COMPUTATIONAL PREDICTIONS OF CELL EFFICIENCY AND FUEL UTILIZATION AS A FUNCTION OF FUEL PROCESSING AND CELL VOLTAGE

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ABSTRACT

This paper presents two computational models that explore operating conditions for SOFC systems. The operating efficiency, defined as the ratio of electrical output to the potential heating value of fully oxidizing the fuel stream, depends strongly on operating voltage. A thermodynamic model predicts maximum possible efficiency and fuel utilization, which are independent of the cell architecture, but depend on fuel composition, temperature, and pressure. The model is used to map maximum efficiency for fuel mixtures of methane-steam, methane-air, and hydrogen-carbon-monoxide. A second model, which includes internal polarization losses, is used to determine cell dimensions needed to achieve certain efficiencies.

INTRODUCTION

Numerous foregoing studies have concentrated on fuel-cell efficiency, including hydrocarbon fuels and co-generation opportunities (1-3). Using two different models, this paper explores the maximum efficiency possible for a range of fuel mixtures, operating temperatures, and cell voltages. The models account for fuel utilization, which has an important influence on efficiency. The net cell efficiency may be represented as

$$\varepsilon = \frac{W_e}{Q_{in}} = \frac{\int iE_{cell} dA}{m_{in} \Delta h_{in}}$$

[1]

where $W_e$ is the electrical work output and $Q_{in}$ is the heat released upon full oxidation of the inlet fuel stream. The inlet fuel mass flow rate is $m_{in}$ and $\Delta h_{in}$ is the specific enthalpy associated with completely oxidizing the fuel stream. The electrical work is the product of the current density $i$ and operating voltage $E_{cell}$, integrated over the active membrane-electrode assembly (MEA) area.

It is useful to think of the net efficiency as a product of three contributing efficiencies (4)

$$\varepsilon = \varepsilon_e \varepsilon_r \varepsilon_u$$

[2]
where $\varepsilon_R$ is the reversible efficiency, $\varepsilon_V$ is a part-load efficiency, and $\varepsilon_U$ is the fuel utilization. The reversible efficiency

$$\varepsilon_R = \frac{\Delta G}{\Delta H} = 1 - T \frac{\Delta S}{\Delta H},$$

is determined thermodynamically from the change in molar enthalpy $\Delta H$ and free energy $\Delta G$ associated with a global electrochemical oxidation reaction. As the operating voltage approaches the open-circuit potential, the reversible efficiency can approach 100%. The part-load (or voltage) efficiency is the ratio of the cell operating voltage and the open-circuit voltage (Nernst potential),

$$\varepsilon_V = \frac{E_{\text{cell}}}{E_{\text{ocv}}},$$

The fuel utilization is written as

$$\varepsilon_U = 1 - \frac{\dot{m}_{\text{out}} \Delta h_{\text{out}}}{\dot{m}_{\text{in}} \Delta h_{\text{in}}},$$

where the “in” and “out” refer to the inlet and outlet of the fuel cell. The $\Delta h$ refers to the specific enthalpy associated complete oxidation of any available fuels. This definition thus accounts for the energy content of any remaining fuels (or fuel byproducts) that leave in the fuel-cell exhaust.

**THERMODYNAMIC EFFICIENCY MODEL**

The thermodynamic analysis begins with a single general global-oxidation reaction as

$$v_f \left( \sum_{k=1}^{K} n_{f,k} \chi_k \right) + v_o \left( \sum_{k=1}^{K} n_{o,k} \chi_k \right) \Leftrightarrow \sum_{k=1}^{K} \nu^f \chi_k + \sum_{k=1}^{K} \nu^o \chi_k,$$

