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# Modelling of a High Temperature Solid Oxide Fuel Cell

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**Abstract**
Solid oxide fuel cell (SOFC) has been considered as one of the most efficient power generation devices for the coming decades. There are various physical phenomena appearing in SOFC in multi-length and -time scales, such as multi-component gas-phase species/charge flow, thermal energy and mass transfer. Meanwhile, generation and consumption of gas and surface phase species together with electric current production are involved at various active sites of different components of SOFC.In this paper, a numerical study of the thermal and electrochemical performance of a single Integrated Planar Solid Oxide Fuel Cell (IP-SOFC) has been performed. The numerical modelling considers internal reforming through the methane reforming and water gas shift reactions in a Ni-YSZ anode. Next to the description of the electrochemical reactions, the methane/steam reforming and shift reactions, the heat-transfer and the mass-transfer processes have also been included in the model.

**Keywords:** Solid oxide fuel cell (SOFC), Integrated Planar Solid Oxide Fuel Cell (IP-SOFC), internal reforming, methane reforming, water gas shift.

## 1. Introduction

Currently, the world's bulk energy requirements are based on the combustion of fossil fuels. Its combustion causes environmental problems particularly air pollution, acid gas emissions, and the emission of greenhouse gases. The demand for energy is increasing day by day, leading to energy crisis. With use of new and alternate energy systems, there is also a question of how to keep our environment clean at the same time. Therefore, there is urgent need of reduction of consumption of energy in developed countries and increase the use of advanced/efficient energy systems at a large scale level. Fuel cell technology is an emerging source of clean energy production without causing any harm to the environment as it does not involve any combustion reaction. A fuel cell is an electrochemical device that converts the chemical energy in fuels such as hydrogen (or hydrogen-rich fuel like methane, butane or even gasoline and diesel) into electrical energy by exploiting the natural tendency of oxygen and hydrogen to react. A single fuel cell is a simple device, containing no moving parts and consists of an electrolyte sandwiched between two thin electrodes (a porous anode and cathode). By controlling the means by which such a reaction occurs and directing the reaction through a device, it is possible to harvest the energy given off by the reaction (Singhal & Kendall 2003).

SOFC is one type of solid-state ionic based fuel cell devices which have all the components in solid state. They operate at very high temperatures typically around 1000ºC allowing them to reform fuels internally, thereby enabling them to use of a variety of fuels and reduces the cost associated with adding a reformer to the system. In addition, they are not poisoned by carbon monoxide (CO), which can even be used as fuel (Kalra et al. 2013). The working principle of an SOFC involves feeding of hydrogen or fuel rich in hydrogen at the anode(fuel electrode) and feeding of oxygen at the cathode (air electrode). An electrons combine with oxygen resulting in the formation of oxide ions. The oxide ions move through the electrolyte which is permeable to these ions reacting on the triple phase boundary formed on the surface of anode in the presence of a catalyst (Nickel on Yittria stabilized Zirconia). The electrons produced due to the reaction of oxide ions with hydrogen from the anode side of the cell cannot pass through the membrane to the positively charged cathode, rather they must travel around it via an electrical circuit to reach the other side of the cell. This movement of electrons is an electrical current. Fig1. shows the principle of operation of SOFC. The electro-chemical reactions occur in the electrodes within a distance of less than 10 – 20 microns from the electrolyte surface referred to as the functional layer. For the electrochemical reaction to occur, the co-existence of the electrolyte, the electron-conducting metal phase, and the gas phase is required. This is referred as the three-phase boundary (TPB) (Mahcene et al. 2006). For a typical Ni/YSZ anode, the region between the electrolyte and the anode where the TPB exists is as shown in fig2.

