PEMFC Model

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1 Model

1.1 Ideal Thermodynamic Efficiency

The hydrogen PEM fuel cell chemical reaction is:

$$\mathrm{H_2 + 1/2O_2 \rightarrow H_2O_{liquid}} \tag{1}$$

At normal temperature and pressure (NTP, which we take as 298.15 K and 101.325 kPa), the heat generated by the reaction is the difference in heat of formation of the products and reactants:

$$\Delta H = \Delta_f H(H_2O_{liquid}) - \Delta_f H(H_2) - 1/2\Delta_f H(O_2) \tag{2}$$

The ideal reversible cell voltage is:

$$E_h = -\frac{\Delta H}{q} \tag{3}$$

where q is the charge transferred by the electrons released by a mole of hydrogen. Faraday's constant (F) – the charge of one mole of electrons – is 96485 Coulomb/mole and hydrogen releases N = 2 electrons per molecule, so the charge released per mole is 2×96845 Coulomb/mole. Thus Equation 3 becomes:

$$E_h = -\frac{\Delta H}{NF} \tag{4}$$

At NTP, $\Delta_f H(H_2O_{liquid}) = -286$ kJ/mole, $\Delta_f H(H_2) = \Delta_f H(O_2) = 0$ kJ/mole and $E_h = 1.48$V.

To calculate the ideal reversible cell voltage at other temperatures and pressures, the enthalpy change from NTP (where the heat of formation was determined) for each product and reactant must be added to each species in the ΔH equation. Enthalpy can be uniquely determined if two other thermodynamic state variables are known (such as pressure and temperature) using equation of state models as are employed in computational tools such as

REFPROP and the open-source Python package CoolProp[1]. CoolProp is used to calculate thermophysical properties as needed in this work. For simplicity later on, we will define these enthalpy change functions in general as:

$$\delta SV_{species}(T,P) = SV_{species}(T,P) - SV_{species}(T = 298.15\text{K}, P = 101.325\text{kPa}) \qquad (5)$$

where SV is the thermodynamic state variable of interest (e.g. enthalpy [h] or Gibbs energy [g]).

In this case,

$$\Delta H = \Delta_f H(H_2O_{liquid}) + \delta h_{H_2O}(T,P) - \delta h_{H_2}(T,P) - 1/2\delta h_{O_2}(T,P) \qquad (6)$$

The heat of reaction (ΔH) is the internal energy contained in the fluid, but not all of this heat can be converted to useful work due to irreversible losses due to entropy. The part that can be converted to useful work is the Gibbs energy change ΔG. At NTP, the Gibbs energy of formation for liquid water is $\Delta_f G(H_2O_{liquid}) = -237.1$ kJ/mole and $\Delta_f G(H_2) = \Delta_f G(O_2) = 0$ kJ/mole. The true reversible cell voltage is:

$$E_r = -\frac{\Delta G}{NF} \qquad (7)$$

At non-standard conditions:

$$\Delta G = \Delta_f G(H_2O_{liquid}) + \delta g_{H_2O}(T,P) - \delta g_{H_2}(T,P) - 1/2\delta g_{O_2}(T,P) + RT\ln\left(\frac{p_{H_2O}}{p_{H_2}p_{O_2}^{1/2}}\right) \qquad (8)$$

where $\delta g(T,P)$s are found in CoolProp and p_is are the partial pressures for each species in atmospheres which are raised to the power of their stoichiometry. Thus $p_{O_2} = x_O \times P$ where x_O is the mole fraction of oxygen in air (0.2095) and P is the stack operating pressure.

The ideal thermodynamic efficiency for the fuel cell is then:

$$\eta_i = \frac{\Delta G}{\Delta H} = \frac{E_r}{E_h} \qquad (9)$$

The ideal thermodynamic efficiency as a function of stack temperature and pressure is shown in Figure 1. The utopia point is $\eta_i = 1$ which in this case is approached by lowering temperature and increasing pressure (top left of graph, yellow). From this result, it would seem that operating the fuel cell as cold as possible would improve performance. However, there is the obvious physical limit that if the temperature drops below the freezing point of water, operation becomes much more challenging if not impossible. Additionally, there are other chemical and practical issues with lowering temperature, which will be discussed in the next section.

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[1] Pure and Pseudo-pure Fluid Thermophysical Property Evaluation and the Open-Source Thermophysical Property Library CoolProp Ian H. Bell, Jorrit Wronski, Sylvain Quoilin, and Vincent Lemort Industrial & Engineering Chemistry Research 2014 53 (6), 2498-2508 DOI: 10.1021/ie4033999

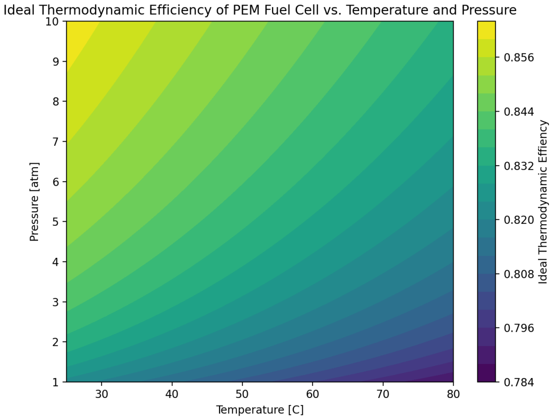

Figure 1: PEM Fuel Cell Ideal Thermodynamic Efficiency vs. Temperature and Pressure. Oxygen is assumed to come from air ($x_O = 0.2095$).

