

25

Term Projects (2): Thermodynamics

25.1 Estimating Combustion Temperatures

25.2 Generating Entropy Data

Term Project 25.1

Estimating Combustion Temperatures

As described in Part II, Chapter 3, Illustrative Open-ended Problem 2, some reasonable assumptions can be made to simplify the rigorous approach to calculating combustion temperatures. These were detailed at that time. When compared to the rigorous approach, a simpler (and in many instances, a more informative) set of equations resulted, which that are valid for purposes of engineering calculation [1,2]. An approximate enthalpy balance ultimately produced Equation 25.1.

$$T = 60 + \frac{\text{NHV}}{(0.3) \left[1 + (1 + \text{EA})(7.5 \times 10^{-4})(\text{NHV}) \right]} \quad (25.1)$$

Based on the above assumptions and development, you are requested to extend the work of Theodore [1–4]. to include other combustible mixtures. In effect, you are being asked to remove the constraint that the combustible mixture consists of only hydrocarbons.

Term Project 25.2

Generating Entropy Data

With unites constant will those provided in Chapter 2. Based on extensive experimental data, Walther Hermann Nernst (1864 – 1941), a German physicist, postulated a “heat theorem” that the entropy change for any chemical reaction at absolute zero temperature; i.e., 0°R or 0K, was zero. Thus,

$$\Delta S = 0 \text{ at } T = 0 \quad (25.2)$$

Planck, another German physicist, further proposed that at absolute zero temperature

$$S = 0 \quad (25.3)$$

Experimental data has verified these two conclusions. The third law of thermodynamics is based on Equation (25.4); i.e., third law of thermodynamics is concerned with the absolute values of entropy. Thus, by definition,

the entropy of all pure crystalline materials at absolute zero temperature is exactly zero and in line with Equation (25.4)

$$S_{-273^{\circ}\text{C}} = S_{0\text{K}} = 0 \quad (25.4)$$

Note, however, that engineers are usually concerned with *changes* in thermodynamic properties. The third law allows one to calculate the entropy at another temperature via the following equation:

$$\Delta S = \int_0^{T_f} \frac{(C_p)_s}{T} dT + \frac{\Delta H_f}{T_f} + \int_{T_f}^{T_v} \frac{(C_p)_l}{T} dT + \frac{\Delta H_v}{T_v} + \int_{T_v}^T \frac{(C_p)_g}{T} dT \quad (25.5)$$

where the first, third, and fifth terms on the right hand side (RHS) represent the entropy change associated with temperature changes for the solid (s), liquid (l), and gas (g) phases, respectively, and the second and fourth RHS terms represent the entropy change associated with fusion and vaporization, respectively. The terms T , C_p and ΔH represent the absolute temperature, and heat capacity at constant pressure, and latent enthalpy change, respectively, in consistent units. Since the entropy is zero at absolute zero:

$$\Delta S = S_T - S_0 = S_T \quad (25.6)$$

The above equation provides the entropy at the temperature in question, T [2,5].

Based on the above (see also Chapter 3), you are requested to obtain *entropy* values for five chemicals (including water) over the temperature range 0K to the boiling point of the material at 1.0 atmospheric pressure plus saturated vapor values above the boiling point. The chemicals can include oxygen (O_2), chlorine (Cl_2), calcium (Ca), sodium chloride (NaCl), etc. Employ both English and SI units.

References

1. L. Theodore and J. Reynolds, *Thermodynamics*, A Theodore Tutorial, East Williston, NY, originally published by the USEPA/APTI, RTP, NC, 1994.
2. L. Theodore, F. Ricci, and T. VanVliet, *Thermodynamics for the Practicing Engineer*, John Wiley & Sons, Hoboken, NJ, 2009.
3. L. Theodore, *Chemical Engineering: The Essential Reference*, McGraw-Hill, New York City, NY, 2014.

4. Personal notes: L. Theodore, East Williston, NY 1976.
5. L. Theodore and J. Reynolds, *Thermodynamics*, A Theodore Tutorial, East Williston, NY, originally published by the USEPA/APTI, RTP, NC, 1991.