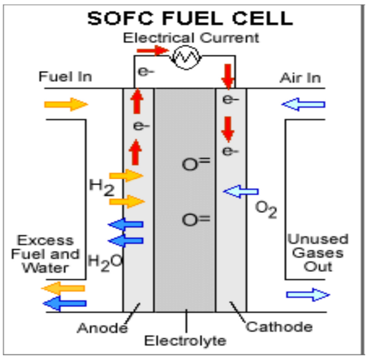

**Fig1. Principle of operation of SOFC**
(Singhal & Kendall 2003)

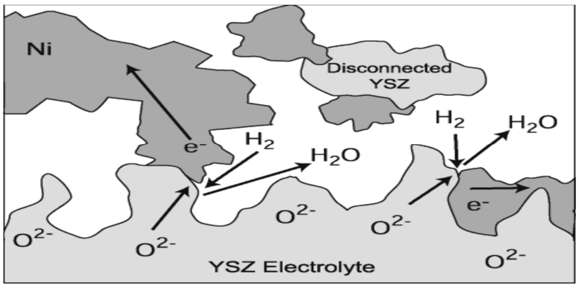

**Fig2. Schematic diagram of anode three-phase boundary**
(McIntosh & Gorte 2004)

Mathematical modelling of SOFCs is a helpful tool in examining various design and operation parameters such as geometry, dimensions, fuels, temperatures, and pressures. With the appropriate models and parameter values influences on gas concentration, temperature, current density, and stress distributions can be determined. Results can be used to optimize designs and select optimal operation conditions. A vast range of models exist today, varying in complexity and in the number of assumptions employed. These range from detailed models on individual components to entire stack models. One-, two-, and three- dimensional, as well as parametric models have been developed for several different geometries. Due to the electrochemical reactions, generation and consumption of chemical species together with electric current production take place at the active surfaces for all kinds of fuel cells. A reliable and predictive well-designed SOFC model requires that the effective heat, mass, species, charge and momentum transport coupled with chemical reactions in the porous substrates (Larminie & Dicks 2003).

Fig3 shows specific Energy balance for a SOFC, the fuel quantity being the reference. The first law of the thermodynamics for the system gives:

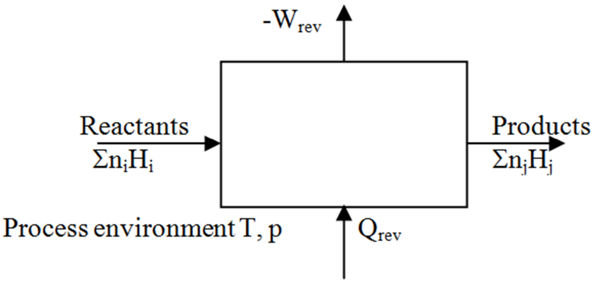

**Fig 3 Energy balance of a reversible fuel cell**
(Kalra et al. 2013).

The reversible efficiency $\eta_{rev}$ of a SOFC is the ratio of the Gibbs enthalpy $\Delta^r G$ and the reaction enthalpy $\Delta^r H$ at the thermodynamic state of the fuel cell gives

$$\eta_{rev} = \frac{\Delta^r G}{\Delta^r H} = \frac{\Delta^r H - T\Delta^r S}{\Delta^r H} \qquad \text{..............(1)}$$

The reaction enthalpy $\Delta^r H$ of the oxidation covers the production of the reversible work and heat.The fuel utilisation $U_f$ is the ratio of the spent fuel flow and the inlet fuel flow and is defined by

$$U_f = 1 - \frac{m_{FAno}}{m_{FI}} \qquad \text{..............(2)}$$

where $m_{FI}$ is the fuel mass flow at the cell's inlet and $m_{FAnO}$ is the fuel mass flow at the outlet of the anode. A similar definition can be made with the molar flow.

The electric current I is a linear function of the molar flow rate of the electrons or the molar flow of the spent fuel

$$I = n_{el}\cdot(-e)N = -n_{el}F = -2n_{H2}.F \qquad \text{..............(3)}$$

*F* being the Faraday constant or the charge on one mole of electrons & N is the Avagadro's No. (Singhal & Kendall 2003). The open circuit voltage generated in a SOFC is given by:

$$E = \frac{-\Delta G_f}{2F} \qquad \text{..............(4)}$$

For a simple system, like that for heat engines- If the maximum temperature of the heat engine is $T_1$, and the heated fluid is released at temperature $T_2$, then the maximum efficiency possible is given by the Carnot efficiency as

$$\text{Carnot efficiency} = \frac{T_1 - T_2}{T_1} \qquad \text{.............(5)}$$

The maximum electrical energy available is equal to the change in Gibbs free energy, maximum possible efficiency is given by

$$\eta_{\max} = \frac{\Delta G_f}{\Delta h_f} \times 100\ \% \qquad \text{.............(6)}$$

This maximum efficiency limit is sometimes known as the 'thermodynamic efficiency' (Brandon 2007)

The four major irreversibilities that are incorporated leading to a reduction in actual efficiency of a SOFC and thus a drop in open circuit voltage are outlined briefly here:

**(i) Activation losses**, $\eta_{Act}$ caused by the slowness of the reactions taking place on the surface of the electrodes.