1.2 Overall Efficiency and Characteristic Curves

The operating cell voltage v_{cell} is the true reversible cell voltage minus activation loss (due to reaction kinetics) Equation 11, ohmic loss (from ionic and electronic resistance) Equation 12, and concentration loss (due to mass transport) Equation 13. These losses are functions of the current density i (A/cm^2) and a leakage current (i_{leak} which is the current lost in side reactions that does not contribute to useful current flowing through the cell). The losses also depend on parameters that are typically identified by curve-fitting test data but can also be modeled with higher fidelity analysis as is done in [2].

$$\begin{aligned} v_{cell} = {} & E_r && (10) \\ & - [a_{anode} + a_{cathode}] - [b_{anode} + b_{cathode}] \ln(i + i_{leak}) && (11) \\ & - iASR_{\Omega} && (12) \\ & - C \ln\left(\frac{i_L}{i_L - (i + i_{leak})}\right) && (13) \end{aligned}$$

The fitting constants depend on material and electrochemical properties of the stack materials as well as operating conditions such as pressure, temperature and humidity[3]. Not all of these dependencies are captured here as they are often experimentally determined, but should be kept in mind. We will further define the activation loss fitting constants (a_{anode}, b_{anode}, $a_{cathode}$, and $b_{cathode}$) as these depend on temperature, which is necessary to show how

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[2] O'Hayre, Ryan P., et al. Fuel Cell Fundamentals. Third edition., Wiley, 2016.

[3] Datta, A. (2021). PEM Fuel Cell Model for Conceptual Design of Hydrogen eVTOL Aircraft.

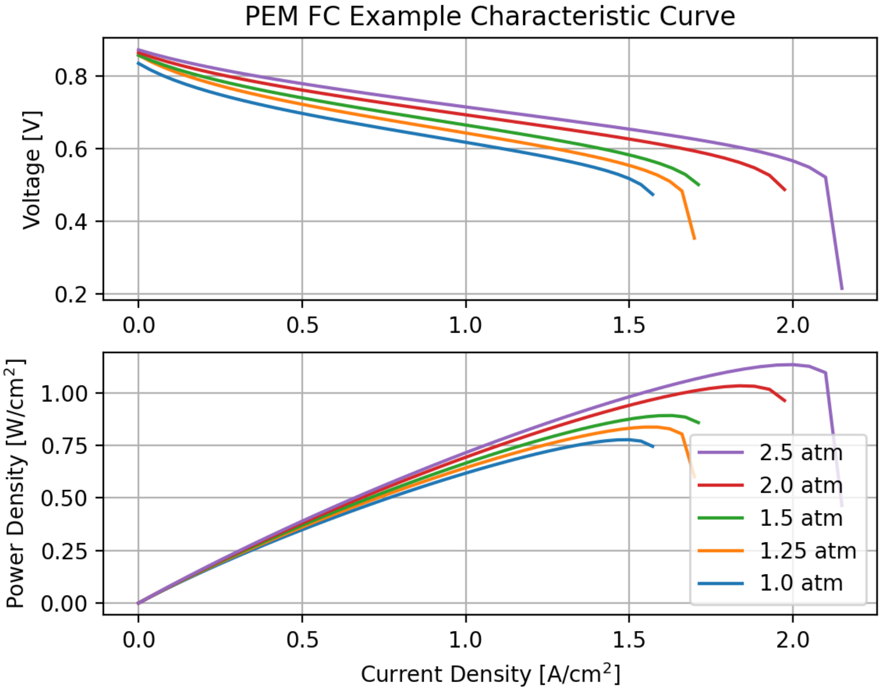

Figure 2: Example Characteristic Curves at 80^{o}C

true efficiency changes with temperature.

$$a_{anode} = -\frac{RT}{\alpha_A n_A F} \ln i_{0_A} \qquad b_{anode} = \frac{RT}{\alpha_A n_A F} \tag{14}$$

$$a_{cathode} = -\frac{RT}{\alpha_C n_C F} \ln i_{0_C} \qquad b_{cathode} = \frac{RT}{\alpha_C n_C F} \tag{15}$$

Once all fitting constants are known, characteristic curves for the specific fuel cell can be made. These characteristic curves show how cell voltage, areal power density, and efficiency vary with the cell's areal current density and are used to choose an operating point when designing the fuel cell system. Example characteristic curves with typical values for the fitting constants are shown in Figure 2. The voltage efficiency is $\eta_r = \frac{v}{E_r}$, and the overall efficiency is $\eta = \eta_i \eta_r$.