The seemingly complicated nomenclature is needed to retain generality in the fuel and oxidizer mixtures (5). Gas-phase species are represented by $\chi_k$, with $\nu$ representing various stoichiometric coefficients. The fuel (anode channel) and oxidizer (cathode channel) molar compositions entering the cell are represented by $n_{f,k}$ and $n_{o,k}$. For example, a fuel stream that is 60% methane and 40% steam would have $n_{f,\text{CH}_4} = 0.6$ and $n_{f,\text{H}_2\text{O}} = 0.4$. The product stoichiometric coefficients $\nu^o$ are subscripted as either “f” or “o” to designate the channel into which a product species appears (e.g., for a proton-conducting membrane electrochemical reaction delivers $\text{H}_2\text{O}$ into the cathode channel whereas SOFC delivers $\text{H}_2\text{O}$ into the anode channel). The reaction can be stated more
compactly as $\sum_{k=1}^{K} \nu_{i,k}^f \chi_{k} \iff \sum_{k=1}^{K} \nu_{i,k}^e \chi_{k}$ with $\nu_{i,k}^f = \nu_{i,k}^f n_{i,k} + \nu_{i,k}^e n_{o,k}$ and $\nu_{i,k}^e = \nu_{i,k}^e n_{o,k} + \nu_{i,k}^e n_{o,k}^r$. By way of example, consider a fuel mixture of 50% CH$_4$ and 50% air in an SOFC with air as the cathode-side oxidizer. The global reaction is stated as

$$\nu_{i,k}^f [0.5CH_4 + 0.5(0.21O_2 + 0.79N_2)] + \nu_{i,k}^e [0.21O_2 + 0.79N_2] \Rightarrow$$

$$\nu_{e,h_{\text{CO}_2}H_2O + \nu_{e,\text{CO}_2}CO_2 + \nu_{e,N_2}N_2}^e$$

[7]

The implementation software is written to determine the stoichiometric coefficients needed to balance the global reaction.

The number of electrons transferred by the global electrochemical reaction is determined from the half-cell reactions. It can be calculated as

$$n_e = \sum_{k=1}^{K} \nu_{i,k}^f z_{i,k} - \sum_{k=1}^{K} \nu_{i,k}^e z_{o,k},$$

where $z_{i,k}$ and $z_{o,k}$ are the charges associated with each fuel and oxidizer species. For example, $z_{CH_4} = 8$ and $z_{O_2} = 4$.

Assuming the global reaction goes to completion within the cell, the net electric current produced can be denoted as $I_e$. It follows from species mass balances in fuel and air channels that

$$\dot{m}_{f,k,\text{in}} - \dot{m}_{f,k,\text{out}} = W_k (\nu_{i,k}^f n_{i,k} - \nu_{i,k}^e n_{o,k}) \frac{I_e}{n_e F},$$

$$\dot{m}_{o,k,\text{in}} - \dot{m}_{o,k,\text{out}} = W_k (\nu_{i,k}^f n_{i,k} - \nu_{i,k}^e n_{o,k}) \frac{I_e}{n_e F}. $$

[9] [10]

The inlet and outlet mass flow rates in the fuel and oxidizer channels are represented as $\dot{m}$, $W_k$ are the molecular weights, and $F$ is the Faraday constant. Multiplying these equations by the species specific enthalpies (i.e., enthalpy per unit mass), which for a uniform-temperature system are constants, and summing over all species yields

$$(\dot{m} h)_{\text{in}} - (\dot{m} h)_{\text{out}} = \frac{I_e}{n_e F} \sum_{k=1}^{K} W_k h_k (\nu_{i,k}^f n_{i,k} - \nu_{i,k}^e n_{o,k}).$$

[11]

$$(\dot{m} h)_{o,\text{in}} - (\dot{m} h)_{o,\text{out}} = \frac{I_e}{n_e F} \sum_{k=1}^{K} W_k h_k (\nu_{i,k}^f n_{i,k} - \nu_{i,k}^e n_{o,k}).$$

[12]

