Lecture 20: PFR Energy Balance

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last updated: October 20, 2009

We proceed in our analysis of the PFR with the following assumptions.

Assumption 1: the internal energy is not a function of molar volume.
Assumption 2: The mixture is an ideal mixture.
Assumption 3: The heat capacity is constant.
Assumption 4: The reactor volume is constant.

In the hand-out titled, "Forms of the Microscopic Energy Balance", we derived previously the PFR energy balance,

$$\rho \frac{\partial\left(\frac{1}{2}v^2 + \hat{H} + \hat{\Phi}\right)}{\partial t} - \frac{\partial p}{\partial t} = -\rho \mathbf{v}\nabla \cdot \left(\frac{1}{2}v^2 + \hat{H} + \hat{\Phi}\right) - \nabla \cdot \mathbf{q} - \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{v}) \quad . \tag{1}$$

Assumption 5: The PFR is at steady state.
Assumption 6: The PFR has variation only in the axial dimension.

At steady state, the accumulation terms are 0. If we assume that there is variation in the axial dimension only, then we have

$$0 = -\rho v_z \frac{\partial}{\partial z}\left(\frac{1}{2}v^2 + \hat{H} + \hat{\Phi}\right) - \frac{\partial q_z}{\partial z} - \frac{\partial \tau_{zz} v_z}{\partial z} \quad . \tag{2}$$

Assumption 7: We neglect heat conduction.
Assumption 8: We neglect viscous heating.
Assumption 9: The pipe is horizontal so that there is no effect of gravity.
Assumption 10: The fluid is incompressible so the change in kinetic energy is negligible.

$$0 = \rho \frac{\partial \hat{H}}{\partial z} = \frac{\partial \rho \hat{H}}{\partial z} \quad . \tag{3}$$

This can also be written on a molar basis as

$$0 = \frac{\partial C_T \underline{H}_{mix}}{\partial z} \quad . \tag{4}$$

where

$$\underline{H}_{mix} = \sum_{i=1}^{N_c} x_i \underline{H}_i = \frac{1}{C_T} \sum_{i=1}^{N_c} C_i \underline{H}_i$$

$$C_T \underline{H}_{mix} = \sum_{i=1}^{N_c} C_i \underline{H}_i$$

$$\frac{\partial C_T \underline{H}_{mix}}{\partial z} = \sum_{i=1}^{N_c} \left(C_i \frac{\partial \underline{H}_i}{\partial z} + \underline{H}_i \frac{\partial C_i}{\partial z} \right)$$

$$\underline{H}_i = C_{p,i}\left(T - T_{ref}\right) + \underline{H}_{f,i}(T_{ref}, p_{ref})$$

$$\frac{\partial \underline{H}_i}{\partial z} = C_{p,i} \frac{\partial T}{\partial z}$$

$$\frac{\partial C_T \underline{H}_{mix}}{\partial z} = \sum_{i=1}^{N_c} \left(C_i C_{p,i} \frac{\partial T}{\partial z} + \underline{H}_i \frac{\partial C_i}{\partial z} \right)$$

We now need to substitute in the mole balance for the PFR, which we derived earlier as

$$v_z \frac{dC_i}{dz} = \nu_i r$$

$$\frac{\partial C_T \underline{H}_{mix}}{\partial z} = \sum_{i=1}^{N_c} \left(C_i C_{p,i} \frac{\partial T}{\partial z} + \frac{\underline{H}_i \nu_i r}{v_z} \right)$$

where

$$v_z = \frac{F}{A_x}$$

so that the energy balance becomes

$$\frac{\partial C_T \underline{H}_{mix}}{\partial z} = \sum_{i=1}^{N_c} \left(C_i C_{p,i} \frac{\partial T}{\partial z} + \frac{\underline{H}_i \nu_i r}{v_z} \right) = 0$$

$$\left(\sum_{i=1}^{N_c} C_i C_{p,i} \right) \frac{\partial T}{\partial z} + \left(\sum_{i=1}^{N_c} \underline{H}_i \nu_i \right) \frac{r}{v_z} = 0$$

$$C_T C_{p,mix} \frac{\partial T}{\partial z} + \Delta H_R \frac{r}{v_z} = 0$$

where

$$\Delta H_R = \sum_{i=1}^{N_c} \left(\underline{H}_i \nu_i \right) \text{ and}$$

$$C_{p,mix} = \sum_{i=1}^{N_c} \left(x_i C_{p,i}(T) \right) \text{ so that}$$

$$C_T C_{p,mix} = \sum_{i=1}^{N_c} \left(C_i C_{p,i}(T) \right)$$

We can rearrange this as

$$\frac{\partial T}{\partial z} = \frac{-\Delta H_R \frac{r}{v_z}}{C_T C_{p,mix}}$$

This is the energy balance for the steady state PFR, given the assumptions above.

However in the interests of maintaining some continuity with Fogler, let’s also consider the following additional analysis.

$$C_A = C_{A,in}\left(1 - X_A\right)$$

$$\frac{dC_A}{dz} = -C_{A,in} \frac{dX_A}{dz}$$

$$-C_{A,in} v_z \frac{dX_A}{dz} = \nu_A r$$

so the reaction rate can be eliminated from the energy balance and written as

$$\frac{dT}{dz} = \frac{\Delta H_R \frac{C_{A,in}}{\nu_A}}{C_T C_{p,mix}} \frac{dX_A}{dz}$$

$$\frac{dT}{\Delta H_R} = \frac{C_{A,in}}{\nu_A C_T C_{p,mix}} dX_A$$

We need to express every variable in terms of temperature, conversion and constants in order to integrate.

