Formulae for Solid Oxide Fuel Cells

Output Voltage

Output Voltage = Nernst Voltage – (Activation Loss + Concentration loss + Ohmic Loss)

$V_{fc} = E_{nernst} – (V_{act} + V_{con} + V_{ohmic})$

Nernst Equation

$$E = E_0 + \frac{RT}{2F} \ln \left(\frac{P_{\mathrm{H_2}} * P_{\mathrm{O_2}}^{0.5}}{P_{\mathrm{H_2O}}} \right)$$

Where

E_0 *= 1.1 V is the standard potential*

R = 8.314 kJ/ kmol .K is the universal gas constant

T = operating temperature of the fuel cell in kelvins

F = 96486 C/mol is the Faraday constant

Output current Density

$$I_{\mathrm{fc}} = I_0 \left(e^{(\alpha_1 nF/RT)V_{\mathrm{act}}} - e^{(-\alpha_2 nF/RT)V_{\mathrm{act}}} \right)$$

where -

I_0 *is the exchange current*

α_i *is the coefficient of charge transfer*

n = 2 is the number of moles of electrons transferred

Exchange Current Density

$I_0 = A(e_{-}Eact)/RT$

where –

A = 101.2 kA/cm^2 *is a preexponential factor obtained by curve fitting with the distributed model*

E_{act} = 120 kJ/mol is the activation energy of the electrochemical reaction

Partial Pressures

$$P_{H2} = \left(\frac{\frac{1}{K_{H2}}}{1+\tau_{H2}} \right) (q_{H2} - 2K_r I_{fc})$$

$$P_{O2} = \left(\frac{\frac{1}{K_{O2}}}{1+\tau_{O2}} \right) (q_{O2} - 2K_r I_{fc})$$

$$P_{H2O} = \left(\frac{\frac{1}{K_{H2O}}}{1+\tau_{H2O}} \right) (2K_r I_{fc})$$

$$q_{H2} = \frac{2K_r}{U_{opt}} \left(\frac{1}{1+\tau_f s} \right)$$

$$q_{O2} = \frac{q_{H2}}{r_{OH}}$$

Where

- *qH2* is the fuel flow rate
- *qO2* is the oxygen flow rate
- *KH2 , KO2 , KH2O* are the molar valve constants of hydrogen, oxygen and water respectively,
- *τH2, τO2 , τH2O,* are the response times of hydrogen, oxygen and water respectively,
- *τf* is the fuel response time in seconds,
- *Uopt* is the optimum fuel utilization,
- *rOH* is the ratio of hydrogen to oxygen
- *Kr* = 1/(8F).

Activation Loss

$$V_{\mathrm{act}} = \frac{RT}{F} \left(z + \sqrt{(1+z^2)} \right)$$

Where

I_0 is the exchange current

α_i is the coefficient of charge transfer

n = 2 is the number of moles of electrons transferred.

Concentration Loss

$$V_{\text{con}} = \frac{RT}{nF} \ln\left(\frac{C_b}{C_\infty}\right)$$

OR

$$V_{conc} = -\frac{RT}{nF} \ln\left(1 - \frac{I_{fc}}{I_L}\right)$$

Where

C_b is the concentration at the triple-phase boundary (tbp) where the gas, electrolyte,

C_∞ is the bulk concentration of reactant

n is the number of moles of electrons participating in the reaction

I_L is the maximum possible current density of the cell at a given flowrate

I_{fc} is the given current density

Ohmic Loss

$$V_{ohmic} = \left(\gamma \exp\left[\beta\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]\right) I_{\text{fc}} = rI$$

where

T is the fuel cell temperature

T_0 = 973 K

γ = 0.2 Ω, and β = −2870 K are the constant coefficients of the fuel cell

r is the internal resistance of the SOFC

Constants and Parameters Used

Parameter	Value	Unit
E_O	1.1	V
R	8.314	KJ/Kmol.K
F	98486	C/mol
K_{H2}	$8.43\text{x}10^{-4}$	Kmol/atm
K_{O2}	$2.81\text{x}10^{-4}$	Kmol/atm
K_{H2O}	$2.52\text{x}10^{-3}$	Kmol/atm
τ_{H2}	26.1	seconds
τ_{O2}	2.91	seconds
τ_{H2O}	78.3	seconds
τ_f	5	seconds
U_{opt}	0.85	-
r_{OH}	1.145	ohm

References:

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