A Thin Film Electrode Solid Oxide Fuel Cell Model

Penyarat Saisirirat a,*

aDepartment of Mechanical Engineering Technology, College of Industrial Technology, King Mongkut’s University of Technology North Bangkok, 1518, PrachaRat 1 Road, Wongswanang, Bangsue, Bangkok, 10800, Thailand

Abstract

Solid oxide fuel cells (SOFCs) are becoming one of the main competitors among environmental friendly energy sources due to low emission rates, high electrical generating efficiency and potential for low operating cost. This work presents systematic to develop and validate the microscopic scale models of a single cell SOFC supplied with humidified hydrogen. The model considers the porous silicon-supported thin film SOFC, in which the electrode microstructure is packed by cylindrical shaped ionic and electronic conducting particles. The model involves mass transfer phenomena inside electrodes coupled with electrochemical reaction, as well as transportation of electrons and ions through the respective electron and ion conducting particles inside the electrodes. The investigation confirms the strong effects of microstructure geometry to improve the SOFC performance, especially the increasing of the electrochemical active surface area. The largest active surface area of electrode is achieved when the size and solid volumetric fraction of ion and electron conducting particles are equal. The accuracy of the model was validated by comparing with published experimental data.

1. Introduction

SOFCs are highly efficient energy conversion devices that transform chemical energy to electrical energy and heat directly from fuels through electrochemical reactions at electrodes. The major limitation using SOFCs is their high operating temperature. As a solution of this drawback and to achieve stability and economics, so the

* Corresponding author. Tel.: +66 2 - 555 -2000 ext. 6353 ; fax: +66 2 - 587- 4350.
E-mail address: penyarat@kmutnb.ac.th , penyarat@gmail.com
Nomenclature

$A_v$  Active surface area per unit volume [m$^2$ m$^{-3}$ or m$^{-1}$]

$\tilde{A}_v$  Dimensionless active surface area of an electrode

$\tilde{A}_{v,0}$  Dimensionless active surface area of a unit particle volume,$V_0$

$D_i$  Binary diffusion coefficient [m$^2$ s$^{-1}$]

$D_{i,k}$  Knudsen diffusion coefficient of the species $i$ [m$^2$ s$^{-1}$]

$D_{i,eff}$  Effective binary diffusion coefficient [m$^2$ s$^{-1}$]

$h_d$  The height of the cylindrical electron conducting particle that contain inside the columnar electrode [m]

$h_{io}$  The height of the cylindrical ion conducting particle that contain inside the columnar electrode [m]

$\bar{h}$  Dimensionless particle height

$J_e$  Electronic current density [A m$^{-2}$]

$J_i$  Ionic current density [A m$^{-2}$]

$J_{H_2}^{ref}$  Reference exchange current density for H$_2$ oxidation [A m$^{-2}$]

$J_{O_2}^{ref}$  Reference exchange current density for O$_2$ reduction [A m$^{-2}$]

$n_{el}$  Number fraction of electron conducting particle in the electrode

$n_{io}$  Number fraction of ion conducting particle in the electrode

$n_t$  Total number of particles in the electrode per unit volume [m$^{-3}$]

$N_i$  Molar flux of species $i$ [mol m$^{-2}$ s$^{-1}$]

$p_{el}$  Probability of percolation of electron conducting particles in the electrode

$p_{io}$  Probability of percolation of ion conducting particles in the electrode

$P_{H_2}$  Partial pressures of H$_2$ within the porous anode

$P_{H_2}^0$  Partial pressures of H$_2$ at the anode surface

$P_{H_2O}$  Partial pressures of H$_2$O within the porous anode

$P_{H_2O}^0$  Partial pressures of H$_2$O at the anode surface

$P_{O_2}$  Oxygen partial pressure in cathode

$r_{el}$  Radius of electron conducting particles in the electrode [m]

$r_{io}$  Radius of ion conducting particles in the electrode [m]