The total mass flow rates and enthalpies in each channel are represented as $\dot{m} = \sum \dot{m}_k$ and $h = \sum Y_k h_k$. Adding these two equations and multiplying by the cell operating potential $E_{\text{cell}}$ yields

$$E_{\text{cell}} [(\dot{m} h)_{\text{in}} - (\dot{m} h)_{\text{out}}] = E_b \dot{W}_e,$$

where $(\dot{m} h)_{\text{in}} = (\dot{m} h)_{\text{in}} + (\dot{m} h)_{o,\text{in}}$ and $(\dot{m} h)_{\text{out}} = (\dot{m} h)_{\text{f,out}} + (\dot{m} h)_{o,\text{out}}$. The net electrical work (power) is written as $\dot{W}_e = I_e E_{\text{cell}}$ and a "reaction voltage" is defined as

$$E_b = \frac{1}{n_e F} \sum_{k=1}^{K} W_k h_k [(\nu_{i,k}^f n_{i,k} + \nu_{i,k}^e n_{o,k}) - (\nu_{i,k}^e n_{o,k} + \nu_{i,k}^e n_{o,k})] \frac{1}{n_e F} \sum_{k=1}^{K} W_k h_k (\nu_{i,k}^f - \nu_{i,k}^e) = -\frac{\Delta H}{n_e F}.$$

[14]

With the open-circuit potential written as $E_{\text{ocv}} = -\Delta G/n_e F$, it is seen that the net cell efficiency can be written as
In other words, the cell efficiency is the product of a reversible efficiency, a voltage efficiency, and a utilization efficiency.

Equation [15] is a closed-form, easily evaluated, expression for fuel-cell efficiency. It does not depend on cell structure and internal polarization losses. It does account for the fuel mixture, operating temperature and pressure, fuel utilization, and cell voltage. Achieving the thermodynamically predicted efficiency requires that the cell be as large as needed, with larger areas needed for cells with higher internal polarization losses.

The definition for \( e_u \) in Eq. [15] appears to be a bit different than the one in Eq. [5]. However, some further manipulation reveals that they are indeed the same. The potential heat release from complete oxidation of the inlet fuel stream can be represented in terms of the enthalpies of fuel, oxidizer, and final products as

\[
(m\Delta h)_{\text{in}} = (m\Delta h)_{\text{full, in}} + (m\Delta h)_{\text{in}} - (m\Delta h)_{\text{out}}.
\]  

[16]

where \((m\Delta h)_{\text{full, in}}\) is an "enthalpy rate" of the oxidizer required to fully oxidize the inlet fuel stream and \((m\Delta h)_{\text{in}}\) is the enthalpy rate of the completely oxidized products of the initial fuel stream. An analogous relationship applies to the exhaust stream, which may contain unspent fuel,

\[
(m\Delta h)_{\text{out}} = (m\Delta h)_{\text{full, out}} + (m\Delta h)_{\text{out}} - (m\Delta h)_{\text{out}}.
\]  

[17]

For a given fuel stream, the fully oxidized products must have the same enthalpy rates at the cell inlet and the cell outlet, i.e., \((m\Delta h)_{\text{full, in}} = (m\Delta h)_{\text{full, out}}\). Furthermore, the difference in the oxidizer required to completely oxidize the inlet and outlet streams must be provided from the cathode stream, i.e., \((m\Delta h)_{\text{in}} - (m\Delta h)_{\text{out}} = (m\Delta h)_{\text{in}} - (m\Delta h)_{\text{out}}\). It follows that

\[
(m\Delta h)_{\text{in}} - (m\Delta h)_{\text{out}} = (m\Delta h)_{\text{in}} - (m\Delta h)_{\text{out}} + (m\Delta h)_{\text{in}} - (m\Delta h)_{\text{out}} = (m\Delta h)_{\text{in}} - (m\Delta h)_{\text{out}}. \]  

[18]

Thus the two representations of \( e_u \) (i.e., Eq. [5] and [15]) are the same.

Figure 2 illustrates predicted thermodynamic efficiencies for four anode streams: 50% CH₄ and 50% air, pure H₂, 50% CH₄ and 50% H₂O, and 50% H₂ and 50% CO. In all cases, the cell is isothermal at 800 °C and uniform pressure of 1 atm, and the cathode stream is undiluted air. The general shape of the voltage-efficiency curve was previously reported and discussed by Sidwell and Coors (6). The effects of the three contributing efficiencies are evident in the figure. At low cell voltage the efficiency increases linearly as a result of \( e_u \). In this region the utilization is nearly 100% and the slope of the efficiency function depends on the reversible efficiency \( e_r \). At around \( E_{\text{cell}} = 0.8 \) V the
utilization begins to fall, which decreases the net efficiency. The utilization decreases because the operating voltage exceeds the open-circuit potential of the partially depleted fuel stream. At sufficiently high voltage, utilization (and hence efficiency) decreases to zero when none of the fuel can be electrochemically oxidized. It is interesting to note that a CH₄-air mixture can deliver higher efficiencies than a pure H₂ fuel.

