Heat balance of reactors

Adiabatic reactors

Derivation

adiabatic means: the heat produced by the reaction is going into the reaction mass (for the continuous types this is the convective flow!!), there is no exchange of heat with the surrounding:

Batch reactor (STR):

$$\frac{d(m \cdot c_p \cdot T)}{dt} = r \cdot (-\Delta H_R) \cdot V_R$$

$$\text{let } c_p \text{ be constant } = \bar{c}_p = \text{ mean value}$$

$$\frac{dT}{dt} = \frac{1}{\bar{c}_p m} r(-\Delta H_R) \cdot V_R = \frac{r(-\Delta H_R)}{\rho \cdot \bar{c}_p}$$

$$\rho = \frac{m}{V}$$

$$\text{the conversion depends on time:}$$

$$dt = c_{A,0} \frac{dU_A}{r_A |\nu_A|}$$

$$\left(\begin{array}{l} from: dt = \frac{dn_A}{V_R \cdot r_A};\ dU_A = -\frac{dn_A}{n_{A,0}}; \\ dt = \frac{dU_A \cdot n_{A,0}}{V_R \cdot r_A} \end{array} \right)$$

$$dT = \frac{c_{A,0}(-\Delta H_R)}{\rho \cdot c_p \cdot \bar{|}\nu_A|} \cdot dU_A$$

ρ and ΔH_R can be considered as nearly constant when the temperature rise is not extremely high. Integration in the boarders T_0 to T and related conversion U_A=0 to U_A gives:

$$T = T_0 + \frac{c_{A,0}(-\Delta H_R)}{\rho \bar{c}_p |\nu_A|} \cdot U_A$$

Total conversion (U_A=1) produces a maximum temperature rise ΔT_{ad} :

$T = T_a + \Delta T_{ad} \cdot U_A$

with: ΔT_{ad} =

$$\frac{c_{A,0}(-\Delta H_R)}{\rho \bar{c}_p |\nu_A|}$$

The continuous reactors:

The TFR:

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In analogy to the material balance for the stationary state:

$$0 = -d\dot{n}_i + r\,\nu_i\,dV_R$$

Convection Reaction

the heat balance for the adiabatic case reads:

$$0 = -d\left(\dot{m}\,\bar{c}_p T\right) + r\left(-\Delta H_R\right)dV_R$$

$$\dot{m}\,\bar{c}_p \cdot \frac{dT}{dV_R} = r\left(-\Delta H_R\right)$$

from the material balance :

$$dV_R = \dot{n}_{A,0}\frac{dU_A}{r\left|\nu_A\right|}$$

$$\left(\begin{aligned} & -d\dot{n}_A = -r_A dV_R;\ dU_A = -\frac{d\dot{n}_A}{\dot{n}_{A,0}}; \\ & \dot{n}_{A,0}\,dU_A = -r_A dV_R \end{aligned}\right)$$

$$dT = \frac{c_{A,0}\left(-\Delta H_R\right)}{\rho\, c_p\left|\bar{\nu}_A\right|}dU_A$$

this is equivalent to the formula of the Batch

(only space and time coordinates are changed):

$$T_{(l=l)} = T_{a(l=0)} + \Delta T_{ad} \cdot U_A$$

The adiabatic CSTR:

$$0 = \left(\dot{m}\, c_p T\right) - \left(\dot{m}\, c_p T\right)_a + r\left(-\Delta H_R\right) V_R$$

$$\dot{m}\, c_p \left(T - T_a\right) = r\left(-\Delta H_R\right) V_R$$

with :

$$r = \frac{c_{A,0} \cdot \dot{v} \cdot U_A}{V_R \left|\nu_A\right|} \quad \textit{from}: \quad \frac{V_R}{\dot{n}_{A,0}} = \frac{U_A}{-r_A}$$

yields :

$$U_A = \frac{\dot{m}\, c_p \left(T - T_a\right) \cdot \left|\nu_A\right|}{\left(-\Delta H_R\right) \cdot c_{A,0} \cdot \dot{v}}$$

$$= \frac{\rho \cdot c_p \cdot \left|\nu_A\right|}{\left(-\Delta H_R\right) \cdot c_{A,0}} \left(T - T_a\right)$$

$$= \frac{1}{\Delta T_{ad}} \left(T - T_a\right)$$

$T = Ta + \Delta T_{ad} \cdot U$

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BACK to main test page