1.3 Stack Sizing

Once the fuel cell is characterized, the stack can be designed by selecting any two of power, current, and voltage. Then the stack area and number of cells in the stack can be calculated:

$$n_{cells} = \frac{V_{overall}}{v_{cell}} \tag{16}$$

$$A_{cell} = \frac{P_{overall}}{n_{cells} p_{cell}} = \frac{I_{overall}}{i_{cell}} \tag{17}$$

$$\eta_{overall} = \frac{v_{cell}}{E_h} \tag{18}$$

For example, suppose we want a 300 V fuel cell with a power output of 100 kW, operating at 1 atm, and we wish to minimize its weight, so we pick to operate at the peak of the power density-current density curve. Then $P_{overall} = 100000W$, the power density and current density are where the curve peaks ($p_{cell} = 0.78W/cm^2$ at $i_{cell} = 1.5A/cm^2$, which corresponds to $v_{cell} = 0.52V$), and the other parameters fall out.

$$n_{cells} = \frac{300}{0.52} = 579\,\text{cells} \tag{19}$$

$$A_{cell} = \frac{100000}{600 * 0.8} = 222cm^2 = \frac{I_{overall}}{1.5} \Rightarrow I_{overall} = 312.5A \tag{20}$$

$$\eta_{overall} = 0.35 \tag{21}$$

Note that this is the overall (or true) efficiency, which is lower than the voltage efficiency which is often reported. Now that the area and number of cells are known, the thickness and density of the components (bipolar plates, gas diffusion layers, catalysts, PEM, gaskets) chosen to make each cell in the stack can be used to calculate the stack weight and volume.

Figure	**Per Cell**	**Stack**
Length [m]	$\sum t_i$	$n_{cells} \sum t_i$
Volume [L]	$A_{cell} \sum t_i$	$n_{cells} A_{cell} \sum t_i$
Mass [kg]	$A_{cell} \sum \rho_i t_i$	$n_{cells} A_{cell} \sum \rho_i t_i$

Finally, the hydrogen and air consumption is calculated. The current ($I_{overall}$) must be produced in each cell, and is proportional to the molar rate of consumption of the reactants. Once the molar rate is known, the mass flow rate can be calculated.

$$I_{overall} n_{cells} = \frac{Q}{s} = NF\nu \tag{22}$$

$$\nu M = \dot{m} \tag{23}$$

$$\dot{m}_{H_2} = \frac{NF}{I_{overall} n_{cells}} * 2.01588 \times 10^{-3} \tag{24}$$

$$\dot{m}_{Air} = f_A * 1/2 * \frac{NF}{x_O I_{overall} n_{cells}} * 28.9655 \times 10^{-3} \tag{25}$$

where f_A is an air utilization factor due to providing more air than is stoichiometrically needed, and is usually ≈ 1.5-2.5. In our example fuel cell, $\dot{m}_{H_2} = 2$ g/s and $\dot{m}_{Air} = 70$ g/s.

2 Parameter Sensitivities for Key FOMs

Based on this PEM fuel cell stack model, we will investigate two key FOMs: overall efficiency and stack specific power.

2.1 Overall Efficiency

First, we expand the equation to show parameter dependencies:

$$\eta_{overall} = \frac{v_{cell}}{E_h} \tag{26}$$

where $E_h = -\frac{\Delta H}{NF}$ is a function of temperature and pressure as shown in Equation 6 and v_{cell} is a function of temperature, pressure, current, and cell characteristics as shown in Equation 10. Expanding, we see:

$$\begin{aligned}
v_{cell} = &-\frac{1}{NF}\left\{-237141 + \delta g_{H_2O}(T,P) - \delta g_{H_2}(T,P) - \tfrac{1}{2}\,\delta g_{O_2}(T,P) + \tfrac{8.314T}{2}\ln\left(\frac{101325}{0.2095\,P}\right)\right\} \\
&-\frac{RT}{F}\left\{\left(-\frac{\ln i_{0_A}}{\alpha_A n_A} - \frac{\ln i_{0_C}}{\alpha_C n_C}\right) + \left(\frac{1}{\alpha_A n_A} + \frac{1}{\alpha_C n_C}\right)\ln(i + i_{leak})\right\} \\
&- i\,ASR_\Omega - C\ln\left(\frac{i_L}{i_L - (i + i_{leak})}\right), \\
E_h = &-\frac{-268000 + \delta h_{H_2O}(T,P) - \delta h_{H_2}(T,P) - \tfrac{1}{2}\,\delta h_{O_2}(T,P)}{NF}
\end{aligned}$$