It is evident that there is a strong maximum in the efficiency as a function of operating voltage. Presumably, it is best to operate a cell near the maximum efficiency. However, one needs to design a cell that can achieve the theoretically optimal performance. The thermodynamic model is silent on MEA structure, charge-transfer kinetics, concentration overpotentials, ohmic losses, and cell dimensions. These issues are addressed later in the paper with the channel-based model. Figures 3, 4, and 5 map
maximum thermodynamic efficiency and utilization for different fuel mixtures and temperature. The top panel of these figures shows the maximum achievable efficiency as a function of fuel mole fraction in a mixture. The lower panel shows the operating voltage at which the maximum efficiency is achieved. The middle panel shows the fuel utilization at maximum efficiency.

CHANNEL MODEL

This paper uses a channel-based model developed previously (7). Considering flow in an individual defined channel (Fig. 1), the species and overall continuity equations may be written as

\[ \frac{d(\rho Y_k u)}{dx} = \frac{P_c}{A_c} J_k^{\text{MEA}} W_k, \]  
\[ \frac{d(\rho u)}{dx} = \sum_{k=1}^K \frac{P_c}{A_c} J_k^{\text{MEA}} W_k. \]

These mass-conservation equations form an initial-value problem that requires specification of the inlet velocity \( u \) and mass fractions \( Y_k \). The channel cross-sectional area is \( A_c \) and the electrochemically active perimeter is \( P_c \). The mole fluxes exchanged between anode and the channel \( J_k^{\text{MEA}} \) are determined from a Dusty-Gas model (8) that predicts the species distributions within the porous anode. This boundary-value problem is solved through the anode thickness at each position \( x \) along the channel length. The mass-conservation equation is

\[ \frac{dJ_k}{dy} = A_c \dot{s}_k, \quad (k = 1, ..., K) \]

where the local mole fluxes \( J_k \) are determined from the following implicit relationship among \( K \) species and the pressure gradients

\[ \sum_{l \neq k} \left[ X_l \frac{J_l}{D_{k,l}^*} - \left( X_l \frac{J_k}{D_{l,k}^*} + J_k \right) \right] = -\frac{d[X_k]}{dy} \frac{[X_k] B_g}{P_c} \frac{dp}{dy}. \]

In these equations \([X_k]\) are molar concentrations, \( D_{k,l}^* \) are effective binary diffusion coefficients, \( D_{k,K}^* \) are Knudsen diffusion coefficients, \( B_g \) is the permeability, \( \mu \) is the mixture viscosity, and \( p \) is the pressure. The effective diffusion coefficients and transport properties are determined from kinetic theory and the porous-media structure. Boundary conditions needed to solve Eq. [21]. The composition at the channel interface is specified to be the local channel composition. The species fluxes at the dense-electrolyte interface are determined from the charge-transfer chemistry.

The molar species production rates \( \dot{s}_k \) within the anode structure are the result of heterogeneous chemistry. Although these rates may be determined from an elementary catalytic reaction mechanism (7), the results in this paper consider the limiting case that the heterogeneous chemistry causes the gas-phase species with the pore spaces to be equilibrated. This is accomplished via three fast, reversible, reactions: \( \text{CH}_4 + \text{H}_2\text{O} \leftrightarrow 3\text{H}_2 + \text{CO} \), \( \text{CO} + \text{H}_2\text{O} \leftrightarrow \text{H}_2 + \text{CO} \), and \( \text{CH}_4 + 2\text{O}_2 \leftrightarrow 2\text{H}_2\text{O} + \text{CO}_2 \). Because these global reactions involve only gas-phase species, the equilibrium constants are easily computed. Thermo-
dynamic and transport properties and chemical reaction rates are calculated using CHEM-KIN software package (9, 10).

