Journal of Power Sources 196 (2011) 4923–4933

Contents lists available at ScienceDirect

Journal of Power Sources

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

Effects of property variation and ideal solution assumption on the calculation of the limiting current density condition of alkaline fuel cells

Ge Zhou[a,1], Lea-Der Chen[a,*,2], James P. Seaba[b]

[a] Department of Mechanical and Industrial Engineering, The University of Iowa, Iowa City, IA 52242, USA
[b] ConocoPhillips Co., 240 PLB, Bartlesville Technology Center, Bartlesville, OK 74004, USA

ARTICLE INFO

Article history:
Received 11 January 2011
Received in revised form 3 February 2011
Accepted 4 February 2011
Available online 12 February 2011

Keywords:
Alkaline fuel cell
Ideal solution
Property effect
Limiting current density

ABSTRACT

A computational study of the electrochemical hydrodynamic process in an alkaline fuel cell was conducted. The computation relaxed the ideal solution assumption, accounted for thermodynamic solubility of the reactants, and allowed for property variations due to temperature and concentration effects. The results showed that the ideal solution assumption is not adequate for calculation of the transport process of the concentrated electrolyte considered, 7 M. The ideal solution formulation resulted in a lower limiting current density condition by about 50% than that predicted by the non-ideal solution formulation. The study also showed that the thermal condition is important to the calculation of the limiting current density condition. The calculated limiting current density increased by about 30% when the boundary condition was changed from isothermal to adiabatic. The computational results suggest that maintaining a uniform KOH concentration in the electrolyte (for example, at design point of 7 M) be an effective measure to increase the limiting current density condition.

© 2011 Elsevier B.V. All rights reserved.

1. Introduction

Stationary fuel cell is a viable option for electrical power generation from renewable sources. For example, H_2 produced by solar or wind turbine based electrolysis can be used to fuel the fuel cells. Among the fuel cell platforms, alkaline fuel cell (AFC) remains a good prospect as it has high reliability and it can use non-precious metal for the electrodes [1–6,23]. However, to be competitive with other power sources, the power density (as well as the cost of manufacturing, operation and maintenance) needs to be improved. A CFD based study of the electrochemical hydrodynamic process that sets the limiting current density condition is conducted. The purpose of this study is to gain a better understanding of the mechanisms critical to setting the limiting current density condition, and to demonstrate the application of CFD based simulation to aid design consideration.

The CFD formation accounts for the electrochemical reaction, charge and species transport, and thermodynamics of gas solubility in the electrolyte. The mathematical models that describe the transport processes are available in the literature, e.g., see [7–13]. However, most transport models were based upon the assumption of ideal solution for the calculation of the transport properties. Error associated with the ideal solution assumption was not assessed. Furthermore, most CFD studies reported in literature assumed an isothermal system. The temperature effects were not evaluated. In this paper, the ideal solution assumption was relaxed and the temperature effects were examined. The objectives of this paper are (a) to examine the effects on CFD calculation due to the ideal solution and isothermal assumptions, and (b) to gain insights into the mechanisms that are critical to setting the limiting current density condition.

2. Formulation

2.1. Transport equations

Major assumptions invoked are (a) Newtonian fluid, (b) negligible pressure effects on enthalpy, (c) negligible magnetic effects due to electrical field, (d) negligible pressure and temperature effects on diffusion transport, (e) negligible viscous dissipation, pressure work, and Dufour effects in energy equation, (f) no homogeneous chemical reactions, (g) electroneutrality, (h) homogeneous and continuous media for gas and liquid phase, (i) local thermal equilibrium, (j) vapor–liquid equilibrium at the gas–liquid interface, and (k) negligible electrical resistance of the electrodes. The governing equations describing the transport of mass, momentum, species, energy and charge balance are summarized in Table 1. The

* Corresponding author. Tel.: +1 361 825 3046; fax: +1 361 825 3056.
E-mail address: ldchen@tamucc.edu (L.-D. Chen).
[1] Currently with UTC Power, 195 Governor's Highway, South Windsor, CT 06074, USA.
[2] Currently with Texas A&M University – Corpus Christi, Corpus Christi, TX 78412, USA.

