ME Grad Assignment 2.2: H2-O2 Fuel Cell Thermodynamics

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1 Introduction

This report analyzes the reversible potential of a hydrogen-oxygen fuel cell using variable specific heat models (NIST Shomate Equations)[1] and a constant C_p model for lower temperature regimes.

2 Thermodynamic Results

2.1 Potential vs. Temperature

Figure 1 shows the reversible potential E_{rev} as a function of temperature. We observe a decrease in potential as temperature increases due to the negative entropy of the reaction ΔS_{rxn}.

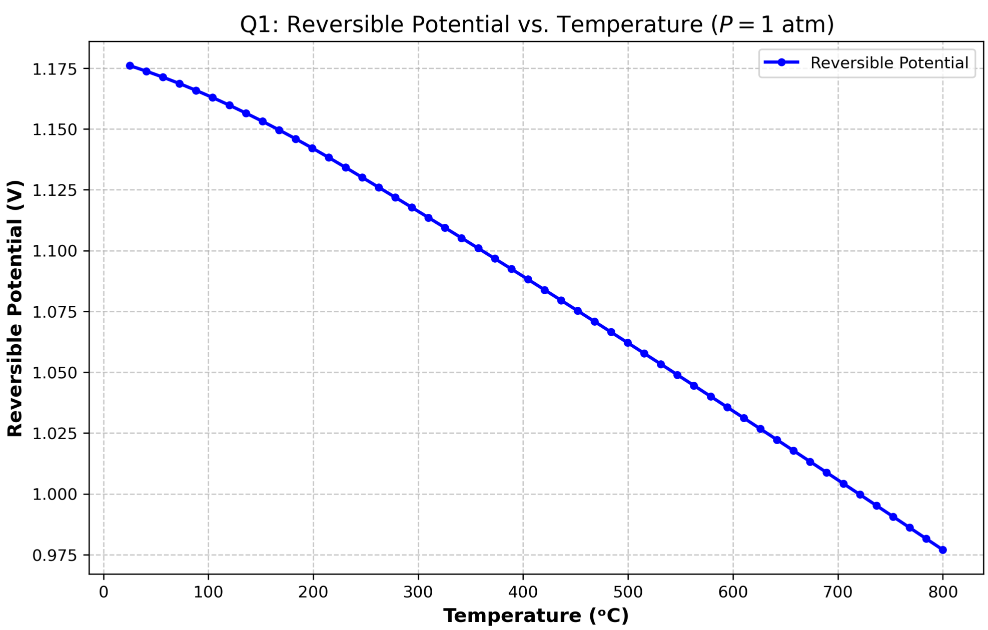

Figure 1: Reversible potential from 25°C to 800°C at $P = 1$ atm.

2.2 Potential vs. Pressure

As shown in Figure 2, the potential increases logarithmically with pressure, consistent with the Nernst relationship.

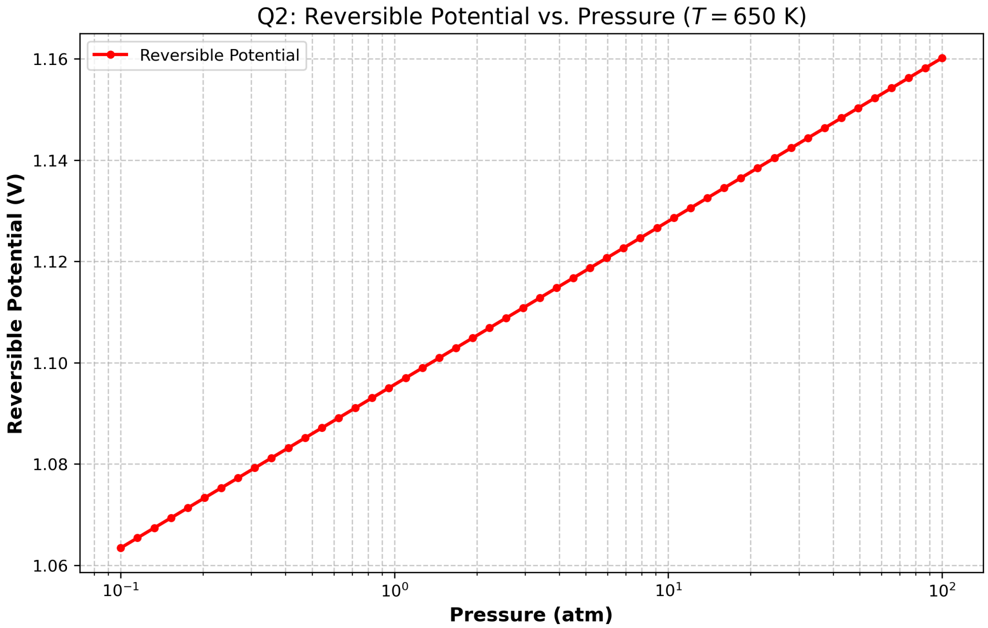

Figure 2: Reversible potential from 0.1 to 100 atm at $T = 650$ K.

3 Mathematical Implementation

The potential was calculated using the Gibbs Free Energy relationship:

$$E_{rev} = -\frac{\Delta G_{rxn}}{nF} = -\frac{\Delta H - T\Delta S}{nF}. \tag{1}$$

The pressure dependence was incorporated using the Nernst equation:

$$E_{rev}(P) = E^0_{rev} - \frac{RT}{nF} \ln\left(\frac{P_{H_2} P_{O_2}^{1/2}}{P_{H_2O}}\right). \tag{2}$$

4 Conclusion

The thermodynamic model successfully captures the voltage drop at higher temperatures and the logarithmic gains with pressure.

5 Code Availability

All Python scripts, thermodynamic coefficients, and diagnostic tools used for this analysis are available on GitHub at: `https://github.com/Ben-JaminRees/Fuel-Cell-Course-Spring-2026/tree/main/Assignment_2_2`.

References

[1] P. J. Linstrom and W. G. Mallard, Eds., *NIST Chemistry WebBook, NIST Standard Reference Database Number 69*. Gaithersburg, MD: National Institute of Standards and Technology. [Online]. Available: https://webbook.nist.gov