Transport phenomena in solid oxide fuel cell electrodes focusing on heat transfer related to chemical reactions

M Navasa, M Andersson, J Yuan and B Sundén
Department of Energy Sciences, University of Lund, Lund 22100, Sweden
E-mail: Maria.Navasa@energy.lth.se

Abstract. Solid oxide fuel cells (SOFCs) are widely studied for their advantages especially at high temperatures. However, operating at high temperatures represents a high cost due to the strict requirements the materials are expected to fulfill. Thus, the main goal in SOFC research has been to decrease the operating temperature so that the range of available materials is widened and hence, the operating cost can be reduced. In this paper, the different heat sources that contribute to the cell energy balance are presented with strong emphasis on the chemical reactions that take place in SOFCs. The knowledge of which heat sources or sinks taking place and their locations within the SOFC can provide useful information for further design and efficiency improvements.

1. Introduction
Solid oxide fuel cells (SOFCs) are high-temperature electrochemical devices which convert the chemical energy of fuels directly into electrical energy in an environmental friendly and efficient manner. For this reason and due to the depletion of fossil fuels, SOFCs are regarded as promising candidates for energy conversion and thus, for being able to obtain electrical power for our society in an environmental friendly way.

When comparing SOFCs to other current fuel cell types, for example, proton exchange membrane fuel cells (PEMFCs), SOFCs present a number of attractive features. SOFCs are fuel flexible, which means that different fuels apart from pure hydrogen can be used due to the tolerance of carbon monoxide (CO), a fuel as well. Then, short-chain hydrocarbon fuels like methane or ethanol among others can be supplied as fuel to SOFCs. Long-chain hydrocarbons can lead to carbon deposition if no previous treatment is done. Moreover, all components are in solid state (there are no liquid electrolytes like for example in alkaline fuel cells), there are no water management issues, which is the main headache for PEMFCs, and the high quality waste heat produced by SOFCs can be utilized effectively for either combined heat and power or for use in hybrid systems together with gas turbines.

Substantial improvements in performance and durability have been made in the last years in SOFCs mainly due to the advances in manufacturing technology. Although other fuel cells are nowadays more technologically developed, for example, molten carbonate fuel cells, SOFCs are widely considered to be one of the two most promising fuel cells together with PEMFCs.
2. Problem Statement

SOFCs are particularly attractive fuel cells compared to other types as mentioned before and thus, they have become an important area of research and development all over the world in the last years and still nowadays [1].

One of the main characteristics of SOFCs is that they are high-temperature devices. The fact that these cells initially operated at temperatures around 1000°C is due to the material of the electrolyte used, yttria stabilized zirconia (YSZ). This is a ceramic material which becomes conductive to oxygen ions at certain temperatures and non-conductive to electrons as well as the anode and cathode materials. Thus, electrochemical reactions can take place at the electrodes without the need of expensive catalysts. In fact, the anode material (YSZ) is catalytic itself for both the internal reforming and electrochemical reactions that take place. The limited range of the available materials to operate at high temperatures is the major limitation to mass production of SOFCs due to the material cost. Nevertheless, long starting times are required for high temperature SOFCs and thermal control becomes difficult despite the high thermal efficiency and long-term stability. In order to be able to mass produce SOFCs, a substantial reduction in the system cost (cell and stack production processes) is required. One way to reduce the costs is by reducing the material costs and increase the durability of the cells. This can be done by reducing the operating temperature to an intermediate temperature, 600-800°C (IT-SOFC), or even lower than 600°C, (LT-SOFC). When the temperature decreases, the overall performance is reduced because the electrolyte resistance increases and the reactions at the electrodes become inactive [1, 2].

However, it is not just a matter of decreasing the operating temperature as other phenomena must be taken into account as well. As well known, the kinetics of the chemical reactions that take place in SOFCs are temperature dependent and this is also a matter of concern. Thus, it is of big interest to know the relationship between the chemical reactions and the heat transfer phenomena.