**(ii) Ohmic losses,** $\eta_{ohm}$ caused due **to** resistance to the flow of electrons through the material of the electrodes and the various interconnections, as well as the resistance to the flow of ions through the electrolyte.

**(iii) Mass transport or concentration losses,** $\eta_{Conc}$ results from the change in concentration of the reactants at the surface of the electrodes as the fuel is used. The concentration affects voltage, and so this type of irreversibility is sometimes called concentration loss (Singhal & Kendall 2003). Fig4 shows the OCV and various losses.

An electrochemical analysis based on deviation from ideal performance is proposed at each slice. Considering the electrodes to be equilibrium surfaces [r] the Nernst voltage is defined by

$$E_{\text{Nernst}} = E^{\circ}_{T,P} + \frac{RT}{nF} \ln \frac{P_{H_2} \times P_{O_2}}{P_{H_2O}} \qquad \text{.............(7)}$$

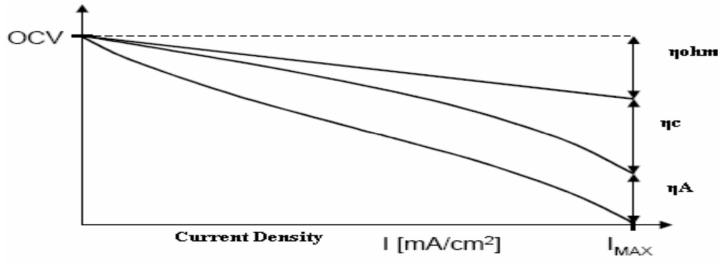

**Fig4: Open circuit voltage fall due to polarization**
(Singhal & Kendall 2003)

at standard temp. & pressure. Substituting the partial pressures of $H_2O$, $H_2$ and $O_2$, we get

$$E_{\text{Nernst}} = E^{\circ}_{T,P} + \frac{RT}{nF} \ln \frac{P^{\frac{1}{2}} . X_{H_2} . X_{O_2}^{\frac{1}{2}}}{X_{H_2O}} \qquad \text{.............(8)}$$

Where p, X and n are gas pressure, mole fraction and no. of electrons flowing in the external circuit.
The cell potential $E$cell is being calculated by subtracting these over-potential from the Nernst potential (*Yuan et al. 2008)*.:

$$E_{cell} = E^{\circ}_{T,P} - \eta_{act} - \eta_{ohm} - \eta_{conc} \qquad \text{.............(9)}$$

The electrical power produced by the fuel-cell is calculated by:

$$W = E_{cell} \times i \qquad \text{.............(10)}$$

## 2. Governing transport equations of SOFC

From perspective of transport, a fuel cell consists of several components: flow channels (the fuel flow channel and air flow channel), electrodes (the anode and cathode), electrolyte, and interconnector. The fuel and air flows gradually across the interfaces, perpendicular to the flow direction, between the flow channels and the electrodes, diffuse through the porous electrodes, and arrive at the interfaces between the electrodes and the electrolyte, where the electrochemical reaction occurs and current is generated (*Lu & Schaefer 2004)*. The details of the two core components and governing equations are given below:

**The flow channels:** The key function of flow channels is to allow the distribution of gases throughout the fuel cell to the porous electrodes with as little losses as possible. The governing transport equations are:

**(i) The conservation of mass:**

$$\frac{\partial \rho}{\partial t} + \nabla .(\rho v) = 0 \qquad \text{.............(11)}$$

where ρ is the density of the flow in the channels, v is the velocity vector.

**(ii) The conservation of momentum:**

$$\frac{\partial}{\partial t}(\rho v) + \nabla .(\rho v v) = -\nabla P + \nabla .\tau \qquad \text{.............(12)}$$

where P is the pressure in the channels and τ is the stress tensor.

