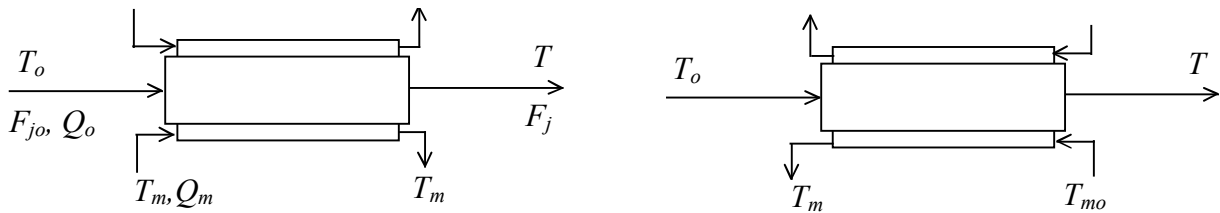


## NONISOTHERMAL OPERATION OF IDEAL REACTORS Plug Flow Reactor



### Assumptions:

1. Homogeneous System
2. Single Reaction
3. Steady State

Two types of problems:

1. Given desired production rate, conversion and kinetics and other parameters, determine the required reactor size, heat duty and temperature profile.
2. Given reactor size, kinetics, etc., determine the composition of the exit stream.

Let us consider a single reaction

$$\sum_{j=1}^s \nu_j A_j = 0 \quad (1)$$

with the rate given by

$$r = k_{10} e^{-E_1/RT} \prod_{j=1}^s C_j^{\alpha_j} - k_{20} e^{-E_2/RT} \prod_{j=1}^s C_j^{\beta_j} \quad (2)$$

with

$$C_j = C_{A_0} \frac{M_{j/A} - \frac{\nu_j}{\nu_A} x_A}{1 + \varepsilon_A x_A} \frac{T_o P}{T P_o} \quad (3)$$

The mass balance in the reactor for species  $j$  can be written as:

$$\frac{dF_j}{dV} = \nu_j r \quad (4)$$

$$\nu = 0 \quad F_j = F_{j_0} \quad (4a)$$

or

$$F_{Ao} \frac{dx_A}{dV} = (-v_A)r = -R_A \quad (4')$$

$$V = 0 \quad x_A = 0 \quad (4'a)$$

The energy balance based on (a) negligible changes in potential and kinetic energy and (b) no work other than flow work is

$$-\frac{d}{dV} \left( \sum_{j=1}^s F_j \tilde{H}_j \right) + \dot{q}_v = 0 \quad (5)$$

$$V = 0 \quad F_j \tilde{H}_1 = F_{jo} \tilde{H}_{jo} \quad (5a)$$

Based on further assumptions of (c) ideal mixtures and (d) ideal gases one gets:

$$-\sum_{j=1}^s F_j C_{p_j} \frac{dT}{dV} - \sum_{j=1}^s H_j \frac{dF_j}{dV} + \dot{q}_v = 0 \quad (6a)$$

Using the idea of (e) mean specific heats which are constant and (f) constant heat of reaction, one gets

$$-(Q\rho)C_p \frac{dT}{dV} + (-\Delta H_r)r + \dot{q}_v = 0 \quad (6)$$

$Q\rho = \dot{m}_{tot}$  is the mass flow rate which is constant

$\dot{q}_v \left( \frac{J}{m^3 s} \right)$  is the rate of heat addition per unit reactor volume

The simplest constitutive relationship for the rate of heat exchange is:

$$\dot{q}_v = U a_v (T_m - T) \quad (7)$$

$a_v \left( \frac{m^2}{m^3} \right)$  - area for heat transfer per unit reactor volume

The equations to be solved simultaneously are:

$$F_{ao} \frac{dx_A}{dV} + v_A r = 0 \quad (A)$$

$$Q\rho C_{p_m} \frac{dT}{dV} - (-\Delta H_r)r + \overbrace{U a_v (T - T_m)}^{-\dot{q}_v} = 0 \quad (B)$$

$$\mp Q_m \rho_m \underline{C}_{p_m} \frac{dT_m}{dV} - \overbrace{U_{av}}^{-q_v} (T_m - T) = 0 \quad (C)$$