The main objective of this article is to describe the major concerns of the chemical reactions in SOFCs relating to thermal issues and thus, describe the major sources for heat transfer in SOFCs. How and where they originate and are located to obtain a detailed model for simulation are important so that the overall cell performance can be improved and the further fuel cell development can be promoted.

3. Chemical reactions: heat transfer effects

SOFCs consist of two porous electrodes (an anode and a cathode) separated by a dense electrolyte and connected into an electrically conducting circuit, see Figure 1. The electrodes must present large reaction sites for the electrochemical reactions having a great number of paths for ion and electron conduction and presenting the appropriate porosity for oxygen, hydrogen and the formed water migration. The required properties for the electrolyte are somehow similar to those required for the electrodes but present some variations. The electrolyte must present a high ionic conductivity, high density, long-term high temperature performance stability and high long-term reliability which means high strength and high durability [3].

One of the major concerns for SOFC technology at the temperatures used nowadays is that the steam reforming (SR) reaction rate is much faster than the electrochemical reaction rate. This fact can be explained by the high nickel (Ni) content which is necessary for the electric conductivity and offers a high number of catalytic sites. The steam reforming reaction (Eq.1) is a highly endothermic reaction ($\Delta H^\circ = 206 \text{ kJ mol}^{-1}$) and thus, consumes energy while the electrochemical reactions produce energy as they are exothermic.
If the steam reforming reaction is faster than the electrochemical, there will be cooling at the inlet of the cell and heating at the outlet resulting in a large temperature gradient in the cell. This temperature gradient can cause thermal stress as well as reduced efficiency [4]. The SR reaction takes place in the anode support layer of the fuel cell (FC) while the electrochemical reactions take place at the three-phase boundaries (TPBs) in the reaction active region or functional layer, see Figure 1.

\[
\text{CH}_4 + \text{H}_2\text{O} \rightleftharpoons \text{CO} + 3\text{H}_2
\]  

(1)

The steam reforming reaction rate needs to be lowered in order to decrease the existing temperature gradients and thus, improve the cell performance. To do so, detailed knowledge of the steam reforming kinetics is required. At present, steam reforming reaction on Ni based catalysts has been widely studied for catalytic reactors because of its industrial importance. However, few studies have been performed for SOFC.

The goal for optimizing the internal reforming reactions for an SOFC is to lower the reaction rate of the steam reforming reaction while maintaining a high electronic conductivity and a high reactivity for the electrochemical reaction. Yet, high reforming reaction rates are still required compared to the electrochemical reaction rates. To reduce the reforming reaction rate, different solutions have been presented [4, 5]:

- Lowering the temperature. The general trend is to lower the operating temperature as SR has a high activation energy (depending on the mechanism 63.3-228 kJ mol\(^{-1}\), Table 1) and the reaction rate decreases rapidly with temperature. The present lower temperature limit for efficient operation is between 650 – 700°C (IT−SOFC) [4, 5] although the current trend is to even decrease it more to 300-600°C (LT−SOFC) by using ceria-based composites as electrolyte [6]. Such low temperatures, close to 300°C, are too low for internal reforming reactions and thus, external reforming is required. The major limitation for decreasing the operating temperature is the ionic conductivity in the electrolyte and thus, the materials used. Different kinetic expressions for the SR reaction over Ni/YSZ anodes have been reported and are shown in Table 1. The different expressions shown seem to vary significantly most probably due to different experimental conditions. Moreover, two types of kinetic expressions are used: power law expressions derived from data fitting from experimental conditions and general Langmuir-Hinshelwood expressions. Furthermore, it was intended to have the same units for the reaction rate in order to be able to compare the different expressions with more precision but the lack of information and the ambiguities with units add difficulty in this task stating that more work needs to be done in this field. Although no activation energy (\(E_A\)) value is shown in expression 5, the stated \(E_A\) value is calculated experimentally by Bebelis et al. [7].