**(iii) The species balance equation:**

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla .(\rho v Y_i) = -\nabla .J_i + r_i \qquad \text{.............(13)}$$

where $Y_i$ is the mass fraction of the ith species in the channels, $J_i$ is the diffusive flux of the ith species, and $r_i$ is the rate of production of species i per unit volume.

**(iv) Energy conservation:**

$$\rho C_P (\frac{dT}{dt} + v.\nabla T) = k\nabla^2 T + q \qquad \text{.............(14)}$$

where $C_p$ is the specific heat, T the temperature, k the thermal conductivity, and q the heat source term per unit volume, in terms of substance in the flow channel.

**The electrodes:** The porous electrodes of fuel cells are where the electrochemical reaction takes place. These electrodes serve several functions- allow for gas transport/ diffusion through the pores to the active sites, and provide a site for the electrochemical reactions to occur. The governing transport equations are:

**The species balance equation:**

$$\varepsilon \frac{\partial}{\partial t}(\rho Y_i) = -\nabla .J_i + r_i \qquad \text{.............(15)}$$

where ε is the porosity of the electrode, and $r_i$ is the rate of production of species i per unit volume within the electrodes. Note only the diffusion is considered in the electrodes.

**Energy conservation:** In the porous structure, the energy conservation can be written by ignoring the convective heat transfer as:

$$\rho C_P \frac{dT}{dt} = k\nabla^2 T + q \qquad \text{.............(16)}$$

where q includes the heat generated by the current flow through the electrodes (Ohmic losses) and the activation losses, and the heat due to chemical reactions. Once again additional terms such as heat terms due to convection and radiation appear as boundary conditions (Singhal 2000).

## 3. Modelling of a One dimensional Planar SOFC

**Assumptions**

1. Chemical Kinetics, conservation of mass and energy equations will be formulated in this model.
2. The study of temperature & bulk concentration distribution will be studied within the SOFC.
3. The rate of diffusion of gases normal to the flow direction will not be considered.
4. The SOFC would be considered to be operating under steady-state conditions.
5. The principal fuel for SOFC would be methane. $H_2$ will be produced by high temperature internal reforming of methane at the cell itself.
8. The performance study will be done by studying the fuel gas composition on a single planar SOFC.
9. The electrodes are sandwiched around a hard ceramic electrolyte like zirconia. The air & fuel flow over the surfaces of cathode & anode respectively.
10. The amount of Polarization losses will be studied by changing the operating conditions & fuel composition.

Various reactions of a single planar SOFC are:

**(i) Methane reforming**

$CH_4 + H_2O \rightarrow 3H_2 + CO \quad \Delta H_{298} = 206$ kJ/mole ......[1]

**(ii) Water gas shift reaction**

$CO + H_2O \rightarrow 2H_2 + CO_2 \quad \Delta H_{298} = -41.1$ kJ/mole ......[2]

**(iii)** The reactions occurring at the anode/cathode and the overall cell reaction are

**Cathode** $\frac{1}{2} O_2 + 2e^- \rightarrow O^{2-}$ ......[3]

The $O^{2-}$ ions migrate through the electrolyte and reach the anode.

**Anode** $H_2 + O^{2-} \rightarrow H_2O + 2e^-$ ......[4]

The overall cell reaction is

**Cell reaction** $H_2 + \frac{1}{2} O_2 \rightarrow H_2O$ ......[5]

Besides these reactions, the oxidation of CO and the reaction of $CH_4$ with steam forming $CO_2$ and $H_2$.

**(iv) Bourdyard reaction** $CO + ½O_2 \rightarrow O_2 + \text{Heat}$ ……[6]

**(v) Methane Reforming2** $CH_4 + H_2O \rightarrow 4H_2 + CO_2$ ……[7]

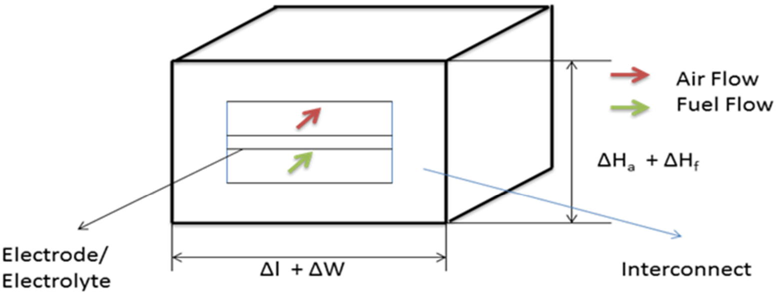

**Fig5. Flow diagram of various components across a single cell planar SOFC**

**3.1 Molar balance of species for an electrochemical steady state model:**The operation of SOFC is based on the variation of concentration of $CH_4$, CO, $CO_2$, $H_2$, $H_2O$ in a node of fuel channel. The variation of mole number for any component I can be written as