$V = 0$ ;  $x_A = 0$ ;  $T = T_o$ , ( $T_m = T_{mo}$  for cocurrent flow)

$V = V$ ; ( $T_m = T_{mo}$  for countercurrent flow) (D)

and

$$G \frac{du}{dz} + \frac{dp}{dz} + F = 0 \quad (E)$$

$G = \rho u$  - mass velocity

$P$  = pressure

$z = \frac{V}{A}$  - axial distance

$u = \frac{Q}{A}$  - velocity

$A$  – cross sectional reactor area

$F$  – frictional losses

Equation (E) is the momentum balance. However this equation is usually solved separately and a mean pressure is selected for evaluation of gas concentrations in eq (3).

For gases the use of mass fractions,  $w_j$ , and extent per unit mass,  $\xi''$  is recommended. (See lecture 1).

The equations can then be written as:

$$G \frac{d\xi''}{dz} = r \quad (8)$$

$$G \frac{dT}{dz} = \beta'' r + q_v'' \quad (9)$$

$$z = 0 \quad \xi'' = 0, \quad T = T_o \quad (10)$$

$$\beta'' = \frac{-\Delta H_r}{\underline{C}_p} \quad ; \quad q_v'' = \frac{q_v}{\underline{C}_p} \quad (11)$$

where the rate is expressed by:

$$r = k_{10} e^{-E_1/RT} \prod_{j=1}^s C_{j0}^{\alpha_j} \left( 1 + v_j \frac{\dot{m}_{tot} \xi''}{F_{j0}} \right)^{\alpha_j} \left[ \frac{T_o P}{T P_o} \frac{1}{1 + \sum_{j=1}^s v_j M_{av_o} \xi''} \right]^{\sum_{j=1}^s v_j} - k_{20} e^{-E_2/RT} \prod_{j=1}^s C_{j0}^{\beta_j} \left( 1 + v_j \frac{\dot{m}_{bot} \xi''}{F_{j0}} \right)^{\beta_j} \left[ \frac{T_o P}{T P_o} \frac{1}{1 + (\sum y) M_{av_o} \xi''} \right]^{\sum v_j} \quad (12)$$

$M_{av_o}$  - average molecular weight at feed conditions

$\dot{m}_{tot}$  = GA – mass flow rate

$$\frac{\dot{m}_{tot}}{F_{j0}} = \frac{M_j}{w_{j0}}$$

$w_{j0}$  – mass fraction of j in the feed.

For liquids one can write

$$\frac{d\xi}{d\tau} = r \quad (13)$$

$$\frac{dT}{d\tau} = \tilde{\beta} r + \tilde{q}_v \quad (14)$$

$$\tau = 0 \quad ; \quad \xi = 0 \quad ; \quad T = T_o \quad (15)$$

$$\tilde{\beta} = \frac{-\Delta H_r}{\rho C_p} \quad ; \quad \tilde{q}_v = \frac{q_v}{\rho C_p} = \frac{Q_v''}{\rho} \quad (16)$$

where the rate is given by

$$r = k_{10} e^{-E_1/RT} \prod_{j=1}^s (C_{j0} + v_j \xi)^{\alpha_j} - k_{20} e^{-E_2/RT} \prod_{j=1}^s (C_{j0} + v_j \xi)^{\beta_j} \quad (17)$$

$$\tau = \frac{z}{u} = \frac{V}{Q} \text{ - residence time along the reactor.}$$

## LECTURE 8

From eqs (8) and (9) or (13) & (14) we can always get the following relationship between temperature and extent

$$T = T_o + \beta'' \xi'' + \frac{1}{G} \int_o^z q_v'' dz \quad (18a)$$

or

$$T = T_o + \tilde{\beta} \xi + \sum_o^{\tau} \tilde{q}_v d\tau \quad (18b)$$

For adiabatic operation ( $q_v'' = 0, \tilde{q}_v = 0$ ) this yields the equation of the adiabatic line, i.e extent and temperature satisfy the relationship below at any and every point of the reactor

$$T = T_o + \beta'' \xi'' \quad (19a)$$

$$T = T_o + \tilde{\beta} \xi \quad (19b)$$

The maximum fractional adiabatic temperature rise is given by the Prater number just like in the case of a CSTR.