$R_a$  Volumetric current density produced due to hydrogen oxidation [A m$^{-3}$]
A technique of thin film fabrication of the electrode and electrolyte of SOFC has been investigated by many researchers. This technique is the thin film deposition that is divided into two technical groups, which are the Liquid-Precursor-Based Deposition technique and Vacuum Deposition technique. The first technique was originally and normally used for the production of electrolyte. Another technique is the vacuum deposition technique, that the whole process takes place in a vacuum chamber. The one technique of vacuum deposition is Physical Vapor Deposition (PVD) provide the films with typical polycrystalline of columnar structure. Thus the grain size can be tailored by varying the deposition conditions, and nano-sized grains are easily obtained, so that the deposited particle sizes and the contact area between the ion and electron conducting particles of the electrode or electrolyte could be easily controlled. The films deposited by PVD methods can be porous or dense depending on the process parameters [2]. Recently, thin film SOFC was fabricated by the PVD films deposition with magnetron source [3]. In 2011, Sochugov et al. [9] use the method of ion-plasma technique for formation of anode-supported thin electrolyte films for IT-SOFC applications. Their method gives the anode electrode and electrolyte with columnar-like structure
similar to Rezugina et al’s work. In this article, the numerical model to predict and to illustrate phenomena inside the thin film SOFC with columnar-shaped microstructure is explained in details.

2. Modeling and governing equations

2.1. The cell geometry

An illustration of physical domain of a SOFC is shown in Fig. 1. Each component thickness used in the modeling is mentioned in Table 1 and 2.

![Fig. 1. The single cell cross section](image)

2.2. The model assumptions

The cell is assumed to operate under steady state. The reactant gas mixtures are approximated as ideal gases. Temperature and total pressure are constant and uniform throughout the entire electrode. The mass transfer process inside the porous electrode is by means of diffusion [5-8]. For the cermet anode and cathode, formed by the mixture of electronic and ionic conductors, the active surface area per unit volume (A_v) could be calculated based on Costamagna et al’s expression, but this work has modified the Costamagna et al’s expression to the domain packed with cylindrical-shaped particles, by assuming that the sizes for both of ion and electron conducting particles are equal, then the A_v becomes,

\[ A_v = \left(2r_{el}h_{el}\right)\left(sin(\theta)\right)n_{el}n_{io}\left(\frac{Z_{el}Z_{io}}{Z}\right)p_{el}p_{io} \]  

(1)

\[ n_{el} = \left(1 - \epsilon\right)\left[\left(\pi r_{el}^2 h_{el}\right)n_{el} + \left(\pi r_{io}^2 h_{io}\right)n_{io}\right] \]  

(2)

\[ \varphi = n_{el} / \left(n_{el} + \left(1 - n_{el}\right)\left(\frac{r_{io}^2 h_{io}}{r_{el}^2 h_{el}}\right)\right) \]  

(3)

\[ n_{el} = \left(\frac{P\varphi}{1 + (P - 1)\varphi}\right); n_{io} = 1 - n_{el}; P = \left(\frac{r_{io}}{r_{el}}\right)^{\frac{2}{Z}} \left(h_{io}/h_{el}\right) \]  

(4)

where, \( n_{el} \) is number of particles per unit volume, \( n_{el} \) and \( n_{io} \) are the fraction number of electron and ion conducting particles, which are related with to the volumetric fraction of electron conducting particles (\( \varphi \)) by the following Eq. (3). The \( r_{el} \) and \( r_{io} \) are the radius of the ion and electron conducting particles. The \( h_{io} \) and \( h_{el} \) are the height of the ion and electron conducting particle. By assuming that the sizes for both of ion and electron conducting particles are equal that the \( A_v \) is shown in equation as above. And where,

\[ Z_{el} = 3 + (Z - 3)\left[\left(n_{el} + \left(1 - n_{el}\right)\left(\frac{r_{io}}{r_{el}}\right)^{\frac{2}{Z}} \right)\right] \]  

(5)
\[ Z_{el} = 3 + \left( (Z-3)(r_{el}/r_{el})^2 \right)^{1/2} \left( (1-n_{el})/(r_{el}/r_{el}) \right) \]  

(6)

The \( Z_{el} \) and \( Z_{io} \) are the average coordination number of electron and ion conducting particles \([9]\). \( Z \) is the total average particle coordination number in electrode equal to 6. The \( p_{el} \) and \( p_{io} \) are the probability probabilities that for an electron and an ion conducting particle to belongs to connecting both ends of the composite, respectively, they are following equation (7) \([9-10, 11-12]\).

\[ p_{el} = \left( 1 - \left( (4.236 - Z_{el, el})/2.472 \right) \right)^{0.4} \quad \text{and} \quad p_{io} = \left( 1 - \left( (4.236 - Z_{io, io})/2.472 \right) \right)^{0.4} \]  

