

## HW6 Batch Reactor Balances

It is not legitimate to simply take the CSTR enthalpy balance and set the flow terms to zero. This is an incorrect enthalpy balance on the reactor in batch mode. See below for a review of how to use thermodynamics in this situation.

Given that there is negligible gas holdup in the reactor:

$$N_B(t) = N_C(t) = 0$$

hence,

$$\frac{dN_B}{dt} = \frac{dN_C}{dt} = 0$$

Enthalpy balance:

$$\frac{dH}{dt} = \frac{d(N_A H_A + N_B H_B + N_C H_C)}{dt} = \frac{d(N_A H_A)}{dt} = \frac{dN_A}{dt} H_A + \frac{dH_A}{dt} N_A$$

$$\frac{dH}{dt} = \dot{Q} - F_B H_B - F_C H_C$$

$$\frac{dN_A}{dt} H_A + \frac{dH_A}{dt} N_A = \dot{Q} - F_B H_B - F_C H_C$$

Batch Reactor mole balances:

$$\frac{dN_A}{dt} = -kN_A$$

$$\frac{dN_B}{dt} = 0 = -F_{B,out} + kN_A$$

$$F_{B,out} = kN_A$$

$$\frac{dN_C}{dt} = 0 = -F_{C,out} + 2kN_A$$

$$F_{C,out} = 2kN_A$$

Plugging in the three mole balance relationships into the enthalpy balance we find:

$$-kN_A H_A + \frac{dH_A}{dt} N_A = \dot{Q} - kN_A H_B - 2kN_A H_C$$

$$\frac{dH_A}{dt} N_A = \dot{Q} - kN_A (H_B + 2H_C - H_A) = \dot{Q} - kN_A \Delta H_{rxn}(T)$$

$$\frac{dH_A}{dt} = c_{p,a} \frac{dT}{dt}$$

$$\frac{dT}{dt} = \frac{\dot{Q} - kN_A \Delta H_{rxn}(T)}{N_A c_{p,a}} = \frac{\dot{Q} - km_A \Delta \hat{H}_{rxn}(T)}{m_A \hat{c}_{p,a}}$$