

# Appendix: Fuel Cell Component Model

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In this appendix, we will describe the ideal characteristics and the relevant loss mechanisms of fuel cells for aeronautical applications. The model presented here was validated against experimental fuel cell data [1, 2] and applied for MW-scale applications in the CHEETA aircraft.

## I. Ideal Cell Voltage

The thermodynamic open-circuit potential ( $e_o$ ) is the theoretical voltage possible for a hydrogen fuel cell based on the Gibbs free energy of formation[3],

$$e_o = \frac{-\Delta g_f}{2F} \quad (1)$$

where  $F$  is Faraday's Constant (96,485 C/mol) and  $\Delta g_f$  is Gibbs function of formation for water. This cell potential can be adjusted for various flight state operating conditions using the Nernst equation,

$$e = e_o + \frac{RT}{2F} \times \ln \frac{cH_2P_{fuel}\sqrt{cO_2P_{air}}}{cH_2OP_{H_2O}} \quad (2)$$

where  $R$  is the universal gas constant (8.314 J/mol-K) and  $e$  is the adjusted ideal cell voltage, henceforth called the Nernst voltage. The partial pressures  $P$  are given in bar or should be normalized to atmospheric reference pressure. This equation captures the voltage change due to variations in operating temperature  $T$ , species mixing ratio  $cX$ , and partial pressure  $P$  [3]. Assuming pure hydrogen fuel, completely liquid water product, and equal air pressure at the inlet and outlet of the fuel cell, we can rewrite (2) as

$$e = e_o + \frac{RT}{2F} \times \ln \frac{P_{fuel}\sqrt{[cO_2]}}{\sqrt{P_{air}}} \quad (3)$$

## II. Ideal Cell Current

The ideal current of a fuel cell is directly related to the mass flow rate of the fuel. Assuming complete fuel usage, we can define the internal current as

$$i_{int} = 2F \times \frac{\dot{m}_{fuel}}{N_c} \times \frac{1000g}{1kg} \times \frac{1mol}{2(MM_H)} \quad (4)$$

where  $N_c$  is the number of cells in the fuel cell stack and  $MM_H$  is the molar mass of hydrogen (1.0079 grams/mol). The real stack current will be somewhat less than this ideal internal current, which we will discuss later. For now, we will define the real current density of the fuel cell stack as

$$i_d = \frac{i + i_x}{A} \quad (5)$$

where  $i$  is the real stack current,  $i_x$  is the lost (crossover) current, and  $A$  is the cell membrane area.

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### III. Loss Mechanisms in Real Fuel Cells

To adequately capture the behavior of real fuel cells, other loss mechanisms must be considered. The main mechanisms are ohmic losses, activation losses, and mass transport losses. Ohmic losses are related to the internal resistance of the device and are described by Ohm's Law,

$$\Delta V_{ohm} = i_d r \quad (6)$$

$$Q_{ohm} = (i_d)^2 A r \times N_c \quad (7)$$

where  $r$  is the internal area resistance per cell ( $\Omega\text{-cm}^2$ ) [3].

Activation losses are overvoltage effects first observed empirically by Tafel [4], of whom the governing equation below is named.

$$\Delta V_{act} = \frac{RT}{2\alpha F} \times \ln\left(\frac{i_d}{i_d^\circ}\right) \quad (8)$$

This equation can be rearranged to solve for the current (then called the Butler-Volmer equation) [3].

$$i_d^\circ = \frac{2Fk[cO_2]P_{t2}}{P_{ref}A} \quad (9)$$

of which  $k$  is an electrochemical rate constant, and

$$z = \frac{2\alpha F \Delta V_{act}}{RT_{t2}} \quad (10)$$

where  $\alpha$  is an empirical charge transfer coefficient. The activation overpotential at the anode can be neglected for hydrogen-powered fuel cells [3]. We can then specify the corresponding power losses due to this activation voltage differential.