(7)

\( Z_{el, el} \) and \( Z_{io, io} \) are the electron conducting particle to electron conducting particle average coordination number and the ion conducting particle to ion conducting particle average coordination number, \([9-12]\).

\[ Z_{el, el} = \left( n_{el} Z_{el} \right)/Z \quad \text{and} \quad Z_{io, io} = \left( n_{io} Z_{io} \right)/Z \]  

(8)

2.3. Mass transfer equations on the anode side

Mass transport through porous medium can be determined using concepts described in Ref. \([5, 6]\). In the steady state, the mass transport equation can be written as

\[ \nabla \cdot N_j = R_i \]  

(9)

where \( N_j \) represent the rate of mass transport (or denotes as the molar flux of each species, \( \text{mol m}^{-2} \text{s}^{-1} \)) into porous media. \( R_i \) is the rate of reaction inside the porous medium (\( \text{mol m}^{-3} \text{s}^{-1} \)). The rates of reaction for \( \text{H}_2\text{O} \) and \( \text{H}_2 \) can be expressed as \( R_{\text{H}_2} = -\left( A J \right)/(2F) \) and \( R_{\text{H}_2\text{O}} = (A J)/(2F) \).

\( N_j \), generally depends on the operating conditions and the microstructure of material. The DGM, was used to develop the expressions for \( N_j \) in this modeling. The mass flux of hydrogen can be determined by the Dusty Gas Model (DGM) as \([8]\).

\[ N_{H_2} = \left( -P/R \right) \left( (1-\alpha y_{H_2}) \right) \left( D_{H_2, H_2}^k \right)^{-1} \left( \frac{dy_{H_2}}{dx} \right) \]  

(10)

where \( \alpha = 1 - \sqrt{M_{H_2}/M_{H_2\text{O}}} \). The parameters \( M_{H_2} \) and \( M_{H_2\text{O}} \) are the molecular weight of \( \text{H}_2 \) and \( \text{H}_2\text{O} \), respectively. The \( D_{H_2, H_2}^k \) and \( D_{H_2\text{O}-H_2}^k \) are the effective Knudsen diffusion coefficient of \( \text{H}_2 \) and the effective binary diffusion coefficient of \( \text{H}_2-\text{H}_2\text{O} \) \([6]\) respectively.

By substituting Eq. (10) into Eq. (9), the governing equation of \( \text{H}_2 \) concentration becomes

\[ \alpha \frac{d^2 y_{H_2}}{dx^2} + \left( \frac{1}{D_{H_2, H_2}^k} \right) \left( \frac{dy_{H_2}}{dx} \right) - \frac{A_J y_{H_2} RT}{2FP} \left( \frac{1}{D_{H_2}^k} + \frac{1 - \alpha y_{H_2}}{D_{H_2\text{O}-H_2}^k} \right) = 0 \]  

(11)

Equation (11), which can be solved by involving the following initial conditions. In Eqs. (12) and (13), Dalton’s law of an ideal gas, \( y_{H_2} = P_{H_2}/P_{H_2}^0 \) and the initial conditions are following as:

\[ \text{IC.1} : y_{H_2} \bigg|_{x=0} = y_{H_2\text{, bulk}} \]  

(12)

\[ \text{IC.2} : \left. \frac{dy_{H_2}}{dx} \right|_{x=0} = -\frac{RT J_{\text{total}}}{2FP} \left( \frac{1 - \alpha y_{H_2, \text{bulk}}}{D_{H_2, H_2}^k} + \frac{1}{D_{H_2}^k} \right) \]  

(13)

the mole fraction of \( \text{H}_2\text{O} \) can be obtained as:

\[ y_{H_2\text{O}} = 1 - y_{H_2} \]  

(14)

In the above equations are dependent of depth in the vertical direction (\( x \)). An iterative scheme is used to solve the non-linear equations. Therefore, the differential equation was solved in MATLAB.