ChatGPT was used to streamline analytical partial derivative calculation and LaTeX formatting. For $\delta g(T,P)$ and $\delta h(T,P)$, finite differences were used to estimate the derivatives

Parameter (p)	**Typical Value**	**Sensitivity** $\left(\frac{\partial SP}{\partial p}\right)$	**Normalized Sensitivity** $\left(\frac{p}{SP}\frac{\partial SP}{\partial p}\right)$
Temperature (T)	350 K	0.00115	0.794
Pressure (P)	1.013e+5 kPa	2.149e-7	0.043
Anode Transfer Coefficient (α_A)	0.5	0.115	0.114
Cathode Transfer Coefficient (α_C)	0.2	1.3	0.514
Anode Exchange Current Density (i_{0A})	0.1	0.218	0.0431
Cathode Exchange Current Density (i_{0C})	1.000e-4	273	0.0539
Ohmic Resistance Loss (ASR_Ω)	0.01 Ωcm^2	-1.09	-0.0214
Concentration Loss Constant (C)	0.1	-1.17	-0.23
Current Density (i)	1.5 A/cm^2	-1.135e-6	-3.360e-6
Leakage Current (i_{leak})	0.1 A/cm^2	-1.098e-6	-2.166e-7
Limiting Current (i_L)	2 A/cm^2	7.509e-7	2.963e-6

Table 1: $\eta_{overall}$ Sensitivity to Parameters Around Typical Values

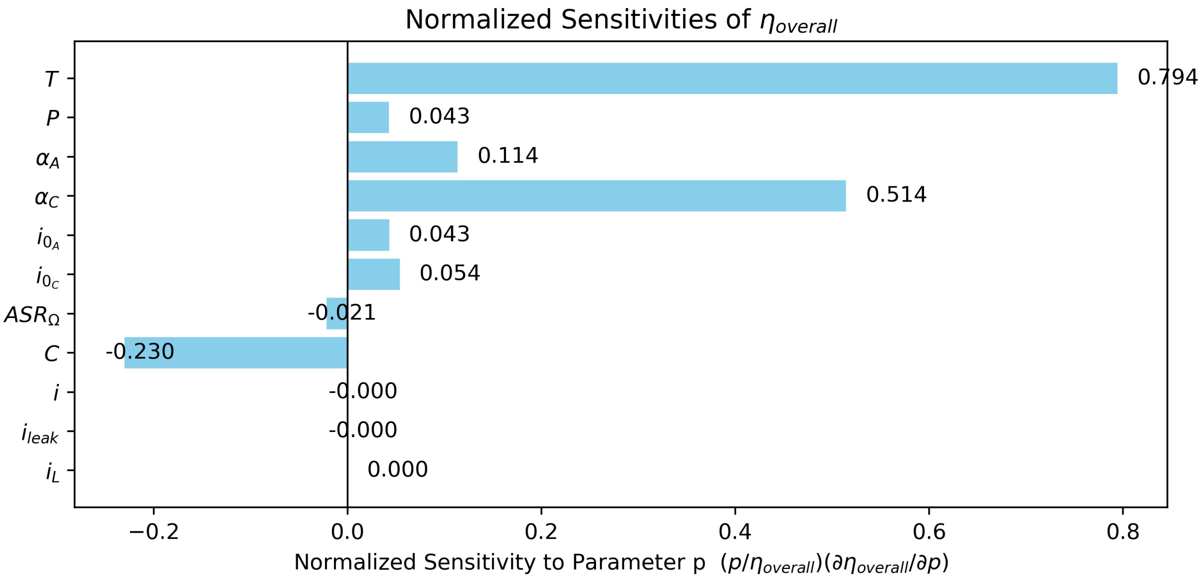

Figure 3: $\eta_{overall}$ Normalized Sensitivity to Parameters

with calls to CoolProp. For all other parameters, analytical partial derivatives were computed (subsection 4.1). A summary of the results using baseline parameter values is provided in Table 1 and the normalized sensitivities are visualized in Figure 3.

From the normalized sensitivities, we see that the overall efficiency actually increases with increasing temperature! This is because of the kinetics and specifically activation overvoltage. There are four main ways to improve kinetic performance: (1) increase the reactant concentration; (2) decrease the activation barrier; (3) increase the temperature; and (4) increase the number of possible reaction sites (i.e., increase the reaction interfaceroughness)[4]. The kinetics also explain why we see an increase in pressure improves efficiency, as an increase in pressure increases the reactant concentration. Figure 3 also illustrates why in fuel cell modeling, anode kinetic losses are often neglected compared to the cathode kinetic losses. The efficiency depends extremely weakly on the current density parameters.