- Reducing the fuel concentration. The fuel concentration can be decreased by recirculating part of the anode exhaust gas, [5].

- Modification of the Ni/YSZ anode or design of other anode materials to decrease the SR activity. Possibility exists to replace some Ni in the anode by copper (Cu) or using...
Cu/CeO$_2$/YSZ among others. The replacement of some Ni particles by Cu seems to be a promising option as it reduces the reforming rate without a significant reduction in the electrochemical reduction. However, more work needs to be done in this field [4, 5].

- Increase the particle size. For the same amount of Ni particles, the surface area decreases for larger Ni particles and thus, there are less active sites. Moreover, if the particle size in the active anode also increases, the TPB, where electrochemical reactions take place, decreases as well. This means that the Ni particle size also influences the electrical conductivity: when the particle size increases, the electrical conductivity decreases [8]. So, increasing the particle size to decrease the SR rate may reduce the cell performance [4]. However, a better alternative is to use functionally graded particle size electrodes. By this way, a large TPB reaction area near the anode-electrolyte can be obtained while avoiding high diffusion losses by using large particles at the electrodes, away from the boundary [9, 10].

Table 1. Steam reforming reaction kinetics reported for SR over Ni/YSZ SOFC anode/anode−supports. $E_A$ in [kJ mol$^{-1}$]

| Expression | $k_0$ | $E_A$ [kC] | $T$ [°C] | $k_0$, k$^{-1}$, k$^+$, k$^-$ | S/C | Ref. |
|------------|-------|------------|---------|-----------------------------|-----|-----|
| $k_0$PC$_H_4$ exp $\left(-\frac{E_A}{RT}\right)$ | 82 | 700–940 | 4274 | 2.6–8 | [11] |
| $k_0$PC$_H_4$H$_2$O exp $\left(-\frac{E_A}{RT}\right)$ | 205 | 600–700 | 30.8 · 10$^1$ | 2–3.5 | [12] |
| $k_0$PC$_H_4$H$_2$O$^{0.35}$ exp $\left(-\frac{E_A}{RT}\right)$ | 95 | 850–900 | 8542 | 1.5–2.5 | [13] |
| $k_{ad}$PC$_H_4$H$_2$O$^{(1.3)}$ exp $\left(-\frac{E_A}{RT}\right)$ | 191 | - | 1.01 · 10$^{-3}$ | - | [14] |
| $k_{ad}$PC$_H_4$H$_2$O$^{(1.3)}$ | 228 | 800–900 | $k_{ad,1073K} = 0.26$ · 10$^{-6}$ | 0–2 | [7] |
| $k_{ad}$PC$_H_4$H$_2$O$^{(1.3)}$ | 63.3 | 650–950 | 498 | 2 | [15] |
| $k_{ad}$PC$_H_4$H$_2$O$^{(1.3)}$ | - | 700–1000 | - | 3–7 | [16] |
| $k_{ad}$PC$_H_4$H$_2$O$^{(1.3)}$ | - | 700–950 | $k_{ad,1073K} = 2.3$ · 10$^{-8}$ | 3 | [17, 18] |
| $k_{ad}$PC$_H_4$H$_2$O$^{(1.3)}$ | - | - | - | - | [19] |

One of the main goals in the fuel cell research is to lower the material cost in order to be able to mass produce SOFC. As seen, the current trend in SOFC development is to decrease the operating temperature. By lowering the operating temperature, other phenomena that take place within the SOFC are also affected. Therefore, the relationship between the chemical and electrochemical reactions with temperature is more than obvious. For this reason, considering heat transfer when performing a numerical simulation of an SOFC is of great interest.

4. Heat transfer in SOFCs affected by various reactions

Different phenomena take place in an SOFC at different length scales. As mentioned, chemical reactions are still the least understood phenomena taking place inside the fuel cell and the need to model at small length scales so that the different chemical species (surface species, ions, etc.) can be distinguished and thus, the existing reaction mechanisms implemented, is more than obvious in order to understand and improve the cell operating conditions if possible. Thus, a good model for the cell microstructure is required. Different models exist based on different time and length scales. Examples are computational fluid dynamics (CFD), Monte Carlo method (MC), Lattice Boltzmann (LB) or coarse-grained molecular dynamics method (CG) among others.