$$I^{out} = I^{in} +/- \Delta mole_{MR} +/- \Delta mole_{WGS} +/- \Delta mole_{BR} +/- \Delta mole_{MR2} \quad \text{……..(17)}$$

For any particular node, the reacted species are related to the current transfer rate across the electrolyte layer of the node & the rate of consumption of species by

$$R = - a\, I/nF \quad \text{……..(18)}$$

Where a = stoichiometeric coefficient, I = current (A) , n= no of electrons per mole of fuel, R= source or sink g-mole/s , F=Faraday constant.The current transfer is due to oxidation of $H_2$ & CO (Singhal 2000).The model can be split into:

### 3.1.1Anode flow model:

For various components at anode $H_2$, $H_2O$, $CO_2$ & CO the rate of consumption is given by

$$R_I = +/- i_I/2F \text{ (Component I consumed or produced)} \quad \text{……..(19)}$$

### 3.1.2 Cathode flow model:

$$R_{O2} = - (0.5\,(i_{H2}+ i_{CO}))/2F \quad \text{(oxygen consumed)} \quad \text{……..(20)}$$

The equilibrium concentrations can be determined by their temperature dependent equilibrium constants for the various reactions, then they can be mathematically represented by

$$K_{MR}= (y_{H2}^3\, y_{CO})/(\, y_{CH4}\, y_{H2O}) = \exp(-\Delta G_{MR}/RT_S) \quad \text{……..(21)}$$

$$K_{WGS}= (y_{H2}^2\, y_{CO2})/(\, y_{CO}\, y_{H2O}^2) = \exp(-\Delta G_{WGS}/RT_S) \quad \text{……..(22)}$$

$$K_{CO\ oxid}= y_{CO2}/(\, y_{CO}\, y_{O2}^{1/2}) = \exp(-\Delta G_{CO\ oxid}/RT_S) \quad \text{……..(23)}$$

$$K_{H2\ oxid}= y_{H2O}/(\, y_{H2}\, y_{O2}^{1/2}) = \exp(-\Delta G_{H2\ oxid}/RT_S) \quad \text{……..(24)}$$

Where y's represents the mole fractions of different gaseous components.

### 3.2 Ideal reversible voltage

The ideal (reversible) is the open circuit voltage of a fuel cell & it is the electric work done per unit charge on one mole of electrons through the fuel cell circuit.

$$E_{rev}= \text{Electrical work}/2F \quad (\text{for } H_2 \text{ oxidation}) \quad \text{……..(25)}$$

Where F is the Faraday constant in the denominator represents the no. of electrons that flow for one mole of $H_2$ oxidized. For an ideal system, the electrical work done during reaction is equal to molar gibb's free released, -ΔG.

$$E_{rev}= - \Delta G/2F \quad \text{……..(26)}$$

The Nernst equation gives the dependence of molar Gibb's free energy on reactant pressure, concentration and temperature (Atkinson et al. 2004).

$$E_{rev} = E_{STP} + (RT_s)/nF \ \ln(\Pi_{\text{reactant activity}})/(\Pi_{\text{product activity}}) \quad \text{……..(27)}$$

The activities of reactants & products are expressed in terms of partial pressure or mole fraction,

$$E_{H2} = E_{STP} + (RT_s)/2F \ \ln(P_{H2}\, P_{O2}^{1/2})/(P_{H2O}) \quad \text{……..(28)}$$

There is a similar Nernst equation for CO oxidation.