2.2 Stack Specific Power

The stack specific power (kW/kg) is:

$$SP = \frac{P_{overall}}{m} = \frac{I_{overall}V_{overall}}{n_{cells}A_{cell}\sum \rho_i t_i} = \frac{n_{cells}A_{cell}i_{cell}v_{cell}}{n_{cells}A_{cell}\sum \rho_i t_i} = \frac{i_{cell}v_{cell}}{\sum \rho_i t_i} \tag{27}$$

Again, expanding this equation we see:

$$\begin{aligned}
&SP = \frac{i}{\sum \rho_i t_i} \times \\
&\Bigg[-\frac{1}{NF}\left\{ -237141 + \delta g_{H_2O}(T,P) - \delta g_{H_2}(T,P) - \tfrac{1}{2}\,\delta g_{O_2}(T,P) + \tfrac{8.314T}{2}\ln\!\left(\frac{101325}{0.2095\,P}\right)\right\} \\
&-\frac{RT}{F}\left\{ \left(-\frac{\ln i_{0_A}}{\alpha_A n_A} - \frac{\ln i_{0_C}}{\alpha_C n_C}\right) + \left(\frac{1}{\alpha_A n_A} + \frac{1}{\alpha_C n_C}\right)\ln(i + i_{leak}) \right\} \\
&- i\,ASR_{\Omega} - C\ln\!\left(\frac{i_L}{i_L - (i + i_{leak})}\right) \Bigg]
\end{aligned}$$

Analytical derivatives are shown in subsection 4.2. Table 2 shows numerical outputs for the partial derivatives and normalized sensitivities, and Figure 4 visualizes the normalized sensitivities.

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[4] O'Hayre, Ryan P., et al. Fuel Cell Fundamentals. Third edition., Wiley, 2016.

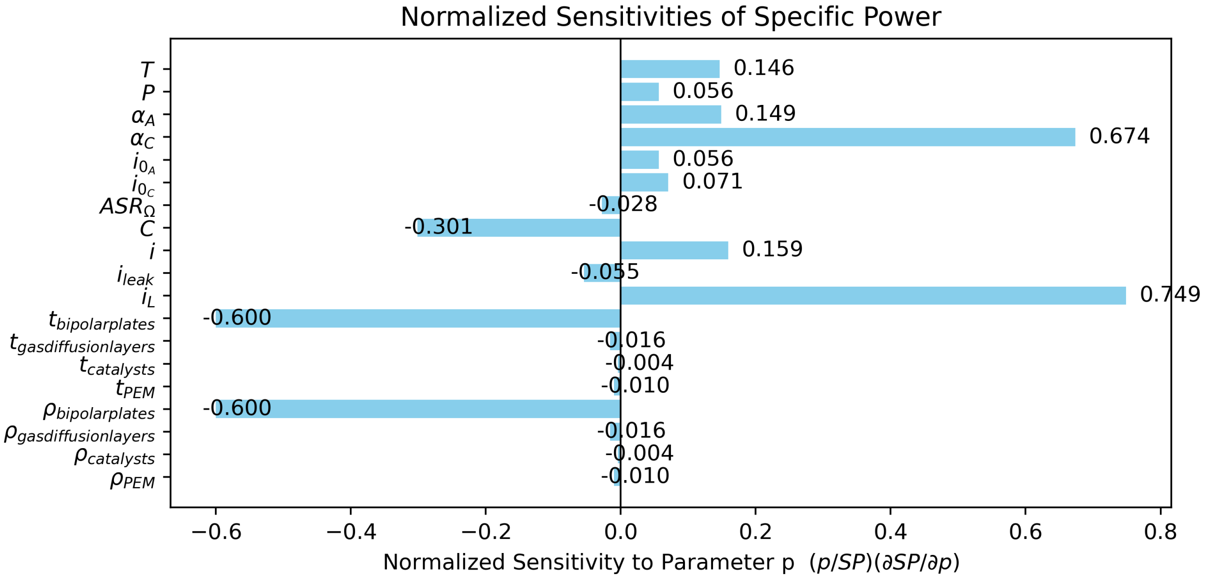

Figure 4: Specific Power Normalized Sensitivity to Parameters

Like with overall efficiency, increasing pressure and temperature increase specific power. Again, cathode kinetic losses are much higher impact than anode kinetic losses. For specific power, the current density parameters are very impactful. Specifically, the limiting current density i_L has a large impact on the specific power, since this is the maximum current density the fuel cell can provide. On the mechanical side, thickness reduction and density reduction increase specific power, with the heaviest components being highest priority (in this case, the bipolar plates).

