Lecture 20: CSTR Energy Balance

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In a CSTR, we have accumulation, in and out terms in the energy balance.

We proceed 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 this case, the accumulation term has the form: (See the Batch Reactor Energy Balance Notes)

$$acc = V\frac{d\left(C_T \underline{H}_{mix}\right)}{dt} = V\frac{d}{dt}\sum_{i=1}^{N_c} C_i\left(C_{p,i}\left(T - T_{ref}\right) + \underline{H}_{f,i}(T_{ref}, p_{ref})\right)$$

$$acc = V\frac{d\left(C_T \underline{H}_{mix}\right)}{dt} = V\left(\sum_{i=1}^{N_c} \underline{H}_i \frac{dC_i}{dt} + \sum_{i=1}^{N_c} C_i C_{p,i}\left(\frac{dT}{dt}\right)\right)$$

In the batch reactor, we had a mole balance that looked like this

$$\frac{dC_i}{dt} = \nu_i r$$

In the CSTR, we have a mole balance that looks like

$$\frac{dC_i}{dt} = \frac{F_{in}}{V}C_{i,in} - \frac{F_{out}}{V}C_i + \nu_i r$$

If we substitute this into the accumulation term, we have

$$acc = V\frac{d\left(C_T \underline{H}_{mix}\right)}{dt} = V\left(\sum_{i=1}^{N_c} \underline{H}_i \left(\frac{F_{in}}{V}C_{i,in} - \frac{F_{out}}{V}C_i + \nu_i r\right) + \sum_{i=1}^{N_c} C_i C_{p,i}\left(\frac{dT}{dt}\right)\right)$$

Rearranging yields

$$acc = V\frac{d\left(C_T \underline{H}_{mix}\right)}{dt} = V\left(\sum_{i=1}^{N_c} \underline{H}_i \left(\frac{F_{in}}{V} C_{i,in} - \frac{F_{out}}{V} C_i\right) + \Delta H_R r + C_T C_{p,mix}\left(\frac{dT}{dt}\right)\right)$$

where

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

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

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

This can also be written as

$$acc = V\frac{d\left(C_T \underline{H}_{mix}\right)}{dt} = V\left(\sum_{i=1}^{N_c} \underline{H}_i \left(\frac{F_{in}}{V} C_{i,in} - \frac{F_{out}}{V} C_i\right) + \Delta H_R r + C_T C_{p,mix}\left(\frac{dT}{dt}\right)\right)$$

The in term has the following form

$$in = F_{in} C_{T,in} \underline{H}_{mix}(C_{i,in}, T_{in}) = F_{in} \sum_{i=1}^{N_c} C_{i,in}\left(C_{p,i}\left(T - T_{ref}\right) + \underline{H}_{f,i}(T_{ref}, p_{ref})\right)$$

$$in = F_{in}\left(C_{T,in} C_{p,mix,in}\left(T_{in} - T_{ref}\right) + \sum_{i=1}^{N_c} C_{i,in} \underline{H}_{f,i}(T_{ref}, p_{ref})\right)$$

That is internal energy can enter as energy stored by the heat capacity of the material, relative to the reference state.

The out term is analogous to the in term

$$out = F_{out} C_T \underline{H}_{mix}(C_i, T) = F_{out}\left(C_T C_{p,mix}\left(T - T_{ref}\right) + \sum_{i=1}^{N_c} C_i \underline{H}_{f,i}(T_{ref}, p_{ref})\right)$$

If we put acc = in – out + generation and set the generation term to zero, we have

$$V\frac{d\left(C_T \underline{H}_{mix}\right)}{dt} = F_{in} C_{T,in} \underline{H}_{mix}(C_{i,in}, T_{in}) - F_{out} C_T \underline{H}_{mix}(C_i, T)$$

Substituting acc, in and out into the energy balance yields

$$V\left(\sum_{i=1}^{N_c}\underline{H}_i\left(\frac{F_{in}}{V}C_{i,in}-\frac{F_{out}}{V}C_i\right)+\Delta H_R r+C_T C_{p,mix}\left(\frac{dT}{dt}\right)\right)$$
$$=F_{in}\left(C_{T,in}C_{p,mix,in}\left(T_{in}-T_{ref}\right)+\sum_{i=1}^{N_c}C_{i,in}\underline{H}_{f,i}(T_{ref},p_{ref})\right)$$
$$-F_{out}\left(C_T C_{p,mix}\left(T-T_{ref}\right)+\sum_{i=1}^{N_c}C_i\underline{H}_{f,i}(T_{ref},p_{ref})\right)$$

We can also substitute in the form of the enthalpy in the accumulation term

$$V\left(\sum_{i=1}^{N_c}\left(C_{p,i}\left(T-T_{ref}\right)+\underline{H}_{f,i}(T_{ref},p_{ref})\right)\left(\frac{F_{in}}{V}C_{i,in}-\frac{F_{out}}{V}C_i\right)+\Delta H_R r+C_T C_{p,mix}\left(\frac{dT}{dt}\right)\right)$$
$$=F_{in}\left(C_{T,in}C_{p,mix,in}\left(T_{in}-T_{ref}\right)+\sum_{i=1}^{N_c}C_{i,in}\underline{H}_{f,i}(T_{ref},p_{ref})\right)$$
$$-F_{out}\left(C_T C_{p,mix}\left(T-T_{ref}\right)+\sum_{i=1}^{N_c}C_i\underline{H}_{f,i}(T_{ref},p_{ref})\right)$$

Rearranging

$$F_{in}\left(C_{T,in}C_{p,mix,in}\left(T-T_{ref}\right)+\sum_{i=1}^{N_c}C_{i,in}\underline{H}_{f,i}(T_{ref},p_{ref})\right)-F_{out}\left(C_T C_{p,mix}\left(T-T_{ref}\right)+\sum_{i=1}^{N_c}C_i\underline{H}_{f,i}(T_{ref},p_{ref})\right)$$
$$+\Delta H_R rV+VC_T C_{p,mix}\left(\frac{dT}{dt}\right)$$
$$=F_{in}\left(C_{T,in}C_{p,mix,in}\left(T_{in}-T_{ref}\right)+\sum_{i=1}^{N_c}C_{i,in}\underline{H}_{f,i}(T_{ref},p_{ref})\right)$$
$$-F_{out}\left(C_T C_{p,mix}\left(T-T_{ref}\right)+\sum_{i=1}^{N_c}C_i\underline{H}_{f,i}(T_{ref},p_{ref})\right)$$

Some terms in the accumulation term cancel with terms in the in and out terms, leaving

$$F_{in}\left(C_{T,in}C_{p,mix,in}\left(T-T_{ref}\right)\right)+\Delta H_R rV+VC_T C_{p,mix}\left(\frac{dT}{dt}\right)=F_{in}\left(C_{T,in}C_{p,mix,in}\left(T_{in}-T_{ref}\right)\right)$$

rearranging we have

$$C_T C_{p,mix}\left(\frac{dT}{dt}\right)=\frac{F_{in}}{V}C_{T,in}C_{p,mix,in}\left(T_{in}-T\right)-\Delta H_R r$$

This is the energy balance for the CSTR.