Nevertheless, when modeling chemical reactions, other transport phenomena, like heat transfer, must be taken into account as chemical reactions are strictly bonded to heat transfer, being special contributors to the global energy balance of the fuel cell.
Heat transfer within the whole FC unit cell consists of convection and conduction. Convection occurs between the gas flow and the solid surfaces while conduction takes place in the solid and in the porous parts. Moreover, radiation also takes place for example, within the electrode-electrolyte structure, from the stack to the surrounding environment and surface to surface radiation in the air and fuel channels. Nevertheless, considering radiation in the model adds a higher degree of complexity to the governing equations [20]. However, radiation should be considered if a detailed model is required. Heat generation or consumption is also present. The general heat conduction equation is used to calculate the temperature distribution for the solid phase in the porous electrodes [21]:

$$\nabla \left( -k_s \cdot \nabla T_s \right) = Q_s$$  \hspace{1cm} (2)

where \(Q_s\) is the heat source, such as the heat transfer between the gas and the solid phases, and the heat generation due to the ohmic polarization and the internal reforming reactions.

The temperature for the gas phase in the porous electrodes (also valid for the air and fuel channels) is governed by [21]:

$$\nabla \left( -k_g \cdot \nabla T_g \right) = Q_g - \rho_g c_{p,g} u \nabla T_g$$  \hspace{1cm} (3)

where \(k_g\) is the gas thermal conductivity and \(Q_g\) is the heat transfer between the gas and the solid phases which is calculated as follows:

$$Q_g = -Q_s = h_v (T_g - T_s) = Avh_{s,g,por} (T_g - T_s)$$  \hspace{1cm} (4)

The subscript \(s\) refers to solid, \(g\) to gas and \(por\) to porous. All previous equations are based on the local temperature non-equilibrium (LTNE) approach where the temperature from the gas- and solid-phases are not assumed to be locally the same as in the local temperature equilibrium (LTE)[22].

It is very important to know where exactly the heat sources in the fuel cell are generated or consumed when modeling at the microscale region (nm and a few \(\mu m\)) in order to obtain an accurate temperature profile in the fuel cell.

There are different mechanisms of heat generation or consumption taking place in an SOFC. Basically, all the heat sources within an SOFC are due to the electrochemical and chemical reactions in an SOFC. Thus, knowledge about these sources is of interest as it can provide information for the overall performance, possible mechanical stresses, etc. The mentioned heat sources will be described in the following sections.

4.1. Methane steam reforming and water-gas shift reforming reactions

SOFCs using methane as fuel need to undergo a reformation process of the fuel as methane cannot be directly used in the FCs. Thus, by reforming methane, carbon monoxide and hydrogen are produced which can now be directly used as fuel. The reforming process can be done internally or externally but SOFCs present the possibility to have internal reforming reaction of methane due to the high operating temperatures. The methane steam reforming (MSR) reaction, Eq. 1, is a highly endothermic reaction \(\Delta H_{1273K} = 227.6\text{ kJ mol}^{-1}\) and thus, introduces a high sink of heat into the cell components involved in the process [23]. The steam reforming reaction of methane takes place in the anode of the fuel cell as it requires the Ni particles which act as catalysts of the reaction. Thus, the steam reforming reaction strictly takes place at the Ni particles’ surface.