3 Discussion

When investigating overall efficiency and specific power, the following strategies for improving performance emerged as having the highest impact:

- Increasing temperature (with higher temperatures having a very strong effect on efficiency specifically)
- Increasing pressure
- Reducing cathode kinetic losses, which are typically more important than anode kinetic losses
- Increasing limiting current (with higher limiting current having a very strong effect on specific power specifically)
- Lightweighting the heaviest components

It should be noted that the technical modeling done here was simplified in many ways. More detailed modeling reveals even more dependencies between different parameters. It is important to remember it is difficult, if not impossible, to address one of the parameters without impacting the others – material, electrochemical, and mechanical properties are highly linked. Additionally, breakpoints such as the freezing and boiling points of water must be considered, as these cause a step-change in behavior. For example, perfluorinated polymers like Nafion are very popular electrolytes, but these must be hydrated with liquid water, restricting the temperatures they can operate at. *Fuel Cell Fundamentals* provides a good discussion of some of these dependencies:

"Many PEMFC electrolytes are polymer materials that rely on water-based vehicle mechanisms for ionic transport. Because water is often intimately involved in the ionic transport chain in these electrolyte materials, ionic conductivity tends to be extremely sensitive to the level of hydration. Operation under dry conditions or at temperatures greater than 100°C is therefore severely limited, if not impossible. Because of these hydration and temperature issues, sophisticated water and temperature management schemes are crucially required for most PEMFC-based systems. Designing a polymer electrolyte material capable of operating above 100°C is highly desirable, as this dramatically simplifies water management, while simultaneously improving electrochemical performance and impurity tolerance (electrochemical reaction rates increase exponentially with temperature). In addition to reducing hydration dependence and increasing operating temperature, candidate PEMFC electrolyte materials must also possess high ionic conductivity and good mechanical properties (so they can be processed into thin, durable membranes) and must be highly stable/durable in the PEMFC environment and reasonably inexpensive"[5].

Similar to what was found in **??**, sensitivity analysis shows that while electrochemical performance is very important, system level considerations greatly impact and potentially constrain electrochemical performance and vice versa. Additionally, careful selection of figures of merit for the specific application is critical to understanding relevant benefits and drawbacks. As we saw in this example, in increasing efficiency a designer would not worry about current density. But if the fuel cell application is on a car or airplane, the current density becomes very important as it greatly impacts the specific power.

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[5] O'Hayre, Ryan P., et al. Fuel Cell Fundamentals. Third edition., Wiley, 2016.

4 Analytical Partial Derivatives

Note: ChatGPT was used to help compute and format the derivatives.

4.1 Overall Efficiency

Introduce symbolic derivatives:

$$\begin{aligned}&\frac{d\delta g_{H_2O}}{dT},\quad \frac{d\delta g_{H_2}}{dT},\quad \frac{d\delta g_{O_2}}{dT},\quad \frac{d\delta h_{H_2O}}{dT},\quad \frac{d\delta h_{H_2}}{dT},\quad \frac{d\delta h_{O_2}}{dT},\\ &\frac{d\delta g_{H_2O}}{dP},\quad \frac{d\delta g_{H_2}}{dP},\quad \frac{d\delta g_{O_2}}{dP},\quad \frac{d\delta h_{H_2O}}{dP},\quad \frac{d\delta h_{H_2}}{dP},\quad \frac{d\delta h_{O_2}}{dP}.\end{aligned}$$

Compute the T- and P-partials of v_{cell} and E_h:

$$\begin{aligned}\frac{\partial v_{cell}}{\partial T} &= \frac{d\delta g_{H_2O}}{dT} - \frac{d\delta g_{H_2}}{dT} - \tfrac{1}{2}\frac{d\delta g_{O_2}}{dT} \;+\; \frac{R}{2}\ln\Bigl(\frac{101325}{0.2095\,P}\Bigr),\\ \frac{\partial E_h}{\partial T} &= \frac{d\delta h_{H_2O}}{dT} - \frac{d\delta h_{H_2}}{dT} - \tfrac{1}{2}\frac{d\delta h_{O_2}}{dT},\end{aligned}$$

and

$$\begin{aligned}\frac{\partial v_{cell}}{\partial P} &= \frac{d\delta g_{H_2O}}{dP} - \frac{d\delta g_{H_2}}{dP} - \tfrac{1}{2}\frac{d\delta g_{O_2}}{dP} - \frac{RT}{2P},\\ \frac{\partial E_h}{\partial P} &= \frac{d\delta h_{H_2O}}{dP} - \frac{d\delta h_{H_2}}{dP} - \tfrac{1}{2}\frac{d\delta h_{O_2}}{dP}.\end{aligned}$$

Now apply the product/quotient rule:

$$\boxed{\frac{\partial \eta_{overall}}{\partial T} = \frac{\bigl(\frac{\partial v_{cell}}{\partial T}\bigr)\,E_h - v_{cell}\bigl(\frac{\partial E_h}{\partial T}\bigr)}{{E_h}^2}}$$