2.4. Mass transfer equations on cathode side

Only the oxygen becomes part of the electrochemical reaction at the cathode. The transport of \( \text{O}_2 \) can be
described by the self-diffusion mechanism,
\[
\frac{dP_{O_{2}}}{dx} = \frac{RT_{\text{eff}} P_{C}}{4FD_{\text{eff}} P_{C}} \left( P_{C} - (D^{\text{eff}}_{O_{2}, L} / (D^{\text{eff}}_{O_{2}, L} + D^{\text{eff}}_{O_{2}, S})) \right) \cdot P_{O_{2}}
\]  
(15)
where \( P_{O_{2}} \) is partial pressure of oxygen at the cathode sites. The boundary condition for the transporting \( O_{2} \) in Eq. (15) is \( P_{O_{2}} = P_{O_{2}}^{0} \) at \( x = 0 \). From Dalton’s law of an ideal gas can be known oxygen mole fraction distribution throughout cathode with the relation as \( y_{O_{2}} = \frac{P_{O_{2}}}{P_{O_{2}}^{0}} \).

2.5. Voltage and current distribution

In this model the electrochemical reaction zones are assumed to occur at the localized three phase boundary (TPB). In the present model the TPB was assumed to be along the whole electrode thickness because the ion and electron conducting particles are treated as shape as columnar along the electrode. In this model, only hydrogen fuel and the oxygen in air was considered. The electrode electrochemical reactions are shown below:

Anode electrochemical reaction:
\[
H_{2} + O^{2-} \rightarrow H_{2}O + 2e^{-}
\]
(16)

Cathode electrochemical reaction:
\[
\frac{1}{2}O_{2} + 2e^{-} \rightarrow O^{2-}
\]
(17)

Overall electrochemical reaction:
\[
H_{2} + \frac{1}{2}O_{2} \rightarrow H_{2}O \ (\text{gas})
\]
(18)

At the anode three phase boundary (TPB):

Electronic charge:
\[
\nabla \cdot (\sigma_{e, a}^{\text{eff}} \nabla \phi_e) = -R_a
\]
(19)

Ionic charge:
\[
\nabla \cdot (\sigma_{i, a}^{\text{eff}} \nabla \phi_i) = R_a
\]
(20)

where \( \sigma_{e, a}^{\text{eff}} \) and \( \sigma_{i, a}^{\text{eff}} \) are the effective electronic conductivities and effective ionic conductivities for porous anode, which are defined as equation below [9]

\[
\sigma_{e, a}^{\text{eff}} = \varphi \left( \frac{(1 - \varepsilon)}{\tau} \right) \left( \left( 9.5 \times 10^{7} / T \right) \exp \left( -1150 / T \right) \right)
\]
(21)

\[
\sigma_{i, a}^{\text{eff}} = (1 - \varphi) \left( \frac{(1 - \varepsilon)}{\tau} \right) \left( 3.34 \times 10^{7} \ exp \left( -10300 / T \right) \right)
\]
(22)

\( R_a \) is volumetric current densities produced in the anode TPB due to \( H_{2} \) oxidation by Butler - Volmer equations:

\[
R_a = A J_{0, a}^{H_{2}} \left( c_{H_{2}} / c_{H_{2, ref}} \right)^{\gamma_{H_{2}}} \left( \exp \left( \left( anF\eta_a \right) / \left( RT \right) \right) - \exp \left( \left( \left( 1 - \alpha \right)nF\eta_a \right) / \left( RT \right) \right) \right)
\]
(23)

\( J_{0, a}^{H_{2}} \) is reference exchange current densities for \( H_{2} \) oxidation at the reference concentrations \( c_{H_{2, ref}} \), \( \alpha \) is charge transfer coefficient uses the value of 0.5, \( R \) is the universal gas constant equal to 8.314 J mol\(^{-1}\) K\(^{-1}\), \( T \) is cell operating temperature (K), \( n \) is number of electrons participating in the electrochemical reaction and \( \eta_a \) is anode activation overpotenetials defined as:

\[
\eta_a = \phi_i - \phi_e
\]
(24)

And at the cathode three phase boundary (TPB):

Electronic charge:
\[
\nabla \cdot (\sigma_{e, c}^{\text{eff}} \nabla \phi_e) = R_c
\]
(25)

