Lecture 20: Temperature Control in Non-isothermal Reactors

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I. Jacketed Batch reactors and CSTRs

Consider a reactor in a jacket. The jacket can either heat or cool the contents of the reactor. The reactor has a surface Area, A_s. There is an overall heat transfer coefficient, U. The coolant (or heating fluid) flows into the jacket at $T_{j,in}$ and flows out at T_j. For simplicity, we assume that heat transfer is determined by the temperature of the reactor, T, which is homogeneous and the outlet temperature of the coolant. In this case, the rate of heat transferred from the reactor to the coolant is

$$\dot{Q} = A_S U \left(T_j - T\right)$$

If the reactor is hotter than the jacket, this is a negative quantity and heat is leaving the system. The material balance on the jacket is

$$\frac{dC_j}{dt} = \frac{F_j}{V_j} C_{j,in} - \frac{F_j}{V_j} C_j$$

The outlet concentration and flowrate of coolant are the same as the inlet concentration and flowrate. In other words, there is no net accumulation of coolant in the jacket, as we expect. The energy balance on the coolant in the jacket is

$$\frac{dC_j \underline{H}_j}{dt} = \frac{F_j}{V_j} C_{j,in} \underline{H}_{j,in} - \frac{F_j}{V_j} C_j \underline{H}_j - \frac{\dot{Q}}{V_j}$$

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

$$\frac{\partial \underline{H}_j}{\partial t} = C_{p,j} \frac{\partial T}{\partial t}$$

$\frac{\partial C_j}{\partial t} = 0$ We assume there is no temperature dependence on the density.

$$\frac{\partial C_j \underline{H}_j}{\partial t} = C_j \frac{\partial \underline{H}_j}{\partial t} + \underline{H}_j \frac{\partial C_j}{\partial t} = C_j C_{p,j} \frac{\partial T}{\partial t}$$

Substitute into the jacket energy balance

$$\frac{\partial T}{\partial t}=\frac{\frac{F_j}{V_j}C_{j,in}\underline{H}_{j,in}-\frac{F_j}{V_j}C_j\underline{H}_j-\frac{\dot{Q}}{V_j}}{C_jC_{p,j}}$$

Substitute for Enthalpy and heat loss

$$\frac{\partial T}{\partial t}=\frac{\frac{F_j}{V_j}C_j\left(C_{p,j}\left(T_{j,in}-T_{ref}\right)+\underline{H}_{f,j}(T_{ref},p_{ref})\right)-\frac{F_j}{V_j}C_j\left(C_{p,j}\left(T_j-T_{ref}\right)+\underline{H}_{f,j}(T_{ref},p_{ref})\right)-\frac{A_SU\left(T_j-T\right)}{V_j}}{C_jC_{p,j}}$$

simplify

$$\frac{\partial T}{\partial t}=\frac{\frac{F_j}{V_j}C_jC_{p,j}\left(T_{j,in}-T_j\right)-\frac{A_SU\left(T_j-T\right)}{V_j}}{C_jC_{p,j}}=\frac{F_j}{V_j}\left(T_{j,in}-T_j\right)-\frac{A_SU\left(T_j-T\right)}{C_jC_{p,j}V_j}$$

This is the jacket energy balance.

The corresponding reactor energy balances are

$$\frac{dT}{dt}=\frac{-V_r\Delta H_Rr+\dot{Q}}{C_TC_{p,mix}V_r}$$ for a batch reactor

$$\frac{dT}{dt}=\frac{F_{in}C_{T,in}C_{p,mix,in}\left(T_{in}-T\right)-V_r\Delta H_Rr+\dot{Q}}{C_TC_{p,mix}V_r}$$ for a CSTR

II. Jacketed PFRs

The difference between batch reactors/CSTRs and PFRs is that the temperature in a batch reactor or CSTR is homogeneous whereas the temperature in a PFR varies along the axial position.

A jacketed PFR can be considered as a shell and tube heat exchanger in which chemical reaction takes place within the tube. The temperature of the jacket may also vary along the axial position, as it does in the reactor. The rate of heat transfer from shell to tube (along the radial dimension) therefore is now a function of axial position.

$$\dot{Q}(z)=A_SU\left(T_j(z)-T(z)\right)$$

The energy balance on the jacket is taken from the “Forms of the Microscopic Energy Balance” handout, where we include an additional energy loss term.

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

When you make all the assumptions that we previously made for the PFR, namely

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

Then you have

$$0=-\rho v_z \frac{d\hat{H}}{dz}-\frac{\dot{Q}}{V_j}$$

converting to moles and subscripting jacket properties with a j in order to distinguish them from reactor properties, we have,

$$0=-C_j v_{z,j}\frac{d\underline{H}_j}{dz}-\frac{\dot{Q}}{V_j}$$

$$\frac{\partial \underline{H}_j}{\partial z}=C_{p,j}\frac{\partial T_j}{\partial z}$$

$$0=-C_j v_{z,j}C_{p,j}\frac{\partial T_j}{\partial z}-\frac{\dot{Q}}{V_j}$$

$$0=-C_j v_{z,j}C_{p,j}\frac{\partial T_j}{\partial z}-\frac{A_S U(T_j-T)}{V_j}$$

$$\frac{\partial T_j}{\partial z}=-\frac{A_S U(T_j-T)}{v_{z,j}C_j C_{p,j}V_j}$$

This is the jacket energy balance. For a cylindrical jacket around a cylindrical reactor, the ratio of the surface area to the volume is

$$\frac{A_S}{V_j} = \frac{2\pi R_r L}{\left(\pi R_j^2 - \pi R_r^2\right)L} = \frac{2R_r}{R_j^2 - R_r^2}$$

The energy balance on the reactor can be derived in a similar fashion. We include the additional heat loss/gain term.

$$\frac{\partial T}{\partial z} = \frac{-\Delta H_R r + \frac{A_S}{V_r} U\left(T_j - T\right)}{v_{z,r} C_T C_{p,mix}}$$

For a cylindrical reactor, the ratio of surface area to volume is

$$\frac{A_S}{V_r} = \frac{2\pi R_r L}{\pi R_r^2 L} = \frac{2}{R_r}$$

The sign on the heat loss is opposite in the reactor energy balance from that in the jacket energy balance since any energy leaving the reactor enters the jacket.