All of the compositions can be written as

$$C_i = C_{i,in} + \frac{\nu_i}{\nu_A}\left(C_A - C_{A,in}\right)$$

$$C_i = C_{i,in} + \frac{\nu_i}{\nu_A}\left(C_{A,in}\left(1 - X_A\right) - C_{A,in}\right) = C_{i,in} - \frac{\nu_i}{\nu_A} C_{A,in} X_A$$

So that

$$C_T C_{p,mix} = \sum_{i=1}^{N_c}\left(C_i C_{p,i}\right) = \sum_{i=1}^{N_c}\left(\left(C_{i,in} - \frac{\nu_i}{\nu_A} C_{A,in} X_A\right) C_{p,i}\right)$$

$$C_T C_{p,mix} = \sum_{i=1}^{N_c}\left(C_i C_{p,i}\right) = \sum_{i=1}^{N_c} C_{i,in} C_{p,i} - \frac{C_{A,in}}{\nu_A} X_A \sum_{i=1}^{N_c} \nu_i C_{p,i}$$

$$C_T C_{p,mix} = \sum_{i=1}^{N_c}\left(C_i C_{p,i}\right) = C_{T,in} C_{p,mix,in} - \frac{C_{A,in}}{\nu_A} \Delta C_p X_A$$

where

$$C_{T,in} C_{p,mix,in} = \sum_{i=1}^{N_c} C_{i,in} C_{p,i}$$

$$\Delta C_p = \sum_{i=1}^{N_c} \nu_i C_{p,i}$$

Furthermore,

$$\Delta H_R = \sum_{i=1}^{N_c}\left(\underline{H}_i \nu_i\right) = \sum_{i=1}^{N_c} \nu_i C_{p_i}\left(T - T_{ref}\right) + \sum_{i=1}^{N_c} \nu_i H_{f,i}\left(T_{ref}\right)$$

$$\Delta H_R = \sum_{i=1}^{N_c}\left(\underline{H}_i \nu_i\right) = \left(T - T_{ref}\right)\Delta C_p + \Delta H_R\left(T_{ref}\right)$$

If we now substitute into our energy balance, we have

$$\frac{dT}{\left(T-T_{ref}\right)\Delta C_p+\Delta H_R\left(T_{ref}\right)}=\frac{C_{A,in}}{\nu_A C_{T,in}C_{p,mix,in}-C_{A,in}\Delta C_p X_A}dX_A$$

Integrate. Both of the integrals have the form

$$\int\frac{dx}{ax+b}=\frac{1}{a}\ln(ax+b) \qquad \text{or} \qquad \int_{x_o}^{x_f}\frac{dx}{ax+b}=\frac{1}{a}\ln\left(\frac{ax_f+b}{ax_o+b}\right)$$

$$\int_{T_{in}}^{T}\frac{dT}{\left(T-T_{ref}\right)\Delta C_p+\Delta H_R\left(T_{ref}\right)}=\frac{1}{\Delta C_p}\ln\left(\frac{\left(T-T_{ref}\right)\Delta C_p+\Delta H_R\left(T_{ref}\right)}{\left(T_{in}-T_{ref}\right)\Delta C_p+\Delta H_R\left(T_{ref}\right)}\right)$$

$$\int_0^{X_A}\frac{dX_A}{\nu_A\frac{C_{T,in}}{C_{A,in}}C_{p,mix,in}-\Delta C_p X_A}=-\frac{1}{\Delta C_p}\ln\left(\frac{\nu_A\frac{C_{T,in}}{C_{A,in}}C_{p,mix,in}-\Delta C_p X_A}{\nu_A\frac{C_{T,in}}{C_{A,in}}C_{p,mix,in}}\right)$$

Equating the two terms

$$\frac{1}{\Delta C_p}\ln\left(\frac{\left(T-T_{ref}\right)\Delta C_p+\Delta H_R\left(T_{ref}\right)}{\left(T_{in}-T_{ref}\right)\Delta C_p+\Delta H_R\left(T_{ref}\right)}\right)=-\frac{1}{\Delta C_p}\ln\left(\frac{\nu_A\frac{C_{T,in}}{C_{A,in}}C_{p,mix,in}-\Delta C_p X_A}{\nu_A\frac{C_{T,in}}{C_{A,in}}C_{p,mix,in}}\right)$$

Simplifying

$$\left(\left(T-T_{ref}\right)\Delta C_p+\Delta H_R\left(T_{ref}\right)\right)\left(\nu_A\frac{C_{T,in}}{C_{A,in}}C_{p,mix,in}-\Delta C_p X_A\right)=\nu_A\frac{C_{T,in}}{C_{A,in}}C_{p,mix,in}\left(\left(T_{in}-T_{ref}\right)\Delta C_p+\Delta H_R\left(T_{ref}\right)\right)$$

Simplify

$$\left(T-T_{in}\right)\nu_A\frac{C_{T,in}}{C_{A,in}}C_{p,mix,in}-\left(\left(T-T_{ref}\right)\Delta C_p+\Delta H_R\left(T_{ref}\right)\right)X_A=0$$

or

$$X_A=\frac{\left(T-T_{in}\right)\nu_A\frac{C_{T,in}}{C_{A,in}}C_{p,mix,in}}{\left(T-T_{ref}\right)\Delta C_p+\Delta H_R\left(T_{ref}\right)}$$

Compare this equation to Fogler, equation (8-29) on page 486. They are completely equivalent.