Ionic charge:
\[
\nabla \cdot (\sigma_{i, c}^{\text{eff}} \nabla \phi_i) = -R_c
\]
(26)

where \( \sigma_{e, c}^{\text{eff}} \) and \( \sigma_{i, c}^{\text{eff}} \) are the effective electronic conductivities and the effective ionic conductivities for porous cathode, which are defined as below [14]:

\[
\sigma_{e, c}^{\text{eff}} = \varphi \left( \frac{(1 - \varepsilon)}{\tau} \right) \left( 4.2 \times 10^{7} / T \exp \left( -1200 / T \right) \right)
\]
(27)

\[
\sigma_{i, c}^{\text{eff}} = (1 - \varphi) \left( \frac{(1 - \varepsilon)}{\tau} \right) \left( 3.34 \times 10^{7} \ exp \left( -10300 / T \right) \right)
\]
(28)

\( R_c \) is volumetric current densities produced in cathode TPB due to \( O_{2} \) reduction by Butler - Volmer equations:
\[
R_c = A_c J_{O_2}^{0,\text{ref}} \left( c_{O_2} / c_{O_2,\text{ref}} \right)^{ \gamma_{O_2} } \left\{ \exp \left( \frac{ \alpha nF \eta_c }{ (RT) } \right) - \exp \left( - \left( (1 - \alpha) nF \eta_c \right) / (RT) \right) \right\} \tag{29}
\]

\( J_{O_2}^{0,\text{ref}} \) is reference exchange current densities for \( O_2 \) reduction at the reference concentrations \( c_{O_2,\text{ref}} \) and \( \eta_c \) is cathode activation overpotenalties defined as:

\[
\eta_c = \phi_e - \phi_i \tag{30}
\]

The electrolyte layer in a SOFC is fully dense with no porosity. A equation governing migration of oxide ion in electrolyte layer is determined by Ohm’s Law and relation between ionic current density and ionic potential.

\[
\nabla \cdot ( \sigma_e \nabla \phi_i ) = 0 \tag{31}
\]

where \( \sigma_e \) is ionic conductivity of electrolyte [14].

\[
\sigma_e = 3.34 \times 10^4 \exp \left( -10300/T \right) \tag{32}
\]

2.6. The boundary conditions

The voltage at the anode and cathode current collectors, \( \varphi_e \) is specified. Current density (\( i \)) at the interface between electrodes and electrolytes; \( i_e = 0 \) and \( i_i = i \) note that \( i_e \) is electronic current density, \( i_i \) is ionic current density.

| Table 1. Standard parameters used in the SOFC microscopic model calculation. |
|---------------------------------|---------------|
| **Operating temperature, \( T \) (\(^\circ\)C)** | **500 - 800** |
| Operating pressure, \( P \) (atm) | 1.0 |
| \( H_2 \) Initial mole fraction, \( y_{H_2}^0 \) | 0.95 |
| \( H_2O \) Initial mole fraction, \( y_{H_2O}^0 \) | 0.05 |
| \( O_2 \) Initial mole fraction, \( y_{O_2}^0 \) | 0.21 |
| Anode electrode layer thickness, \( t_{an} \) (\( \mu \)m.) [16] | 0.7 |
| Cathode electrode layer thickness, \( t_{cat} \) (\( \mu \)m.) [16] | 0.7 |
| Porosity of anode, \( e_{an} \) | 0.5 |
| Porosity of cathode, \( e_{cat} \) | 1.4 |
| Si-substrate thickness, \( t_s \) (\( \mu \)m.) [3] | |
| Porosity of Si-substrate, \( e_s \) [3] | 0.5 |
| Tortuosity of Si-substrate, \( \tau_s \) [3] | 1.4 |
| Radius of electronic conducting particle, \( r_{e} \) (nm.) [16] | 10 |
| Radius of ionic conducting particle, \( r_{i} \) (nm) [12] | 10 |
| Contact angle between \( e \) and \( O^2- \) conducting particles, \( \theta (\,^\circ) \) [10] | 15 |
| Volumetric fraction of electronic conducting particle [10] | 0.5 |
| Volumetric fraction of ionic conducting particle [5] | 0.5 |
| Reference \( H_2 \) concentration, \( c_{H_2,\text{ref}} \) (mol m\(^{-3}\)) [14] | 10.78 |
| Reference \( O_2 \) concentration, \( c_{O_2,\text{ref}} \) (mol m\(^{-3}\)) [14] | 2.38 |
Reference exchange current density for H₂ oxidation, 2H₀,refJ (A m⁻²) [14] 1320
Reference exchange current density for O₂ reduction, 2O₀,refJ (A m⁻²) [14] 400
Reaction order for H₂ oxidation, γₜ₁ [14] 0.5
Reaction order for O₂ reduction, γ₀₂ [14] 0.5

