].

Another key area has become popular recently is related to the analysis and optimization of warm-up strategy during the start-up period of a HT-PEMFC [7]. Conceptually, there are number of ways of starting up the HT-PEMFC and generally, two main parameters define a heating strategy. Firstly, the mode of operation of the fuel cell during the cold start-up process, which can be set by controlling the extracted current or voltage (holding either one of them at a constant value or setting at any desired profile) [8–10]. Secondly, the set temperature during the warm-up period, above which the fuel cell is put on operation, is another key factor. As far as this is concerned, there are three different methods for start-up, i.e., (a) the fuel cell to be heated up to a temperature above the boiling point of water, after which the fuel cell is operated, (b) similar to (a) but the fuel cell is operated below the boiling

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