Similarly for pressure:

$$\boxed{\frac{\partial \eta_{overall}}{\partial P} = \frac{\bigl(\frac{\partial v_{cell}}{\partial P}\bigr)\,E_h - v_{cell}\bigl(\frac{\partial E_h}{\partial P}\bigr)}{{E_h}^2}}$$

$$
\begin{aligned}
\frac{\partial \eta_{overall}}{\partial T} &= \frac{-\Bigg(\dfrac{d\delta g_{H_2O}}{dT} - \dfrac{d\delta g_{H_2}}{dT} - \frac{1}{2}\dfrac{d\delta g_{O_2}}{dT} + \dfrac{R}{2}\ln\Big(\frac{101325}{0.2095P}\Big)\Bigg)\ E_h}{{E_h}^2} \\
&- \frac{\frac{NR}{F}\Bigg(\Big(-\frac{\ln i_{0_A}}{\alpha_A n_A} - \frac{\ln i_{0_C}}{\alpha_C n_C}\Big) - \Big(\frac{1}{\alpha_A n_A} + \frac{1}{\alpha_C n_C}\Big)\ln(i + i_{leak})\Bigg) E_h}{{E_h}^2} \\
&- \frac{v_{cell}\Big(\dfrac{d\delta h_{H_2O}}{dT} - \dfrac{d\delta h_{H_2}}{dT} - \frac{1}{2}\dfrac{d\delta h_{O_2}}{dT}\Big)}{{E_h}^2}
\end{aligned}
$$

$$
\frac{\partial \eta_{overall}}{\partial P} = \frac{\Big(\dfrac{d\delta g_{H_2O}}{dP} - \dfrac{d\delta g_{H_2}}{dP} - \frac{1}{2}\dfrac{d\delta g_{O_2}}{dP} - \dfrac{RT}{2P}\Big) E_h \ - \ v_{cell}\Big(\dfrac{d\delta h_{H_2O}}{dP} - \dfrac{d\delta h_{H_2}}{dP} - \frac{1}{2}\dfrac{d\delta h_{O_2}}{dP}\Big)}{{E_h}^2}
$$

$$
\frac{\partial \eta_{overall}}{\partial \alpha_A} = -\frac{RT}{F\alpha_A^2 n_A E_h}\left(\ln i_{0_A} - \ln(i - i_{leak})\right),
$$

$$
\frac{\partial \eta_{overall}}{\partial \alpha_C} = -\frac{RT}{F\alpha_C^2 n_C E_h}\left(\ln i_{0_C} - \ln(i - i_{leak})\right),
$$

$$
\frac{\partial \eta_{overall}}{\partial i_{0_A}} = \frac{RT}{F\alpha_A n_A E_h i_{0_A}},
$$

$$
\frac{\partial \eta_{overall}}{\partial i_{0_C}} = \frac{RT}{F\alpha_C n_C E_h i_{0_C}},
$$

$$
\frac{\partial \eta_{overall}}{\partial ASR_\Omega} = -\frac{i}{E_h}
$$

$$
\frac{\partial \eta_{overall}}{\partial C} = -\frac{1}{E_h}\ \ln\Big(\frac{i_L}{i_L - (i + i_{leak})}\Big),
$$

$$
\frac{\partial \eta_{overall}}{\partial i} = \frac{1}{NFE_h}\left(-\frac{\frac{RT}{\alpha_A n_A F} + \frac{RT}{\alpha_C n_C F}}{i + i_{leak}} - ASR_\Omega - \frac{C}{i_L - (i + i_{\text{leak}})}\right),
$$

$$
\frac{\partial \eta_{overall}}{\partial i_{leak}} = \frac{1}{NFE_h}\Bigg(-\frac{\frac{RT}{\alpha_A n_A F} + \frac{RT}{\alpha_C n_C F}}{i + i_{leak}} - \frac{C}{i_L - (i + i_{leak})}\Bigg),
$$

$$
\frac{\partial \eta_{overall}}{\partial i_L} = \frac{1}{NFE_h}\Bigg(-C\Big(\frac{1}{i_L} - \frac{1}{i_L - (i + i_{leak})}\Big)\Bigg).
$$

4.2 Specific Power

$$\begin{aligned}\frac{\partial SP}{\partial T} &= -\frac{i}{\sum \rho_i t_i} \times \left\{ \frac{1}{NF} \left[\frac{d\delta g_{H_2O}}{dT} - \frac{d\delta g_{H_2}}{dT} - \tfrac{1}{2}\frac{d\delta g_{O_2}}{dT} + \frac{R}{2}\ln\left(\tfrac{101325}{0.2095P}\right) \right] \right. \\ &\quad \left. + \frac{R}{F}\left[\left(-\frac{\ln i_{0_A}}{\alpha_A n_A} - \frac{\ln i_{0_C}}{\alpha_C n_C} \right) - \left(\frac{1}{\alpha_A n_A} + \frac{1}{\alpha_C n_C} \right) \ln(i + i_{leak}) \right] \right\}\end{aligned}$$

$$\frac{\partial SP}{\partial P} = -\frac{i}{NF\sum \rho_i t_i} \times \left\{ \frac{d\delta g_{H_2O}}{dP} - \frac{d\delta g_{H_2}}{dP} - \tfrac{1}{2}\frac{d\delta g_{O_2}}{dP} + \frac{RT}{2P} \right\}$$