As the SR reaction is endothermic, the heat absorbed or consumed by the reaction in \(W_m\) can be determined by the reaction rate and the enthalpy of reaction. Different expressions for the reaction rate can be found in Table 2.

$$Q_{MSR}^{w} = r_{MSR} \Delta H_{MSR} A v_m$$  \hspace{1cm} (5)
Anyhow, the SR reaction of methane is accompanied by the water-gas shift (WGS) reaction. The WGS is slightly exothermic ($\Delta H_{1273K} = -31.8 \text{ kJ mol}^{-1}$) and it is usually assumed to be in equilibrium as it is a much faster reaction than the SR reaction [17, 23–26].

$$\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2 \quad (6)$$

The heat generated by the WGS reaction can be expressed as follows.

$$Q''_{WGS} = r_{WGS}\Delta H_{WGS}A\nu_{an} \quad (7)$$

The equilibrium approach can be modeled as [25].

$$r_{WGS} = k_{WGS}P_{\text{CO}} \left( 1 - \frac{P_{\text{CO}}P_{\text{H}_2}}{K_{e,WGS}P_{\text{H}_2}\text{O}} \right) \quad (8)$$

$$K_{e,WGS} = \exp \left( \frac{4276}{T} - 3.961 \right) \quad (9)$$

where $k_{WGS}$ is the reaction rate constant and can be calculated according to Haberman and Young [25] and $K_{e,WGS}$ is the equilibrium constant for the WGS reaction.

### 4.2. Entropy changes due to the electrochemical reactions

The oxidation of hydrogen is the driving reaction of the energy conversion in an SOFC device. This process can be written as a general reaction as follows:

$$\text{H}_2 + \frac{1}{2}\text{O}_2 \rightleftharpoons \text{H}_2\text{O} \quad (10)$$

Nevertheless, this general electrochemical reaction consists of two semi-reactions that take place in different parts of the fuel cell. The reduction of oxygen, Eq. 11, takes place in the active layer of the triple-phase boundaries (TPBs) of the cathode while the oxidation of hydrogen, Eq. 12, takes place at the anodic TPBs.

$$\frac{1}{2}\text{O}_2 + 2e^- \rightarrow \text{O}^2^- \quad (11)$$

$$\text{H}_2 + \text{O}^2^- \rightarrow \text{H}_2\text{O} + 2e^- \quad (12)$$

Although the global electrochemical reaction is highly exothermic ($\Delta H_{1273K} = -250 \text{ kJ mol}^{-1}$), only a part can be converted into electric work. The maximum work that can be obtained is given by the Gibbs free energy ($\Delta G$).

$$\Delta G_{ER} = \Delta H_{ER} - T\Delta S_{ER} \quad (13)$$

where the subscript $ER$ refers to electrochemical reaction and the term ($-T\Delta S_{ER}$) is the change of entropy released as heat due to the electrochemical reaction.

Despite the fact that most models assume that the heat associated with the general electrochemical reaction is assigned to the anodic TPB, this heat is generated at the two different electrodes and in different amounts. Therefore, if a detailed model is desired, one should take into account the entropy changes for each semi-reaction and thus, calculate the heat generation due to the electrochemical reaction for each electrode as follows. However, one must consider the reaction sites as infinitely thin layers and thus, the released heat per unit volume [$W/m^3$], by considering TPBs reaction area, can be calculated [23].

$$Q''_{ER} = \frac{j}{2F} \left( -T\Delta S_{ER} \right) A\nu_{an,cat} \quad (14)$$

where $j$ is the local current density. Moreover, Fischer et al. [23] showed that the amounts of heat released or absorbed by the semi-reactions are the most important sources or sinks of heat in the fuel cell.
4.3. **Concentration polarizations**

Concentration polarizations are those polarizations associated with the variation of concentration of the critical species due to mass transfer processes. There are basically two main sources due to mass transport: transport of reactants and products through the electrodes and diffusion between the bulk flows and cell surfaces. Thus, concentration polarizations are highly dependent on the diffusion length, the pore volume percentage of the components as well as the gases involved [27]. Therefore, these concentration polarizations give a surplus heat at the anodic and cathodic reaction sites which can be calculated as follows [23].

\[
Q_{\text{conc}}^{m, an, cat} = j \eta_{\text{conc}}^{an, cat} A_{\text{e}, an, cat}
\]