0378-7753/$ – see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.jpowsour.2011.02.026

Nomenclature

a_k	activity of species k
$a_{\beta\gamma}$	specific interfacial area between phase β (liquid) and phase γ (gas) (m^{-1})
$a_{\beta\sigma}$	specific interfacial area between phase β (liquid) and phase σ (solid) (m^{-1})
C_k	molar concentration of species k ($kmol\,m^{-3}$)
C_p	specific heat ($J\,kg^{-1}\,K^{-1}$)
D_k	diffusion coefficient of species k into the solution/mixture ($m^2\,s^{-1}$)
D_{kj}	multicomponent Maxwell–Stefan binary diffusion coefficient ($m^2\,s^{-1}$)
d_f	fiber diameter (m)
E	electric potential (V)
F	Faraday constant ($C\,kmol^{-1}$)
$\boldsymbol{g}$	gravitational acceleration ($m\,s^{-2}$)
H	Henry's constant ($kmol\,m^{-3}\,atm^{-1}$)
i	current density ($A\,m^{-2}$)
i_0	exchange current density ($A\,m^{-2}$)
$\boldsymbol{i}$	vector quantity of current density ($A\,m^{-2}$)
i_n	current density at solid–liquid interface ($A\,m^{-2}$)
$\boldsymbol{j}_k$	vector quantity of mass flux of species k ($kg\,m^{-2}\,s^{-1}$)
K	absolute permeability (m^2)
k^r	relative permeability
k_K	Kozeny constant
k_{scx}	Setschenow salt effect parameter
M_k	molecular weight of species k ($kg\,kmol^{-1}$)
m	molality ($mol\,kg^{-1}$)
n	number of electron transfer
p	pressure (Pa)
p_c	capillary pressure (Pa)
p_s	saturation vapor pressure (Pa)
q_k	stoichiometric coefficient of species k
R_u	universal gas constant ($J\,kmol^{-1}\,K^{-1}$)
S	entropy ($J\,kmol^{-1}\,K^{-1}$)
S_r	reduced phase saturation
s	saturation
s_{im}	immobile saturation
s_k	stoichiometric coefficient of species k
T	temperature (K)
t	time (s)
t_k	transference number of species k
U	open cell potential (V)
u_k	mobility of species k ($m\,s^{-1}\,kmol\,N^{-1}$)
$\boldsymbol{v}$	velocity vector ($m\,s^{-1}$)
x_k	mole fraction of species k
Y_k	mass fraction of species k
z_k	charge number of species k

Greek

α	transfer coefficient
δ	film thickness (m)
$\gamma_{\pm,C}$	mean activity coefficient based on molarity
ε	porosity
η	local overpotential (V)
κ	electrical conductivity ($S\,m^{-1}$)
κ^D	diffusion conductivity ($A\,m^{-1}$)
λ	thermal conductivity ($W\,m^{-1}\,K^{-1}$)
λ_k^0	limiting ionic equivalent conductance of ion k ($S\,m^2\,kmol^{-1}$)
μ	dynamic viscosity ($kg\,s^{-1}\,m^{-1}$)
μ_k	chemical potential of species k ($J\,kmol^{-1}$)
υ	stoichiometric coefficient
υ_k	number of cation or anion produced by the dissociating electrolyte
θ_c	contact angle
ρ	density ($kg\,m^{-3}$)
σ	surface tension ($N\,m^{-1}$)
τ	normal or shear stress ($N\,m^{-2}$)
Φ	electric potential at electrolyte phase (V)

Subscripts

a	anode
c	cathode
e	electrolyte
g	gas
i,j,k	species
l	liquid
m	mixture
nw	non-wetting
T	total
w	wetting
β	liquid phase
γ	gas phase
σ	solid phase
0	standard state, pressure at 1 atm or solvent or reference value
+	cation
−	anion

Superscripts

a	anode
c	cathode
eff	effective
h	energy
i	charge
m	mass
r	reference state
β	liquid phase
γ	gas phase
σ	solid phase
0	standard state, pressure at 1 atm, or solvent/reference state

respective source terms are given in Table 2. The source terms account for (a) mass and species addition or removal due to gas solubility and H_2O phase change, (b) momentum exchange due to Darcian flow in porous electrodes, (c) energy source or sink terms due to heat and entropy generation at catalyst layer, Joule heating in separator and catalyst layer, and latent heat of H_2O phase change, and (d) charge generation at catalyst layer. The constitutive equations describing the reaction rate (Butler–Volmer equation), capillary pressure (Leverett–J function), and physical properties are given in Table 3. Conservation equation of the liquid-phase species is solved only for OH^-. The mass fraction of K^+ is calculated from electroneutrality.

2.2. Electrochemical reaction

One-step electrochemical reactions are assumed for anode and cathode electrodes,

Anode:

$$H_2 + 2OH^- \rightarrow 2H_2O + 2e^- \quad (1)$$

Download English Version:

https://daneshyari.com/en/article/1284757

Download Persian Version:

https://daneshyari.com/article/1284757

Daneshyari.com