$$Q_{act} = (i_d A) \Delta V_{act} \times N_c \quad (11)$$

A lower bound on these activation power losses is set by the exchange current density. As mentioned previously,  $i_d^\circ$  is the minimum current density required for activation losses to be present [3]. As we shall see, this threshold will always be met by fuel crossover, thereby justifying this lower bound.

$$Q_{act} = (i_d^\circ A) \Delta V_{act} \times N_c \quad (12)$$

There is also a non-negligible amount of fuel that crosses through the membrane (in addition to neglected secondary reactions, electrical short-circuiting, and oxygen crossover) [5]. These fuel crossover effects reduce the open-circuit voltage of the device by approximately 0.2 V [3]. To account for this effect, we can specify a fuel utilization factor  $\mu_{fuel}$  to determine the actual stack current  $i$ .

$$\mu_{fuel} = \frac{i}{i + i_x} = \frac{i}{i_{int}} \quad (13)$$

If  $\mu_{fuel}$  is not known (or cannot be assumed), then we can estimate the crossover current  $i_x$  based on the approximation below (where short circuiting effects through the membrane are insignificant) [5]

$$i_x = \frac{2Fk_{H_2}P_{fuel}}{L_m} \quad (14)$$

where  $L_m$  is the membrane thickness (cm) and  $k_{H_2}$  is the approximate permeability of hydrogen through a Nafion membrane [6]. The low-temperature Nafion membrane may not be representative of high-temperature PEM fuel cells, so we characterize fuel crossover effects using an assumed fuel utilization.

$$k_{H_2} = 6.6 \times 10^{-8} \exp\left(\frac{-21030}{RT}\right) \frac{\text{mol}}{(\text{bar})(\text{cm})(\text{s})} \quad (15)$$

The presence of this crossover current causes an activation voltage drop,  $V_{act}$ . As such, there are significant losses even at an 'idle' power condition, as captured by the lower bound on activation losses.

At high current densities, there are also significant mass transport losses associated with the membrane concentrations of reactants and transport of liquid water products away from the cell [3]. Mass transport losses are typically accounted for with the following empirical relation [7, 8]:

$$\Delta V_{trans} = m e^{n i_d} \quad (16)$$

where  $m$  and  $n$  are empirical constants of approximate value  $3 \times 10^{-5} \text{V}$  and  $8 \times 10^{-3} \frac{\text{cm}^2}{\text{mA}}$ , respectively [3].

#### IV. Real Fuel Cell Performance

Tying together the ideal cell behavior and corresponding loss mechanisms, we can characterize the real cell voltage  $V_c$  using Kirchoff's Voltage Law,

$$e = V_c + \Delta V_{ohm} + \Delta V_{act} \quad (17)$$

and

$$V = V_c N_c \quad (18)$$

where  $V$  is the fuel cell stack voltage.

For a given gross stack power, we can relate the stack voltage to our real current (and therefore our internal current and fuel mass flow rate) by the definition of electrical power,

$$V = \frac{P_{gross}}{i} \quad (19)$$

We can quantify the efficiency of the fuel cell by relating the gross output power of the device to the ideal chemical power of the hydrogen mass flow. The waste heat to the heat exchanger system can be determined based on the loss mechanisms and the lost fuel energy.

$$\eta_{fc} = \frac{P_{gross}}{h_{fuel} \dot{m}_{fuel}} \quad (20)$$

$$\dot{Q} = Q_{ohm} + Q_{act} \quad (21)$$

$$\dot{Q} = (1 - \eta_{fc}) P_{gross} \quad (22)$$

For the MW-scale stacks used on the CHEETA aircraft, we must also account for the power losses of the other components such as the air compressor, hydrogen fuel recycler, coolant pump. We can consider the compressor power draw based on an input pressure ratio and efficiency, and the other components using a parasitic loss factor ( $x_{para} = 0.03$ ).