(15)

4.4. **Activation polarizations**

The activation polarizations can be considered as the extra potential needed in order to overcome the activation energy \(E_A\) or energy barrier of the rate-determining step to a value that the reaction proceeds at a desired rate [22, 27]. The activation polarizations are described by the Butler-Volmer equation [22, 23, 27].

\[
\dot{j} = j_0 \left\{ \exp \left( \frac{n_e F \eta_{\text{act}}^{an, cat}}{RT} \right) - \exp \left( - \frac{(1 - \alpha) n_e F \eta_{\text{act}}^{an, cat}}{RT} \right) \right\}
\]

(16)

where \(n_e\) is the number of electrons participating in the reaction, \(\alpha\) the charge transfer coefficient, usually assumed to be 0.5 in FCs and \(j_0\) the exchange current density.

The heat generated by these irreversible polarizations is released at the anodic and cathodic catalyst particle surfaces. Thus, the heat source will be \([W/m^3]\) [23].

\[
Q_{\text{act}}^{m, an, cat} = j \eta_{\text{act}}^{an, cat} A_{\text{e}, an, cat}
\]

(17)

4.5. **Ohmic polarizations**

The ohmic polarizations are due to the joule heating effect or, in other words, they are due to the resistance to ion transfer through the electrolyte (YSZ), electron transfer through the electrodes (Ni or strontium doped lanthanum manganate, LSM) and current collectors and also by the contact resistance between the different cell components. Thus, they are characteristic for the solid parts of the FC and they lead to a release of heat which can be determined by the local current density and the material conductivity [22, 23, 27].

\[
Q_{\Omega}^{m} = \frac{1}{\sigma} \dot{j}^2
\]

(18)

where \(Q_{\Omega}^{m}\) is the local heat source \([W/m^3]\).

4.6. **Comparison of different heat sources**

In Table 2, the different kinds of heat generation or consumption within SOFCs are summarized. Moreover, in the last column, the percentage contributed by each one in absolute values is shown. The sum of all contributions adds up to 100%. These values are estimated for the model used by Andersson et al. [28], in which reforming reactions take place through the whole cell operating a 30% pre-reformed natural gas as fuel.

The results show that the main contribution to heat generation or consumption is by the electrochemical reactions. It must be pointed out that this is the net contribution from both semi-reactions, that is why it is considered as a heat source (positive values) because, as mentioned previously, the different semi-reactions take place at different electrodes (one being endothermic and the other exothermic). Nevertheless, still electrochemical reactions are the main contributors. The second most important is the methane steam reforming reaction, which
is the heat sink of the SOFC as it is a strong endothermic reaction. Thus, as electrochemical and reforming reactions are the main contributors, it is reasonable that the major concerns of nowadays technology are that the SR reaction is much faster than the electrochemical reaction and the need of lowering the SR reaction rate. Activation polarizations are quite significant as they are directly related to the chemical reactions. The contribution from the WGS reaction and the ohmic polarizations are quite similar while the contribution from the concentration polarizations is less than 1%.

Table 2. Mechanisms and relative contribution of specific reactions to the total heat (source or sink) in SOFCs

| Mechanism                  | Symbol | Location          | Expression                                                                 | Heat source/sink | % Relative contribution |
|----------------------------|--------|-------------------|---------------------------------------------------------------------------|------------------|--------------------------|
| MSR reaction               | $Q_{MSR}^\prime$ | anodic active layer | $r_{MSR}\Delta H_{MSR}Ae^{an}$                                          | sink             | 27                       |
| WGS reaction               | $Q_{WGS}^\prime$ | anodic active layer | $r_{WGS}\Delta H_{WGS}Ae^{an}$                                          | source           | 6                        |
| Electrochemical reaction   | $Q_{ER}^{an,cat}$ | active layer electrodes’ TPBs | $J_{ER}^{an,cat} \Delta S_{ER}^{an,cat}$                                | source           | 47                       |
| Concentration polarizations| $Q_{conc}^{an,cat}$ | electrodes’ reaction sites | $j_{conc}^{an,cat} A_{an,cat}$                                         | source           | < 1                      |
| Activation polarizations   | $Q_{act}^{an,cat}$ | electrodes’ reaction sites | $j_{act}^{an,cat} A_{an,cat}$                                         | source           | 16                       |
| Ohmic polarizations        | $Q_{V}$   | solid cell components | $J_{V}$                                                                 | source           | 3                        |

