**Equivalence of Notation between Introductory Chemical Engineering Thermodyanamics (Elliott and Lira) and Elements of Chemical Reaction Engineering (Fogler, 3rd ed.) for Energy Balance in Reacting Systems.**

The presentation of the reacting system energy balance differs in chemical engineering textbooks, which can be confusing when first learning the material. This handout compares the notation in two textbooks to help students compare and make the transition between textbooks. The first part of the handout starts with the energy balance from Introductory Chemical Engineering Thermodynamics (E&L), and results in an equation using the notation used in Elemements of Chemical Reaction Engineering (Fogl). The second part of the handout starts from Elements of Chemical Reaction Engineering, and results in the same equation. This handout considers a single reaction.

Consider the reaction

$$a\mathrm{A} + b\mathrm{B} = c\mathrm{C} + d\mathrm{D} \tag{1}$$

The energy balance in Introductory Chemical Engineering Thermodynamics uses reactions in this generic form. To use Fogler's notation, once the limiting reactant is identified, it is designated as A. All of Fogler's notation is for the reaction written as

$$\mathrm{A} + (b/a)\mathrm{B} = (c/a)\mathrm{C} + (d/a)\mathrm{D} \tag{2}$$

First of all, a table is presented to compare notation from the two textbooks.

**Table 1: Comparison of notation between the two texts.**

| | E & L | Fogler |
|---|---|---|
| Stoichiometric number | $\nu_i$ | $-a, -b, c, d$ |
| Molar flowrate of A into reactor. | $\dot{n}_A^{in}$ | $F_{A0}$ |
| Molar flowrate of A out of reactor. | $\dot{n}_A^{out} = \dot{n}_A^{in} - a\dot{\xi}$ | $F_A = F_{A0}(1-X)$ |
| Heat of reaction | $\Delta H^o_{298} = a\Delta H^o_{Rx}(T_R)_{\text{Fogl}}$ | $\Delta H^o_{Rx}(T_R)_{\text{Fogl}} = \dfrac{\Delta H^o_{298}}{a}$ |
| Reaction Coordinate/Conversion | $\dot{\xi} = \dfrac{F_{A0}X}{a}$ | $X_A = \dfrac{a\dot{\xi}}{\dot{n}_A^{in}}$ |

The energy balance from Introductory Chemical Engineering Thermodyanamics, Eqn. (14.36) pg 496 is

$$0 = \sum_i \dot{n}_i^{in}\int_{298}^{T^{in}} C_{P,i}\,dT - \sum_i \dot{n}_i^{out}\int_{298}^{T^{out}} C_{P,i}\,dT + \dot{Q} - \dot{\xi}\Delta H^o_{298} \tag{3}$$

For a single rxn $\dot{n}^{out} = \dot{n}^{in} + \nu_i\dot{\xi}$, and using the shorthand notation, $\sum_i \nu_i C_{P,i} = \Delta C_P$ the energy balance becomes,

$$0 = \sum_i \dot{n}_i^{in} \int_{T^{out}}^{T^{in}} C_{P,i} dT - \dot{\xi} \int_{298}^{T^{out}} \Delta C_P dT + \underline{\dot{Q}} - \dot{\xi} \Delta H^o_{298} \tag{4}$$

to adapt some of Fogler notation, $n_i^{in} = F_{i0} = F_{A0}\Theta_i$, resulting in

$$\boxed{0 = F_{A0}\left[\sum_i \Theta_i \int_{T^{out}}^{T^{in}} C_{P,i} dT - \frac{X}{a}\int_{298}^{T^{out}} \Delta C_P dT\right] + \underline{\dot{Q}} - \frac{F_{A0}}{a}\Delta H^o_{298} X} \tag{5}$$

ignoring the difference in heat capacities between the feed and products, and using a mean specific heat for the feed and products,

$$\boxed{0 = \dot{m} C_{Pm}(T^{in} - T^{out}) + \underline{\dot{Q}} - \frac{F_{A0}}{a}\Delta H^o_{298} X} \tag{6}$$

The energy balance in Elements of Chemical Reaction Engineering is given in Eqn. (8-30) on pg 435 (dropping the work term) as

$$0 = -F_{A0}\left[\sum_i \Theta_i \tilde{C}_{Pi}(T - T_{i0})\right] - F_{A0} X \Delta \hat{C}_P (T - T_R) + \dot{Q} - F_{A0} X \Delta H^o_{Rx}(T_R) \tag{7}$$

where $\dot{Q}_{\text{Fogl}} = \underline{\dot{Q}}$ is the total heat transfer rate, and Fogler uses

$$\sum_i (v_i/a) C_{P,i} = \Delta C_{P,\text{Fogler}} = \Delta C_P / a \tag{8}$$

The heat capacity terms are given by Fogler's (8-28) $\Delta \hat{C}_P (T - 298.15) = \frac{1}{a}\int_{298}^{T^{out}} \Delta C_P dT$, and Eqn. (8-29), $-\tilde{C}_{Pi}(T - T_{i0}) = \int_{T^{out}}^{T^{in}} C_{P,i} dT$. Plugging in these terms, and the relation for the heat of reaction, results in Eqn (5).

$$\boxed{0 = F_{A0}\left[\sum_i \Theta_i \int_{T^{out}}^{T^{in}} C_{P,i} dT - \frac{X}{a}\int_{298}^{T^{out}} \Delta C_P dT\right] + \underline{\dot{Q}} - \frac{F_{A0}}{a}\Delta H^o_{298} X} \tag{9}$$