The charge-transfer chemistry is represented in a modified Butler-Volmer form that is derived from an elementary reaction mechanism with an assumed rate-limiting step (7, 11),

$$i = i_0 \left[ \exp \left( \frac{3F\eta_a / 2}{RT} \right) - \exp \left( -\frac{F\eta_a / 2}{RT} \right) \right],$$

$$i = i_{H_2}^* \left( \frac{p_{H_2}^*/p_{H_2}}{1 + \left( p_{H_2}^*/p_{H_2}^* \right)^{1/2}} \right).$$  [23]

For the results in this paper $i_{H_2}^* = 1.54 \text{ A/cm}^2$. At 600°C $p_{H_2}^* \approx 0.36$ atm, 700°C $p_{H_2}^* \approx 1.5$ atm, 800°C $p_{H_2}^* \approx 4.7$ atm, and 900°C $p_{H_2}^* \approx 12.3$ atm. The activation overpotential $\eta_a = E_a - E_{a,eq}$ is defined in the ordinary way as the difference between the electric-potential difference between the anode and the electrolyte and the equilibrium electric-potential difference between the anode and the electrolyte.

It is assumed here that the air flow is sufficiently great that oxygen depletion in the cathode channel is negligible. The oxygen reduction is represented in a Butler-Volmer form as

$$i = i_0 \left[ \exp \left( \frac{F\eta_c / 2}{RT} \right) - \exp \left( -\frac{F\eta_c / 2}{RT} \right) \right],$$

$$i = i_{H_2}^* \left( \frac{p_{O_2}^*/p_{O_2}}{1 + \left( p_{O_2}^*/p_{O_2}^* \right)^{1/2}} \right).$$  [24]

For the results shown in this paper, $i_{H_2}^* = 2.8$ A/cm² and $p_{O_2}^* = 4.9E8 \exp (-200 \text{ kJ}/RT)$.

Figure 6 illustrates the voltage-current performance of an MEA structure operating on hydrogen-steam mixtures similar to ones discussed by Jiang and Virkar (12). The physical MEA structure is modeled to represent the Jiang and Virkar experiments. Predicting the performance of dilute fuel streams is central to understanding the cell efficiency in a full fuel cell, where fuel dilution plays an important role.

**CHANNEL PERFORMANCE**

While the theoretical efficiencies are a good guide to what is theoretically achievable, actual performance depends on the details of cell construction and materials. Figure 7 illustrates the results of a channel simulation for a fuel stream of 50% CH₄ and 50% air. In this simulation the cell is running at 0.8V, which is near maximum efficiency. The channel is assumed to have a square cross section of 1 mm² and the channel is 8 cm long. The cell is isothermal at 800°C and the inlet velocity is 10 cm/s. The anode is presumed to be a porous structure that is 1.2 mm thick. The electrochemically active perimeter $P_e = 1.2$ mm. The anode pore structure has porosity $\phi = 0.35$, tortuosity $\tau = 0.35$, aver-
Figure 7. Channel-model simulation of a fuel cell operating on an inlet fuel mixture of 50% CH₄ and 50% air. The top panel shows gas-phase mole fractions and current density along the anode channel. The drop-down panels show gas-phase composition with the anode pore structure at selected locations along the channel.

Age pore radius \( r_\text{p} = 0.5 \, \mu\text{m} \), and primary particle diameter \( d_\text{p} = 2.5 \, \mu\text{m} \). These parameters affect the species transport within the anode and hence the effective concentration overpotential. Since the transport and thermal chemistry within the anode is modeled, there is no need to evaluate concentration overpotentials. Rather, the charge transfer is evaluated in terms of the H₂ concentration at the dense-electrolyte interface. In this model the gas-phase species are drive to local equilibrium via heterogeneous reactions within the anode pore spaces.

