

## Equivalence of Notation between Introductory Chemical Engineering Thermodynamics (Elliott and Lira) and Chemical Reaction Engineering (Levenspiel, 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 Chemical Reaction Engineering (Lev). The second part of the handout starts from Chemical Reaction Engineering, and results in the same equation. This handout considers a single reaction.

Consider the reaction



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



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	Lev
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.	$\dot{n}_A^{out} = \dot{n}_A^{in} - a\dot{\xi}$	$F_A = F_{A0}(1 - X_A)$
Heat of reaction	$\Delta H_{298}^o = a\Delta H_{298}^o(\text{Lev})$	$\Delta H_{298}^o(\text{Lev}) = \frac{\Delta H_{298}^o}{a}$
Reaction Coordinate/Conversion	$\dot{\xi} = \frac{F_{A0}X_A}{a}$	$X_A = \frac{a\dot{\xi}}{\dot{n}_A^{in}}$

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

$$0 = \sum_i \dot{n}_i^{in} \int_{298}^{T^{in}} C_{P,i} dT - \sum_i \dot{n}_i^{out} \int_{298}^{T^{out}} C_{P,i} dT + \dot{Q} - \dot{\xi} \Delta H_{298}^o \quad (3)$$

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,

$$0 = \sum_i \dot{n}_i^{in} \int_{T^{out}}^{T^{in}} C_{P,i} dT - \xi \int_{298}^{T^{out}} \Delta C_P dT + \underline{\dot{Q}} - \xi \Delta H_{298}^o \quad (4)$$

to adapt some of Lev. notation,  $n_i^{in} = F_{i0} = F_{A0}(M_i)$  where the variable  $M$  has been generalized to  $M_i = F_{i0}/F_{A0}$ , resulting in

$$0 = F_{A0} \left[ \sum_i M_i \int_{T^{out}}^{T^{in}} C_{P,i} dT - \frac{X_A}{a} \int_{298}^{T^{out}} \Delta C_P dT \right] + \underline{\dot{Q}} - \frac{F_{A0}}{a} \Delta H_{298}^o X_A \quad (5)$$

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

$$0 = \dot{m} C_{Pm} (T^{in} - T^{out}) + \underline{\dot{Q}} - \frac{F_{A0}}{a} \Delta H_{298}^o X_A \quad (6)$$

Starting with the notation from Chemical Reaction Engineering, the heat capacities are per mole of A in the feed, therefore,

$$C_P' = \sum_i M_i C_{P,i}, \quad C_P'' = \sum_i \left( M_i + \frac{v_i}{a} \right) C_{P,i} = C_P' + \frac{\Delta C_P}{a}, \quad (7)$$

The energy balance in Chemical Reaction Engineering is given on pg 225 as

$$0 = C_P''(T_2 - T_1)X_A + C_P'(T_2 - T_1)(1 - X_A) + Q - \Delta H_{r1}X_A \quad (8)$$

where  $Q$  is the heat transfer per mole of A. This equation may be expressed as

$$0 = C_P'(T_2 - T_1) + (\Delta C_P/a)(T_2 - T_1)X_A + Q - \Delta H_{r1}X_A \quad (9)$$

The heat of reaction at  $T_1$  is  $\Delta H_{r1}$ , which can be related to the heat of reaction at any reference temperature  $T_R$ ,

$$\Delta H_{r1} = C_P'(T_1 - T_R) + \Delta H_R^o + C_P''(T_R - T_1) = (\Delta C_P/a)(T_R - T_1) + \Delta H_R^o(\text{Lev}) \quad (10)$$

Plugging this into (9) results in

$$0 = C_P'(T_2 - T_1) + X_A(\Delta C_P/a)(T_2 - T_R) + Q - \Delta H_R^o(\text{Lev})X_A \quad (11)$$

Inserting the following E&L notation, and using 298.15 K as the standard state temperature,

$$\Delta H_R^o(\text{Lev}) = \Delta H_R^o/a, \quad Q(\text{Lev}) = \underline{\dot{Q}}(\text{E\&L})/F_{A0} \quad (12)$$

results in

$$0 = \sum_i M_i \int_{T^{out}}^{T^{in}} C_{P,i} dT - \frac{X_A}{a} \int_{298}^{T^{out}} \Delta C_P dT + \frac{\underline{\dot{Q}}}{F_{A0}} - \frac{X_A}{a} \Delta H_{298}^o \quad (13)$$

which results in Eqn. (5) when multiplied by  $F_{A0}$ .