5. Conclusions

The research done lately in the FC field has allowed a decrease in the operating temperature of SOFCs. This has resulted in a big gain for SOFCs as internal reforming of natural gas is possible, cheaper materials can be used for the FC and also higher stability of the overall fuel stack. This is indeed an important path for improving SOFC performance to increase the future potential market.

Special attention has been given to the kinetics of the internal reforming reaction as it is believed to be one of the main issues for improving the SOFC performance. Different kinetic expressions based on the overall reaction schemes have been found in the literature for SR in Ni-YSZ catalysts on SOFC anodes. However, these expressions differ ones from each other making comparison difficult as the conditions they are derived from are also different.

Moreover, the different heat sources that take place within an SOFC have been described together with the place at which they are located as well as their relationship with the chemical and electrochemical reactions in an SOFC. From the different heat sources, the heat originated or consumed due to the electrochemical reactions at the two electrodes is the main contributor followed by the steam reforming reaction.

In order to perform a detailed simulation of an SOFC, heat transfer phenomena must be taken into account as well as a detailed reaction mechanism for each reaction. If a detailed heat transfer analysis is implemented, with special details on where the heat sources are located, detailed reaction mechanisms for the different chemical reactions are also required. This means modeling probably at nanometer scales and the computational cost may be increased. However, it is a good chance for obtaining a detailed model of the chemistry and temperature distribution so that the SOFC performance can be further improved.
Nomenclature

| Symbol | Description |
|-------|-------------|
| $A_v$ | Active surface area to volume ratio, $[m^2/m^3]$ |
| $C_p$ | Specific heat at constant pressure, $[kJ/kg-K]$ |
| $E_A$ | Activation energy, $[kJ/mol]$ |
| $F$ | Faraday constant, $[sA/mol]$ |
| $\Delta G$ | Gibbs free energy of reaction, $[kJ/mol]$ |
| $h$ | Heat transfer coefficient, $[W/m^2K]$ |
| $\Delta H$ | Enthalpy change of reaction, $[kJ/mol]$ |
| $j$ | Current density, $[A/m^2]$ |
| $k$ | Thermal conductivity, $[W/mK]$ |
| $k_i$ | Reaction rate constant, $[mol^3Pa^{-2}s^{-1}]$ |
| $K_e$ | Equilibrium constant, dimensionless |
| $n_e$ | Number of electrons, dimensionless |
| $P_i$ | Partial pressure, [bar] or [Pa] |
| $Q$ | Heat flow, [W] |
| $r$ | Reaction rate, mainly $[mol^2m^{-2}s^{-1}]$ |
| $R$ | Gas constant, $[J/molK]$ |
| $\Delta S$ | Entropy of reaction, $[J/molK]$ |
| $T$ | Temperature, $[^\circ C]$ or [K] |
| $u$ | Velocity vector, $[m/s]$ |

Greek symbols

| Symbol | Description |
|-------|-------------|
| $\alpha$ | Charge transfer coefficient, dimensionless |
| $\eta$ | Voltage loss, [V] |
| $\rho$ | Density, $[kg/m^3]$ |
| $\sigma$ | Conductivity, $[S/m]$ |

Superscripts

| Symbol | Description |
|-------|-------------|
| $an$ | Anode |
| $cat$ | Cathode |
| $0$ | Standard conditions |
| $m$ | Per unit volume |

Subscripts

| Symbol | Description |
|-------|-------------|
| $act$ | Activation polarizations |
| $conc$ | Concentration polarizations |
| $ER$ | Electrochemical reaction |
| $g$ | Gas |
| $i$ | Gas species |
| $por$ | Porous |
| $\Omega$ | Ohmic |
| $0$ | Standard conditions |

Acknowledgments

The financial support from the European Research Council (ERC-226238-MMFCs) and the Swedish Research Council (VR-621-2010-4581) is gratefully acknowledged.