As the methane-rich fuel-air mixture enters the anode channel it is thermally oxidized very rapidly to form H₂, CO and H₂O. The drop-down panels in Fig. 7 show the gas-phase composition with the anode structure. The CH₄ profile in left-hand panel indicates a diffusive flux of methane out of the channel and into the anode. The H₂ has a peak concentration within the anode, indicating flux back to the channel and toward the dense-electrolyte interface at the lower edge of the anode. The H₂ is formed by partial oxidation and reforming chemistry within the anode. The H₂ at the electrolyte interface participates in charge-transfer chemistry (see Fig. 2), where H₂O is formed. Water-gas-shift chemistry reacts CO and H₂O to form CO₂, which is transported back toward the fuel channel.

By about \( x = 0.5 \, \text{cm} \) from the channel entrance the CH₄ has been essentially consumed, forming substantial concentrations of H₂ and CO in the fuel channel. As the H₂ and CO are consumed via electrochemical and thermal processes, the current density decreases and the product concentrations of H₂O and CO₂ increase. By about \( x = 6 \, \text{cm} \) from the inlet the fuels are largely consumed and the current density has nearly vanished. However, had the cell been shorter (say only 4 cm long), then there would be significant unspent H₂ and CO exhausted, with a resulting decrease in efficiency.
Figure 8 compares directly results from the thermodynamic and channel models for a cell operating on a fuel mixture of 50% CH₄ and 50% air at 800°C. The models predict nearly identical efficiency and utilization performance. This excellent comparison is observed over very large ranges of fuels and operating conditions.

Inlet flow velocities are an important variable in the channel model. Figure 8 shows model results for inlet velocities of 10 cm/s and 20 cm/s. The predicted efficiency and fuel utilization (as a function of operating voltage) are virtually identical. Of course, the composition profiles within the flow channel and the anode are very different for different flow velocities. The channel model can be used to determine the cell length needed to achieve the maximum efficiency, something the thermodynamic model cannot do. The results in Fig. 8 show predicted channel lengths for inlet velocities of 10 cm/s and 20 cm/s. Here the effective cell length is taken to be the length at which 95% of the available electric power has been produced.

The length required to deliver the available power has an interesting, and unexpected, profile as a function of operating voltage. At voltages below that needed achieve maximum efficiency, the cell length increases with increasing cell voltage. This is the expected result, because at low voltage the electrochemistry proceeds rapidly and expends the fuel early in the channel. Beyond the peak efficiency, where fuel utilization is decreasing, the required cell length decreases toward a local minimum. At very high voltages approaching the Nernst potential the required length increases rapidly.

Figure 9 shows mole-fraction and current-density profiles along the channel length for operating voltages around the maximum efficiency. These profiles provide some quantitative insight regarding the channel-length predictions. As the operating voltage increase, the current densities have flatter profiles. In all cases the channel is made sufficiently long so that the current density approaches zero toward the end of the channel. At low voltages, the fuel is nearly all oxidized.
dized so that utilization is high and there is no fuel in the exhaust stream. At the lowest voltage shown in Fig. 9 (0.8V), the exhaust contains about 5% H2. At higher voltages the exhaust contains a great deal of fuel (i.e., low fuel utilization). Because the operating voltage exceeds electrochemical potential of the depleted and diluted fuel stream, the charge-transfer reactions can no longer proceed. It is interesting to note the fundamental change in profile shape for the H2 mole fractions at voltages above 0.95 V. On the scale shown in Fig. 9, it is difficult to see the channel lengths from the current-density profiles. However, by observing where the profiles flatten to asymptotically unchanging values, the needed channel lengths can be observed from the H2 profiles.

CONCLUSIONS

Two models are developed and used to predict SOFC efficiencies for a wide range of fuels and operating conditions. The net efficiency is the product of a reversible efficiency, voltage efficiency, and fuel utilization. Cell efficiency is a strong function of operating voltage, with maximum efficiency achieved at cell voltages in the range of 0.8 V. The thermodynamic model predicts best possible performance, independent of specific cell design. The channel-based model incorporates details of MEA structure, fluid transport, and charge-transfer kinetics. The channel model can be used to guide cell design and optimization.

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