3. Model validation

This work validated the results with an available experimental data by Barnett et al. [15]. By using parameters are listed in Table 2.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
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<tr>
<td>Total pressure, P (atm)</td>
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<td>Inlet fuel compositions, γᵣ₁, γᵣ₂, η₁, η₂</td>
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<tr>
<td>Inlet air composition, γₒ₁, γₒ₂</td>
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<td>Anode electrode layer thickness, tₑ₁ (µm.)</td>
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<td>Cathode electrode layer thickness, tₑ₂ (µm.)</td>
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<td>Electrolyte thickness, tₑₑ (µm.)</td>
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<td>Porosity of anode and cathode, ε</td>
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<tr>
<td>Tortuosity of anode and cathode, τ</td>
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<tr>
<td>Contact angle between e⁻ and O₂⁻ conducting particles, θ (°) [10, 14]</td>
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<tr>
<td>Si-substrate thickness, tₛ (µm.) [3]</td>
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<tr>
<td>Porosity of Si-substrate, εₛ [3]</td>
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<tr>
<td>Tortuosity of Si-substrate, τₛ [3]</td>
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<tr>
<td>Radius of electronic conducting particle, rₑ (nm.) [16]</td>
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<td>Radius of ionic conducting particle, rᵢ (nm) [16]</td>
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<tr>
<td>Volumetric fraction of electronic conducting particle, φ [10]</td>
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<td>Volumetric fraction of ionic conducting particle, 1-φ [10]</td>
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<tr>
<td>Reference H₂ concentration, cₑ₁,ref (mol m⁻³) [14]</td>
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<tr>
<td>Reference O₂ concentration, cₒᵢ,ref (mol m⁻³) [14]</td>
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<td>Reference exchange current density for O₂ reduction, 2O₀,refJ (A m⁻²) [14]</td>
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<tr>
<td>Reaction order for H₂ oxidation, γᵣ₁ [14]</td>
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<tr>
<td>Reaction order for O₂ reduction, γₒ₂ [14]</td>
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</table>
4. Results and discussion

This numerical study was employed to gain an understanding of the coupled mass transfer and electrochemical phenomena in the electrodes of SOFCs. Moreover, parametric analyses were performed to investigate the effects of operating parameters on SOFC performance. The model was considered at steady state. The other input parameters used in this study are displayed in Table 1.

4.1. The effect of electrode particle shape and size on the electrode performance

This section is to optimize the cylindrical particle sizes inside the electrode as shown in Fig. 1 with the objective to maximize the cell performance. This study is motivated by the need to develop a methodology that provides an optimum cylindrical particle size directly from the electrochemical laws and geometrical variables. Some useful dimensionless variables were introduced in order to represent characteristics of cell. Figure 3 shows the effect of cylindrical particle shape on the active surface area. The dimensionless height \( \tilde{h} \) is defined as \( \tilde{h} = \frac{h}{(V_0)^{1/3}} \) and \( V_0 = \pi r^2 h \) is the particle volume that is finite and fixed and the term \( (V_0)^{1/3} \) that is used to non-dimensionalize all of the length geometry. Also, the dimensionless particle radius \( \tilde{r} \) is defined as \( \tilde{r} = \frac{r}{(V_0)^{1/3}} \). The projected views of Fig. 3 are shown in Fig. 4, which illustrates the existence of the optimal geometric shape of electrode particles. Figure 4 is the projection plot between the electrode dimensionless particle radius \( \tilde{r} \) and the dimensionless active surface area of the electrode \( \tilde{A}_\nu \), while Fig. 4 (b) is the projection plot between the dimensionless particle height \( \tilde{h} \) and the dimensionless active surface area of the electrode \( \tilde{A}_\nu \). The maximum electrochemical active surface area occurs when the electrode contains the particles size with the dimensionless particle radius \( \tilde{r} \) of 0.072 and the dimensionless particle height \( \tilde{h} \) of 22.7, providing the maximum dimensionless active surface area \( \tilde{A}_\nu \) of \( 2.8630 \times 10^{19} \). The dimensionless active surface area of an electrode is defined as \( \tilde{A}_\nu = \frac{A_\nu}{(V_0)^{2/3}} \).
Next results are the effect of the cylindrical particle shape and size on the current density. All of the results are in the dimensionless forms. In Fig. 5, the x-axis represents the electrode dimensionless particle radius ($\tilde{r}$), whereas the y-axis represents the electrode dimensionless particle height ($\tilde{h}$) which relate to the dimensionless current density ($\tilde{R}_c$) produced by the electrode electrochemical reaction. Again, the relation in Fig. 5 is projected onto the principal axis as shown in Fig. 6. Figures 6 (a) and (b) show the maximum dimensionless current density ($\tilde{R}_c$) produced by the electrode electrochemical reaction of $1.0175 \times 10^{-3}$ occurs at the dimensionless particle radius ($\tilde{r}$) of 0.0720 and the dimensionless particle height ($\tilde{h}$) of 22.7. The dimensionless current density is defined as shown in Eq. (33) and (34):
\[ \tilde{R}_a = \frac{R_u}{\left(J_{0,ref}^H n_1(V_0)^{2/3}\right)} \]  