$$\frac{\Delta T_{ad \max}}{T_o} = \beta = \frac{(-\Delta H_r) C_{A_o}}{(-v_A) T_o \rho C_p} \quad (20)$$

### Basic types of problems

#### 1. The temperature in the reactor is prescribed

- $T(z) = T_o$  – isothermal reactor. Integrate (8) or (13) and find extent along the reactor. From eq. (9) or (14) find the heat addition/removal requirement along the reactor and the overall heat duty for the reactor.
- $T(z)$  specified. Integrate (8) or (13) find  $\xi(z)$ . Use  $\xi(z)$  and  $T(z)$  in eq (9) or (14) to get  $q_v(z)$

#### 2. The heat addition (removal) rate is prescribed

- Adiabatic operation.  $T = T_o + \beta'' \xi''$  or  $T = T_o + \tilde{\beta} \xi$ . Substitute into eq (8) or (13) and integrate
- Heat duty is prescribed.  $q_v''(z)$  or  $\bar{q}_v(z)$  prescribed. Simultaneously integrate (8) or (9) or substitute

$$T = T_o + \beta'' \xi'' + \frac{1}{G} \int_o^z q_v'' dz \text{ into (8) and integrate.}$$

3. Rate of heat addition (removal) controlled by another equation

$$\dot{q}_v = Ua_v(T - T_m)$$

- a)  $T_m = \text{const.}$  Integrate eqs (8) and (9) or eqs (13) and (14) simultaneously.  
This is the case when reactor tubes are immersed in boiling medium or condensing medium.
- b)  $T_m$  determined with  $T$  and  $\xi''$  by equations (A) to (E).

$$G_m \frac{dT_m}{dz} = \mp \kappa'_m (T_m - T) \quad \kappa'_m = \frac{Ua_{v_m}}{C_{p_m}} \quad G_m = \frac{Q_m \rho_m}{A_m}$$

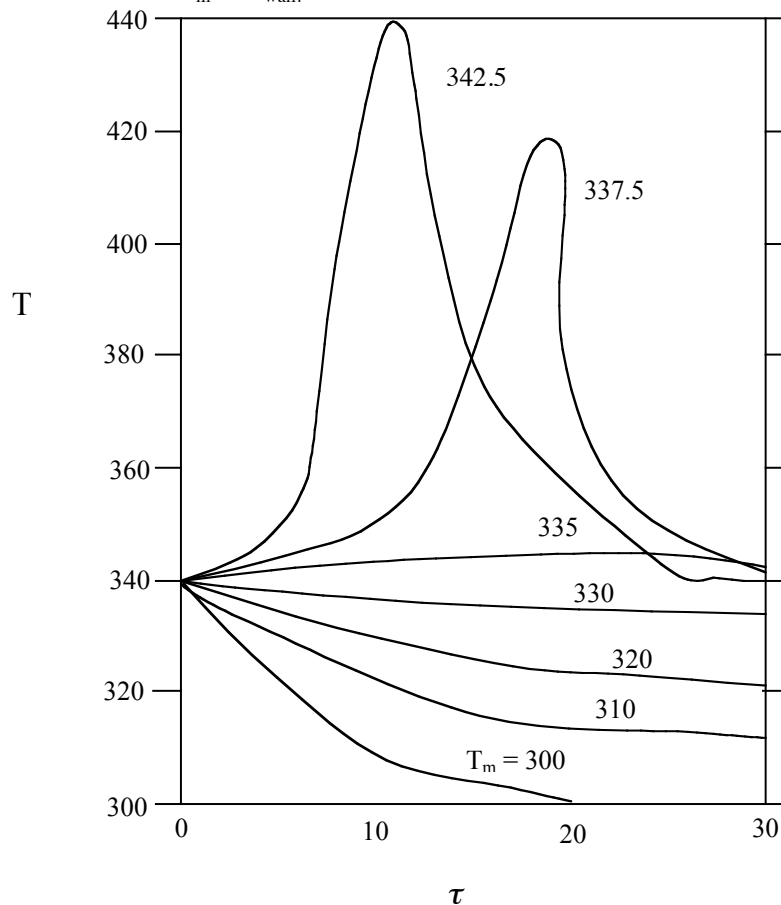
Note: With cocurrent cooling a PFR can be kept isothermal with countercurrent cooling it cannot in the case of n-th order reactions. Prove that for an exercise.