$$P_{comp} = \dot{m} \Delta h_t \quad (23)$$

$$P_{comp} = \frac{\dot{m} C_p \Delta T_t}{\eta_{comp}} \quad (24)$$

$$P_{comp} = \dot{m} C_p T_{t\infty} \left( \frac{T_{tc}/T_{t\infty} - 1}{\eta_{comp}} \right) \quad (25)$$

$$P_{comp} = \dot{m}_{air} C_p T_{t\infty} \left( \frac{\Pi_c^{(\gamma-1)/\gamma} - 1}{\eta_{comp}} \right) \quad (26)$$

$$P_{parasitic} = x_{para} P_{gross} \quad (27)$$

Taking these power draws from the gross stack power, we can determine a net power system output power and efficiency.

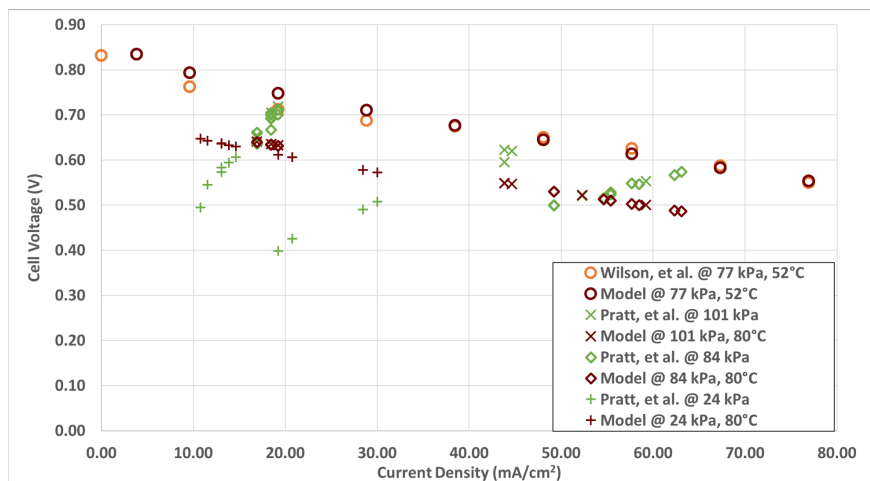
$$P_{gross} = P_{out} + P_{comp} + P_{para} \quad (28)$$

$$\eta_{net} = \frac{P_{out}}{h_{fuel} \dot{m}_{fuel}} \quad (29)$$

#### V. Model Validation

The fuel cell model has been validated against two experimental studies by configuring model parameters to match the configurations studied in the literature [1, 2]: one test by Wilson *et al* was done at constant operating conditions (temperature and pressure) for varied output power and the other by Pratt *et al* was done at variable conditions (air pressure, humidity, and airflow rate with uncontrolled temperature) for varied output power. Given that these experiments were conducted using the same fuel cell design, we will assume the parameters are the same for both baselines: membrane area ( $13 \text{ cm}^2$ ), cell internal resistance ( $2.7 \Omega - \text{cm}^2$ ), cathode exchange current density (varies with air pressure [1],  $10^{-6} \text{ mA/cm}^2$ ), and charge transfer coefficient (0.50). Anode activation losses can be neglected for hydrogen-fueled PEM fuel cells [3]. Mass transport losses were found to be negligible, given the low current density at which these fuel cells were tested.

The results of these experiments and the corresponding predictions of our model are shown in Figure 1, within 5% accuracy for the constant operating conditions case and within 15% for the varied operating conditions. The greater differences in the comparison with the latter experiment could be due to the uncontrolled temperature of the fuel cell stack [1] or membrane dehydration occurring at low pressures, although our assumption of a constant operating temperature of 80°C captures the behavior reasonably well. The fuel cell model is sufficiently accurate for our purposes except at very low air pressures, and this low-pressure regime is not important for the current study due to the integration of an air compression system for the CHEETA application.



**Fig. 1** Modeled cell voltage for varied current density is shown against experimental data [1, 2] at various operating conditions.

## References

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