\[ \tilde{u}_a = R_a\left(J_{0,ref}^H n_1(V_0)^{2/3}\right) = \left(\frac{\alpha}{c}\right)\left(\frac{c_{H_2}/c_{H_2,ref}}{V_0}\right)^{2/3} \times \exp\left(\frac{\alpha n F \eta_a}{(V_a T)}\right) - \exp\left(-(1 - \alpha)n F \eta_a \right)/\left(\eta_a T\right)\right) \]  

Fig. 5. Dimensionless particle radius ( \( \tilde{r} \) ) and particle height ( \( \tilde{h} \) ) effect on dimensionless current density ( \( \tilde{R}_a \) )

At the optimum particle shape, it will be given the maximum active surface area that means the maximum current density. The high zone of dimensionless current density ( \( \tilde{R}_a \) ) produced by the electrode electrochemical reaction occurs when the dimensionless particle radius ( \( \tilde{r} \) ) is in the range of 0.06 - 0.08 and the dimensionless particle height ( \( \tilde{h} \) ) is in the range of 14 - 28. In the high electrochemical zone, the cylindrical size and height of electrode particles packed to form electrode provides sufficient pore size and number of conduction materials. Thin film deposition techniques as applied to the Micro Solid Oxide Fuel Cells ( \( \mu \) SOFCs) fabrication is an emerging and highly active field of research that is attracting greater and greater attention. At the present time, the thickness of electrodes created by PVD method is nearly 1 µm [3]. For calculation in this work, the typical grain size of 20 nm [3] and the typical thickness of 0.7 µm [16] were used. Therefore, the corresponding particle volume of 2.199×10^{-22} m^3 was selected as our optimization constraint.
Fig. 6. (a) Dimensionless particle radius (\(\tilde{r}\)) and dimensionless current density (\(\tilde{R}_c\)); (b) Dimensionless particle height (\(\tilde{h}\)) and dimensionless current density (\(\tilde{R}_c\)).

Fig. 7. Cylindrical particle radius (r) and height (h) effect on the active surface area of electrode (A_v) when each particle contained inside the electrode has its volume of 2.199\(\times10^{-22}\) m\(^3\). The results shown in Figs. 7 and 8 illustrate the maximum active surface area of 104304 m\(^2\)/m\(^3\) at the particle height of 1.37 \(\mu\)m and radius of 4.34 nm. The regular thickness of the thin film SOFC is normally fabricated at 1.39 \(\mu\)m [3].

Fig. 8. (a) Particle radius (r) and active surface area of electrode (A_v); (b) Particle height (h) and active surface area of electrode (A_v) when each particle contained inside electrode has its volume of 2.199\(\times10^{-22}\) m\(^3\).
5. Conclusion

A mathematical model of a planar SOFC has been developed for a simplified one cell design of a co-flow pattern based on the microscale modeling of multi-physical transport phenomena. The model focuses on the porous silicon-supported thin film SOFC, in which the electrode microstructure is packed by cylindrical shaped ionic and electronic conducting particles. The investigation shows, the optimal size ratio between ion and electron conducting particles is equal to one. For a conventional thin film SOFC, the optimal thickness of the electrode particles in a SOFC film for both anode and cathode sides should be 1370 nm with the optimal radius of cylindrical shaped particles of 4.34 nm.

References