There is always a unique steady state in a PFR. Main problem with PFR's is:

- hot spot formation
- parametric sensitivity and temperature runaway.

Classical example of temperature runaway presented by Bilous & Amundson (AIChE J., 2, 117 (1956)).

PFR cooled from the wall t constant  $T_m = T_{\text{wall}}$ .



## LECTURE 8

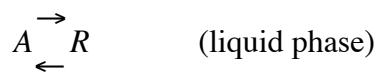
A “hot spot” is formed due to a very small change in wall temperature. The system shows extreme parameter sensitivity.

Reaction runaway is the phenomenon when a small change in feed concentration, temperature, flow rate or in coolant temperature triggers a dramatic change in the temperature profile and leads to runaway reactions and explosions. Exact criteria for runaways are difficult to develop.

Approximate criteria are given on the enclosed graph.

Example 1

A reversible first order reaction (considered earlier in a CSTR) is now to be performed in a PFR.



$$k_1 = 5 \times 10^8 e^{-12,500/RT} \text{ (min}^{-1}\text{)}$$

$$k_2 = 3.4 \times 10^{21} e^{-32,500/RT} \text{ (min}^{-1}\text{)}$$

$$\Delta H_r = -20,000 \text{ cal/mol} \quad \Delta G_{298}^{\circ} = -2,500 \text{ cal/mol}$$

$$\rho C_p = 2,000 \text{ (cal/lit}^{\circ}\text{C)}$$

$$C_{A0} = 2 \text{ (mol/lit)}$$

If the feed rate is  $Q = 100$  (lit/min) and the PFR size is  $V = 1,500$  (lit):

- find final conversion in an isothermal reactor operated at 0, 10, 20, 100°C
- determine conversion in an adiabatic reactor if the feed is at i) 0°C, ii) 20°C,
- if the maximum permissible temperature is 80°C determine the optimal temperature profile along the reactor necessary to maximize exit conversion.
- If the desired conversion is 85% find the minimum reactor volume and the desired heat removal rate along the reactor. Permissible temperature range is 0° to 100°C.

Solution

- For an isothermal reactor only the mass balance has to be solved

$$\tau = \frac{V}{Q_0} = C_{A0} \int_0^{x_A} \frac{dx_A}{-r_A}$$

$$-r_A = k_1 C_A - k_2 C_R = C_{A0} [k_1(1 - x_A) - k_2 x_A]$$

$$-r_A = k_1 C_{A0} \left[ 1 - x_A - \frac{x_A(1 - x_{Ae})}{x_{Ae}} \right] \quad \text{since} \quad k_2 = \frac{k_1}{K} = \frac{k_1(1 - x_{Ae})}{x_{Ae}}$$

$$(-r_A) = \frac{k_1 C_{A0}}{x_{Ae}} (x_{Ae} - x_A) \quad x_{Ae} = \frac{K}{1 + K} = \frac{k_1}{k_1 + k_2}$$

$$(-r_A) = (k_1 + k_2)C_{A0}(x_{Ae} - x_A)$$

$$\tau = \frac{1}{k_1 + k_2} \int_0^{x_A} \frac{dx_A}{x_{Ae} - x_A} = \frac{1}{k_1 + k_2} \ln \left( \frac{x_{Ae}}{x_{Ae} - x_A} \right)$$

Solve for conversion

$$x_A = \left[ 1 - \exp \left( -k_1 \left( 1 + \frac{1}{K} \right) \tau \right) \right]$$

$$= x_{Ae} \left[ 1 - \exp \left( \frac{-k_1}{x_{Ae}} \tau \right) \right] \quad \tau = \frac{1500}{100} = 15 \text{ min}$$