### 3.3 Electrical Analog

The total current can be represented by summation of the current due to $H_2$ and CO oxidation. An electrical analog of the how current is distributed can be represented by the fig6 below:

The three currents can be calculated from the following equation

$I = I_{CO} + I_{H2}$ ……..(29)

$V = V_{rev,H2} - (R_c + R)\, I - R_A\, I_{H2}$

$= V_{rev,CO} - (R_c + R)\, I - R_A\, I_{CO}$

$V = V_{rev,H2} - \eta_C + R\, I - R_A\, I_{H2}$

$V = V_{rev,CO} - \eta_C + R\, I - R_A\, I_{CO}$ ……..(30)

$R_C$ – resistance due to concentration loss

R = Surface specific resistance

$\eta_C$ = voltage loss due to concentration polarization

$R_A$ I – voltage loss due to activation polarization.

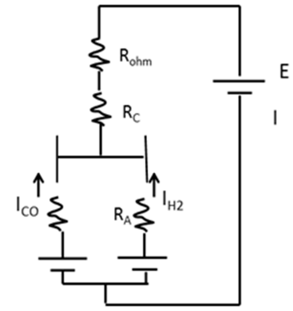

**Fig6 Electrical Analog**

### 3.4 Continuity Equations:

The continuity equation for one dimension is given by

$\partial u/\partial x = 0$ ……..(31)

The dynamic flow model are given by the mass, momentum & energy equations. For an $i^{th}$ component, the conservation of mass this becomes

$\partial \rho_i/dt + u\, \partial \rho_i/dx = (1/V)\ \Sigma\, r_{a,i}$ ……..(32)

$\rho_i$- molar density, U = average velocity, $m_i$ - species mole fraction, n- no of species, $r_{a,i}$- rate of reaction of species I, $\Sigma\, r_{a,i}$- summation of rate of reaction of all species.

The conservation equation for species I is given by:

$\partial c_i/dt + u\, \partial c_i/dx = 1/V\ \Sigma\, r_{a,i}$ ……..(33)

Where ci – molar concentration of species i.

The conservation equations for $O_2$

$\partial m_{O2}/dt + u_C\, \partial m_{O2}/dx = (RT_S)/(P_C\, V_C)\ r_{O2,\ reacted}$ ……..(34)

The amount of oxygen reacting is predicted by Faraday's law as:

$r_{O2,\ reacted} = R_{O2} = -I_{H2}/4F$ ……..(35)

Anode flow model: The conservation equations are written for various components i.e. $H_2$, $H_2O$, CO, $CO_2$, $CH_4$, for a general component I

$\partial m_I/dt + u_a\, \partial m_I/dx = (RT_S)/(P_C\, V_C)\ r_{I,\ reacted}$ ……..(36)

$u_a$ = gas velocity at the anode surface

$r_{H2,\ reacted} = R_{MR} + R_{WGS} + R_{cell\ reaction} + R_{MR2}$

$= r_{MR} + r_{WGS} - I_{H2}/2F + r_{MR2}$ ……..(37)

$r_{H2O,\ produced} = R_{MR} + R_{WGS} + R_{cell\ reaction} + R_{MR2}$

$= r_{MR} + r_{WGS} + I_{H2}/2F + r_{MR2}$ ……..(38)

$r_{CO,\ reacted} = R_{WGS} + (-R_{MR}) + R_{BR}$ ……..(39)

$r_{CO2,\ produced} = R_{WGS} + R_{BR} + R_{MR2}$ …….(40)

$r_{CH4,\ reacted} = R_{MR} + R_{MR2}$ ……..(41)

$u_a$ = gas velocity at the anode surface

$r_{H2,\ reacted} = R_{MR} + R_{WGS} + R_{cell\ reaction} + R_{MR2}$

$= r_{MR} + r_{WGS} - I_{H2}/2F + r_{MR2}$ ……..(42)

$r_{H2O,\ produced} = R_{MR} + R_{WGS} + R_{cell\ reaction} + R_{MR2}$

$= r_{MR} + r_{WGS} + I_{H2}/2F + r_{MR2}$ ……..(43)

$r_{CO,\ reacted} = R_{WGS} + (-R_{MR}) + R_{BR}$ ……..(44)

$r_{CO2,\ produced} = R_{WGS} + R_{BR} + R_{MR2}$ ……..(45)

$r_{CH4,\ reacted} = R_{MR} + R_{MR2}$ ……..(46)

### 3.5 Polarization effect on Planar SOFC

(i) **Ohmic loss $\eta_{ohm}$ :** $\eta_{ohm} = I\, R_{el}$ ……..(47)

