# ME-5895 Fuel Cells: Assignment 2.2

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**Problem 1**

(a) Plot equilibrium (thermodynamic) potential of $H_2-O_2$ fuel cell as a function of temperature between $25-800°C$.
(b) Plot equilibrium potential of $H_2-O_2$ fuel cell as a function of pressure between 0.1 atm-100 atm at 650 K. Both reactants and products are at the same pressure.
All reactants and products are gas and at 1 atm. You should consider specific heats as variable. Analytical or numerical integration is acceptable.

The overall reaction is defined by

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$$

we define thermodynamic potential as

$$E_{\text{th}} = \frac{-\Delta G}{zF} \tag{1}$$

where $\Delta G$ is the maximum work that is thermodynamically possible for a given reaction. We can write this as the difference between the heat of the reaction and the minimum entropy generation written as

$$\Delta G = \Delta H - T\Delta S \tag{2}$$

which is ultimately a function of temperature since heat of reaction is just

$$\Delta H = \bar{h}_{H_2O} - (\bar{h}_{H_2} + \frac{1}{2}\bar{h}_{O_2})$$

and the heat of formation is

$$\bar{h}_{H_2O} = \bar{h}^{\circ}_{f,H_2O} + \left(\bar{h}(T,p) - \bar{h}(T_0,p_0)\right)_{H_2O}.$$

Obviously, the second term can be written as

$$\Delta\bar{h} = \int_{T_0}^{T} \bar{c_p} dT \tag{3}$$

Similarly, we can define the change in entropy in terms of $c_p$ because

$$\Delta S = \bar{s}_{H_2O} - \left(\bar{s}_{H_2} + \frac{1}{2}\bar{s}_{O_2}\right)$$

where

$$\bar{s}_{H_2O} = \bar{s}^{\circ}_{H_2O} + \left[\bar{s}(T,p) - \bar{s}(T_0,p_0)\right]_{H_2O}$$

and just like before, the second term on the RHS is a function of temperature:

$$\Delta\bar{s} = \int_{T_0}^{T} \frac{c_p}{T} dT \; + \bar{R}\ln\frac{p}{p_0} \tag{4}$$

(assuming ideal gas); for constant pressure we know $p/p_0 = 1$ making the natural log term 0.

Equations (3)-(4) have been solved and are called the Shomate equations, which I used for this analysis. For each species $i \in \{H_2O, H_2, O_2\}$, the Shomate forms are

$$H_i^\circ(T) = A_i t + \frac{B_i t^2}{2} + \frac{C_i t^3}{3} + \frac{D_i t^4}{4} - \frac{E_i}{t} + F_i - H_i \qquad \text{[kJ/mol]} \tag{5}$$

and

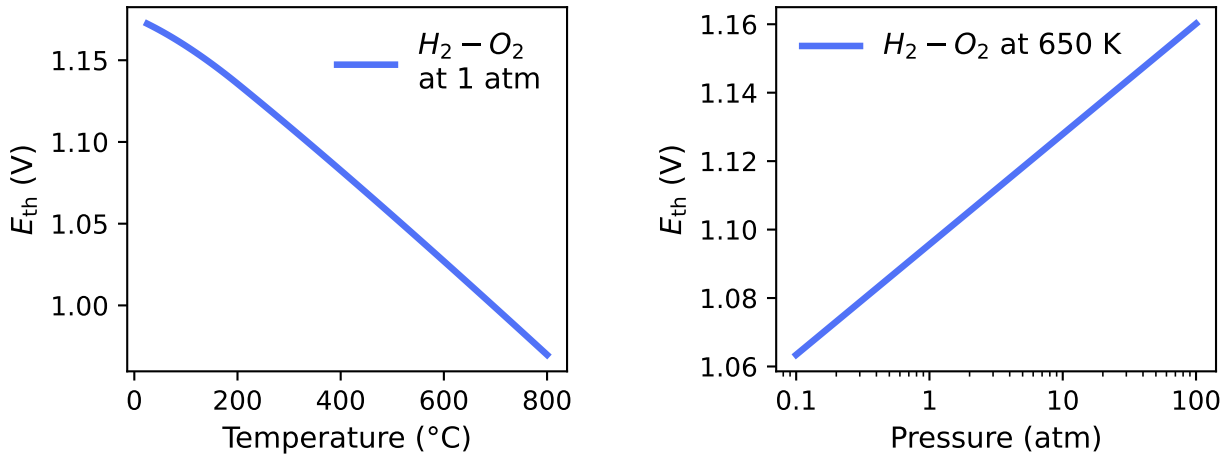
$$S_i^\circ(T) = A_i \ln t + B_i t + \frac{C_i t^2}{2} + \frac{D_i t^3}{3} - \frac{E_i}{2t^2} + G_i \qquad \text{[J/(mol K)]}. \tag{6}$$

The coefficients for these shomate equations for each species are included in the Appendix Table 2 Finally, the thermodynamic (reversible) fuel-cell potential is

$$E_{\text{th}}(T) = -\frac{1}{2F}\left[\Delta H^\circ(T) - \frac{T}{1000}\,\Delta S^\circ(T)\right], \tag{7}$$

with Faraday constant $F$ and $z = 2$ electrons per mole of $H_2$.

I assumed that $C_p$ was constant for $H_2O\,(g)$ from 298K-500K since the shomate equation is defined only from 500K-1078K. This might be a bad assumption.




(a) Thermodynamic potential as a function of temperature

(b) Thermodynamic potential as a function of pressure

**Figure 1:** understanding the impact of different operating conditions on the efficacy of a hydrogen-oxygen fuel cell

## References


Glassman, I., Yetter, R. A., and Glumac, N. G. (2014). *Combustion*. Academic press.

Linstrom, P. J. and Mallard, W. G. (2025). Nist chemistry webbook. NIST Standard Reference Database Number 69, National Institute of Standards and Technology, Gaithersburg, MD, USA. https://webbook.nist.gov/chemistry/.

# Appendix

| | $\Delta h_f$ (kJ/mol) | $S_f^\circ$ (J/mol*K) |
|---|---|---|
| $H_2O$ | -241.83 | 188.84 |
| $H_2$ | 0 | 130.68 |
| $O_2$ | 0 | 205.15 |

**Table 1:** Table values from Glassman et al. (2014)

| Species | $H_2O$ | $H_2$ | $O_2$ |
|---|---|---|---|
| Temperature (K) | 500–1700 | 298–1000 | 298–700 |
| A | 30.09200 | 33.066178 | 31.32234 |
| B | 6.832514 | -11.363417 | -20.23531 |
| C | 6.793435 | 11.432816 | 57.86644 |
| D | -2.534480 | -2.772874 | -36.50624 |
| E | 0.082139 | -0.158558 | -0.007374 |
| F | -250.8810 | -9.980797 | -8.903471 |
| G | 223.3967 | 172.707974 | 246.7945 |
| H | -241.8264 | 0.0 | 0.0 |

**Table 2:** Shomate coefficients Linstrom, P. J. and Mallard, W. G. (2025)

Code used to generate plots can be found here:
https://github.com/mohammadmundiwala/fuel-cells