We get the following results:

T	K	k <sub>1</sub>	x <sub>ae</sub>	x <sub>a</sub>
273	1494	0.0498	0.999	0.526
283	407	0.112	0.998	0.813
293	121	0.239	0.992	0.965
303	40	0.486	0.975	0.974
313	13.5	0.943	0.931	0.931
323	5.0	0.755	0.833	0.833
333	2.0	3.149	0.662	0.662
343	0.81	5.46	0.448	0.448
353	0.35	9.17	0.262	0.262
363	0.16	15.0	0.139	0.139
373	0.08	23.8	0.071	0.071

Same as equilibrium conversion

The reactor space time is so large that above 50°C practically equilibrium conversion is obtained.

a) The adiabatic operating line is

$$T = T_o + \tilde{\beta}_A C_{A0} x_A$$

$$\tilde{\beta}_A = \frac{-\Delta H_{r_A}}{\rho C_p} = \frac{20,000}{2,000} = 10 \left( \frac{\text{lit}^\circ \text{C}}{\text{mol}} \right)$$

$$C_{A0} = 2 \left( \frac{\text{mol}}{\text{lit}} \right)$$

$$T = T_o + 20 x_A$$



Substitute this relationship into the mass balance and integrate:

$$C_{Ao} \frac{dx_A}{d\tau} = (k_1 + k_2)C_{Ao}(x_{Ae} - x_A) = k_1C_{Ao} - (k_1 + k_2)C_{Ao}x_A$$

$$\tau = 0 \quad x_A = 0$$

$$k_1 = k_{10}e^{E_1/RT_{ad}} = k_{10}e^{-E_1/R(T_o + 20x_A)}$$

$$k_2 = k_{20}e^{-E_2/R(T_o + 20x_A)}$$

$$x_{Ae} = \frac{K}{1 + K} = \frac{k_1}{k_1 + k_2}$$

Thus integrate numerically

$$\frac{dx_A}{d\tau} = k_{10}e^{-E_1/RT(T_o + 20x_A)} - \left( k_{10}e^{-E_1/R(T_o + 20x_A)} + k_{20}e^{-E_2/R(T_o + 20x_A)} \right) x_A ; \tau = 0 \quad x_A = 0$$

$$\frac{dx_A}{d\tau} = 5x10^8 e^{-\frac{12,500}{1.987(T_o + 20x_A)}} - \left[ 5x10^8 e^{-\frac{12,500}{1.987(T_o + 20x_A)}} + 3.4x10^{21} e^{-\frac{32,500}{1.987(T_o + 20x_A)}} \right] x_A ; \tau = 0 \quad ; \quad x_A = 0$$

Desired result is obtained at  $\tau = 15$ .

Alternatively we could solve by trial and error the following integral:

$$\tau = 15 = \int_0^{x_A} \frac{dx}{5x10^8 e^{-\frac{12,500}{1.987(T_o + 20x)}} - \left[ 5x10^8 e^{-\frac{12,500}{1.987(T_o + 20x)}} + 3.4x10^{21} e^{-\frac{32,500}{1.987(T_o + 20x)}} \right] x}$$

We find:

- i)  $T_o = 0^\circ\text{C} = 273 \text{ K}$     $x_A = 0.78$   
 $\Delta T_{adiabatic} = 15.7\text{K} = 16\text{K}$     $T = 289 \text{ K}$
- ii)  $T_o = 20^\circ\text{C} = 293 \text{ K}$     $x_A = 0.94 = x_{Ae}$   
 $\Delta T_{adiabatic} = 18.8 = 19\text{K}$     $T = 292\text{K}$

c) To maximize conversion at given space time we should follow the line of maximum rates.

$$T_m = \frac{(E_2 - E_1/R)}{\ln \frac{k_{20}E_2}{k_{10}E_1} + \ln \frac{x_A}{1 - x_A}} = \frac{10,065}{30.51 + \ln \left( \frac{x_A}{1 - x_A} \right)}$$

Since maximum permissible temperature is  $80^\circ\text{C}$  (353 K) we have to preheat the feed to 33 K, cool the reactor and keep it isothermal a 353 K until the locus of maximum rate is reached and then run along the locus of maximum rates.