References

[1] Kawamoto H 2008 Sci. Technol. Trends 47 52–70
[2] Nielsen J, Jacobsen T and Wandel M 2011 Electrochim. Acta 56 7963–7974
[3] Services E T 2004 Fuel Cell Handbook 7th ed (U.S. Dep. Energy Office of Fossil Energy Nat. Energy Technol. Lab.)
[4] Mogensen D, Grunwaldt J D, Hendriksen P V, Dam-Johansen K and Nielsen J U 2011 J. Power Sources 196 25–38
[5] Andersson M, Paradis H, Yuan J and Sundén B 2011 Int. J. Energ. Res. 35 1340–1350
[6] Zhu B 2006 Int. J. Energy. Res. 30 895–903
[7] Bebelis Zeritis T N 2000 Ind. Eng. Chem. Res. 39 7
[8] Simwonis D, Tietz F and Stöver D 2000 Solid State Ionics 132 241–251
[9] Liu L, Flesner R, Kim G Y and Chandra A 2012 Fuel Cells 12 97–108
[10] Ni M, Leung M K H and Leung D Y C 2007 Chem. Eng. Technol. 30 587–592
[11] Achenbach E and Riensche E 1994 J. Power Sources 52 283–288
[12] Leinfelder R 2004 Reaktionskinetische untersuchung zur methan-damp-reformierung und shift-reaktion an anoden oxidkeramischer brenstoffzellen Doctoral dissertation, Der Technischen Fakultät der Universität Erlangen-Nürnberg

[13] Ahmed K and Foger K 2000 Catal. Today 63 479–487

[14] Yakabe H, Ogiwara T, Hishinuma M and Yasuda I 2001 J. Power Sources 102 144–154

[15] Boder M and Dittmeyer R 2006 J. Power Sources 155 13–22

[16] Peters R, Dahl R, Klüttgen U, Palm C and Stolten D 2002 J. Power Sources 106 238–244

[17] Lehnert W, Meusinger J and Thom F 2000 J. Power Sources 87 57–63

[18] Drescher I, Lehnert W and Meusinger J 1998 Electrochim. Acta 43 3059–3068

[19] Drescher I 1999 Kinetik der Methan-Dampf-Reformerung Doctoral dissertation, Forschungszentrums Jülich

[20] Damm D L and Fedorov A G 2005 J. Power Sources 143 158–165

[21] Sohn S, Nam J H, Jeon D H and Kim C J 2010 Int. J. Hydrogen Energ. 35 11890–11907

[22] Andersson M 2011 Solid Oxide Fuel Cell Modeling at the Cell Scale Focusing on Species, Heat, Charge and Momentum Transport as well as the Reaction Kinetics and Effects Doctoral dissertation, Lund University

[23] Fischer K and Seume J R 2009 J. Fuel Cell Sci. Technol. 6 011002

[24] Klein J M, Bultel Y, Georges S and Pons M 2007 Chem. Eng. Sci. 62 1636–1649

[25] Haberman B A and Young J B 2004 Int. J. Heat Mass Transfer 47 3617–3629

[26] Aguiar P, Adjiman C S and Brandon N P 2004 J. Power Sources 138 120–136

[27] Hajimolana S A, Hussain M A, Daud W M A W, Soroush M and Shamiri A 2011 Renew. Sust. Energ. Rev. 15 1893–1917

[28] Andersson M, Yuan J and Sundén B 2012 International Journal of Heat and Mass Transfer 55 773–788