$$\frac{\partial SP}{\partial \alpha_A} = -\frac{iRT}{F\alpha_A^2 n_A \sum \rho_i t_i}\left(\ln i_{0_A} - \ln(i - i_{leak})\right),$$

$$\frac{\partial SP}{\partial \alpha_C} = -\frac{iRT}{F\alpha_C^2 n_C \sum \rho_i t_i}\left(\ln i_{0_C} - \ln(i - i_{leak})\right),$$

$$\frac{\partial SP}{\partial i_{0_A}} = \frac{iRT}{F\alpha_A n_A \sum \rho_i t_i i_{0_A}},$$

$$\frac{\partial SP}{\partial i_{0_C}} = \frac{iRT}{F\alpha_C n_C \sum \rho_i t_i i_{0_C}},$$

$$\frac{\partial SP}{\partial ASR_\Omega} = -\frac{i^2}{\sum \rho_i t_i}$$

$$\frac{\partial SP}{\partial C} = -\frac{i}{\sum \rho_i t_i}\ln\left(\frac{i_L}{i_L - (i + i_{leak})}\right)$$

$$\begin{aligned}\frac{\partial SP}{\partial i} &= \frac{1}{\sum \rho_i t_i} \times \\ &\left\{ -\frac{1}{NF}\left(-237141 + \delta g_{H_2O}(T,P) - \delta g_{H_2}(T,P) - \tfrac{1}{2}\,\delta g_{O_2}(T,P) + \tfrac{8.314T}{2}\ln\left(\frac{101325}{0.2095\,P}\right) \right) \right. \\ &\quad - \left[-\frac{RT}{\alpha_A n_A F}\ln i_{0_A} - \frac{RT}{\alpha_C n_C F}\ln i_{0_C} \right] - \left[\frac{RT}{\alpha_A n_A F} + \frac{RT}{\alpha_C n_C F} \right] \left(\frac{i}{i + i_{leak}} + \ln(i + i_{leak}) \right) \\ &\quad \left. - 2i\,ASR_\Omega - C\left(\frac{i}{i_L - (i + i_{leak})} + \ln\left(\frac{i_L}{i_L - (i + i_{leak})}\right) \right) \right\}\end{aligned}$$

$$\frac{\partial SP}{\partial i_{leak}} = \frac{i}{\sum \rho_i t_i} \times \left\{ -\frac{\frac{RT}{\alpha_A n_A F} + \frac{RT}{\alpha_C n_C F}}{i + i_{leak}} - C\frac{1}{i_L - (i + i_{leak})} \right\}$$

$$\frac{\partial SP}{\partial i_L} = \frac{i}{\sum \rho_i t_i} \times \left\{ -C \frac{i + i_{leak}}{(i + i_{leak}) i_L - i_L^2} \right\}$$

$$\frac{\partial SP}{\partial \rho_j} = -t_j SP$$

$$\frac{\partial SP}{\partial t_j} = -\rho_j SP$$

Parameter (p)	**Typical Value**	**Sensitivity** $\left(\frac{\partial SP}{\partial p}\right)$	**Normalized Sensitivity** $\left(\frac{p}{SP}\frac{\partial SP}{\partial p}\right)$
Temperature (T)	350 K	5.323e-4	0.146
Pressure (P)	1.013e+5 kPa	7.060e-7	0.0562
Anode Transfer Coefficient (α_A)	0.5	0.379	0.149
Cathode Transfer Coefficient (α_C)	0.2	4.28	0.674
Anode Exchange Current Density (i_{0A})	0.1	0.718	0.0564
Cathode Exchange Current Density (i_{0C})	1.000e-4	898	0.0706
Ohmic Resistance Loss (ASR_Ω)	0.01 Ωcm^2	-3.57	-0.0281
Concentration Loss Constant (C)	0.1	-3.83	-0.301
Current Density (i)	1.5 A/cm^2	0.135	0.159
Leakage Current (i_{leak})	0.1 A/cm^2	-0.696	-0.0547
Limiting Current (i_L)	2 A/cm^2	0.476	0.749
Bipolar Plates Density (ρ_{BP})	3 g/cm^3	-0.254	-0.6
Gas Diffusion Layers Density (ρ_{GDL})	0.4 g/cm^3	-0.0509	-0.016
Catalyst Layers Density (ρ_{cat})	0.4 g/cm^3	-0.0127	-0.004
PEM Density (ρ_{PEM})	2 g/cm^3	-0.00636	-0.01
Bipolar Plates Thickness (t_{BP})	0.2 cm	-3.82	-0.6
Gas Diffusion Layers Thickness (t_{GDL})	0.04 cm	-0.509	-0.016
Catalyst Layers Thickness (t_{cat})	0.01 cm	-0.509	-0.004
PEM Thickness (t_{PEM})	0.005 cm	-2.54	-0.01

Table 2: Specific Power Sensitivity to Parameters Around Typical Values