$R_{el}$ - electrolyte area specific resistance = $l_e/\sigma_e$, le - electrolyte thickness

σe - electrical conductivity of the cell material

(ii) **Activation Polarization $\eta_{act}$ :** $\eta_{act} = (R\, T_s/n_e\, \beta\, F)\ \ln (i/i_0)$ ……..(48)

$i_0$ - total current density, $n_e$ - no. of electrons for 1 mole of $H_2$ oxidation

F- Faraday's constant , β = 0.5, Ts- Temperature of the cell

(iii) **Concentration Polarization $\eta_{conc}$ :**

$\eta_{conc\ cathode} = (R\, T_s/4\, F)\ \ln (1 - i/i_{cs})$ ……..(49)

$\eta_{conc\ anode} = (R\, T_s/2\, F)\ \ln (1 - i/i_{as}) - (R\, T_s/2\, F)\ \ln (1 + (P_{H2}\, i)/(P_{H2} i_{as}))$ ……..(50)

$i_{as}$, $i_{CS}$ are the limiting current densities for anode & cathode respectively.

i – total current density developed

The net voltage output for each cell

$V = V_0 - \eta_{act} - \eta_{conc} - \eta_{ohm}$ ……..(51)

### 3.6 Fuel utilization Coefficient ($\mu_F$) and Fuel cell efficiency ($\eta$):

The fuel utilization coefficient $\mu_F$ is defined as

$\mu_F$ = (Mass of fuel reacted in the cell) / (Mass of fuel input in the cell) ……..(52)

The mass of fuel reacted can be improved with a fuel containing higher percentage of hydrogen. The cell efficiency is given by:

$\eta = (\mu_F V)/V_0$ ……..(53)

$\mu_F$ is the fuel utilization coefficient
V is the net voltage
$V_0$ is the ideal voltage developed.

### 3.7 Steady state heat Transfer

Assumptions for heat transfer

- The electrodes, electrolyte & interconnect are solid materials & therefore would be involved in conduction.
- The convection heat transfer is in the fuel & air channels.
- The exothermic heat involved during electrochemical reactions i.e. $H_2$, CO as well as water gas shift serve as heat source.
- The reforming reactions are endothermic in nature & tends to balance the heat generated by other reactions.

The convective heat transfer based on the laminar flow of fluids is

$Nu = (hd_h)/k$ ……..(54)

The convective heat transfer is given by

$Q = h(T_S - T_{air/fuel})$ ……..(55)

If $Q_{source}$ is the heat dissipated by reaction in the anode/electrolyte surface i.e fuel cell reaction, CO oxidation, Water gas shift and Methane reforming.

ΔG of the total energy obtained goes as electrical work done by the fuel cell. The remaining sustains the high temperature operation of SOFC. The governing energy equations are as follows:

$Q_{source} = -T_S \Delta S_{cell} \Delta U - T_S \Delta S_{WGS} \Delta V - T_S \Delta S_{CO,\,oxid} \Delta W + T_S \Delta S_{MR1} \Delta X + T_S \Delta S_{MR2} \Delta Y$ ……..(56)
$\Delta H_{cell} = [\text{Enth } H_2O\ (T_{fuel}) - \text{Enth } H_2\ (T_{fuel}) - 0.5 \text{ Enth } O_2\ (T_{air})]\ \Delta U$ ……..(57)
$\Delta H_{WGS} = [2\times \text{Enth } H_2(T_{fuel}) + \text{Enth } CO_2(T_{fuel}) - 2\times \text{Enth } H_2O\ (T_{fuel}) - \text{Enth CO}\ (T_{air})]\ \Delta V$ ……..(58)
$\Delta H_{CO,\,oxid} = [\text{Enth } CO_2\ (T_{fuel}) - \text{Enth CO}\ (T_{fuel}) - 0.5 \text{ Enth } O_2\ (T_{air})]\ \Delta W$ ……..(59)
$\Delta H_{MR1} = [3 \times \text{Enth } H_2\ (T_{fuel}) + \text{Enth CO}\ (T_{fuel}) - \text{Enth}CH_4(T_{fuel}) + \text{Enth } H_2O(T_{cell})]\ \Delta X$ ……..(60)
$\Delta H_{MR2} = [4\times \text{Enth}H_2\ (T_{cell}) + \text{Enth } CO_2\ (T_{cell}) - \text{Enth } CH_4(T_{fuel}) - 2\times \text{Enth } H_2O(T_{cell})]\ \Delta Y$ ………(61)

Similarly, the entropy change for various reactions gives:

$\Delta S_{cell} = [\text{Entr } H_2O\ (T_{fuel}) - \text{Entr}H_2\ (T_{fuel}) - 0.5 \text{ Entr}O_2\ (T_{air})]\ \Delta U$ ……..(62)
$\Delta S_{WGS} = [2\times \text{Entr}H_2(T_{fuel}) + \text{Entr } CO_2\ (T_{fuel}) - 2\times \text{Entr } H_2O\ (T_{fuel}) - \text{EntrCO}\ (T_{air})]\ \Delta V$ ……..(63)
$\Delta S_{CO,\,oxid} = [\text{Entr } CO_2\ (T_{fuel}) - \text{Entr CO}\ (T_{fuel}) - 0.5 \text{ Entr } O_2\ (T_{air})]\ \Delta W$ ……..(64)
$\Delta S_{MR1} = [3\times \text{Entr } H_2\ (T_{fuel}) + \text{Entr CO}\ (T_{fuel}) - \text{Entr } CH_4(T_{fuel}) + \text{Entr}H_2O(T_{cell})]\ \Delta X$ ……..(65)
$\Delta S_{MR2} = [4 \times \text{Entr } H_2\ (T_{cell}) + \text{Entr } CO_2\ (T_{cell}) - \text{Entr}CH_4(T_{fuel}) - 2\times \text{Entr } H_2O(T_{cell})]\ \Delta Y$ ……..(66)

The radiation heat transfer occurs between cell surface to the interconnect surface is

$Q_{rad} = A_1 F_{12} (\varepsilon_1 \sigma T_1^4 - \varepsilon_2 \sigma T_2^4)$ ……..(66)

the interconnect & separator plate to be black surfaces & view factor F12 can be assumed to be 1.

$Q_{rad} = A_1 \sigma (T_1^4 - T_2^4)$ ……..(67)

### 3.8 Energy Equations for different channels:

Air Channel: $\rho_a C_{pa} V_a (\partial T_a/ \partial t) = \rho_a C_{pa} V_a u_a (\partial T_a/ \partial x) - h_a \times A\,(Ts - Ta)$ ……..(68)
Interface: $\rho_S C_{pS} V (\partial T_S/ \partial t) = k_S V(\partial^2 T_S/ \partial x^2) - h_a \times A_{Ca}(Ts - Ta) + h_f \times A_{Cf}(Ts - T_f) + Q_{source}$ ……..(69)
Fuel channel: $\rho_f C_{pf} V_S (\partial T_f/ \partial t) = \rho_f C_{pf} V u_f (\partial T_f/ \partial x) - h_f \times A_{Sf}\,(Ts - Tf)$ ……..(70)

## 4. CONCLUSIONS AND FUTURE WORK

A one –dimensional model was developed to comprehensively describe the electrochemistry, hydrodynamics and multi-component transport of SOFC. The model would be implemented into the commercial CFD software Ansys Fluent. The CFD model would to be able to predict the current-voltage characteristics of SOFC, in addition to the detailed reactant and product distributions in the cell. This data makes it possible to analyze SOFC operation in detail.The CFD model described in this study is intended to present a tool for design optimization of SOFCs. To achieve this and fully utilize this tool, the model can be used to perform parametric and sensitivity studies of varying operating conditions and cell designs.

The present CFD model also has the energy equation built in to resolve the temperature distribution. However, a detailed account of various heat generating sources such as irreversible and reversible (entropic) heat as well as ohmic heating has not been accounted in the equations. The temperature distribution can be used to couple to stress analyses, thereby providing a comprehensive computer-aided engineering (CAE) tool for SOFC design and operation. The present model can be easily extended to include multiple fuels such as H2 and CO. Finally, the present model would serves as a building block to build a comprehensive CFD-based model for 3-dimensional SOFC with internal reforming on the anode. In such a situation, convectional & diffusional transport of various chemical species in all the three dimensional have to be taken into account.

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