The intersection of the isothermal line  $T = 353$  K and the  $T_m$  line determines up to which point the reactor has to be run isothermally.

$$T = 353 = T_m = \frac{10,065}{30.51 + \ln\left(\frac{x_A}{1-x_A}\right)}$$

$$x_A = \frac{\exp\left(\frac{10,065 - 353 \times 30.51}{353}\right)}{1 + \exp\left(\frac{10,065 - 353 \times 30.1}{353}\right)} = 0.119$$

$$\tau = \frac{1}{k_1 + k_2} \int_0^{0.119} \frac{dx}{(x_{Ae} - x_A)} = \frac{1}{(k_1 + k_2)} \ln\left(\frac{x_{Ae}}{x_{Ae} - x_A}\right)$$

At 80°C (353 K) from the table given earlier

$$\tau = \frac{1}{9.17\left(1 + \frac{1}{0.35}\right)} \ln\left(\frac{0.262}{0.262 - 0.119}\right) = 0.017(\text{min})$$

The isothermal operation should occur in the very entry section of the reactor. After that the  $T_m$  line should be followed.

$$\frac{dx_A}{d\tau} = 5 \times 10^8 e^{-\frac{12,500}{1.987T_m}(1-x_A)} - 3.42 \times 10^{21} e^{-\frac{32,500}{1.987T_m}x_A}$$

$$T_m = \frac{10,065}{30.51 + \ln\left(\frac{x_A}{1-x_A}\right)}$$

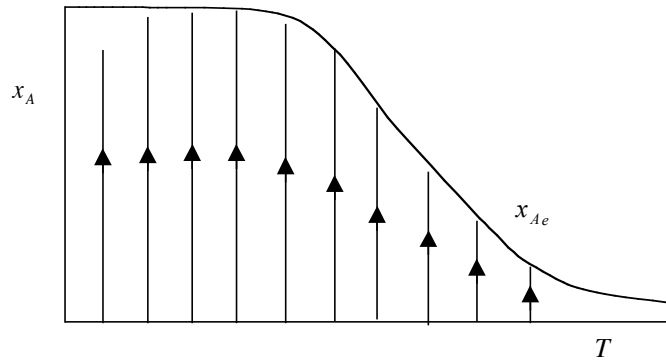
$$\tau = 0.017 \quad x_A = 0.119$$

Desired result at  $\tau = 15$

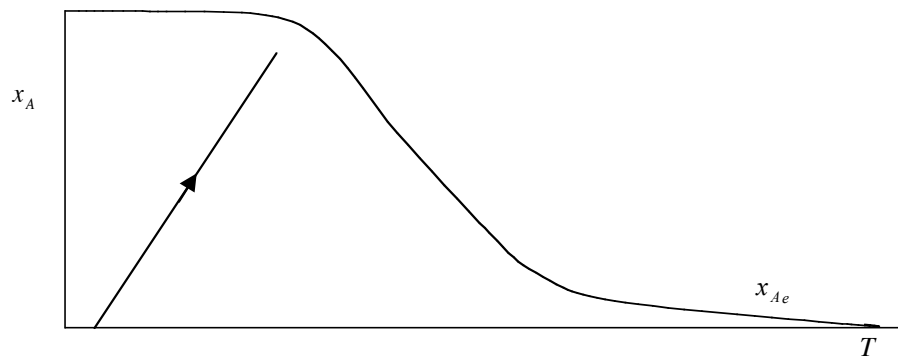
$$x_{A=0.988} \quad T_{\text{exit}} = 288\text{K}$$

Really one should preheat only to adiabatic line. Adiabatic line should end at  $T = 353$  K,  $x_A = 0.119$ . Hence, the fluid must be preheated up to  $T_o = T - \tilde{\beta}_A C_{A_o} x_A = 353 - 20 \times 0.119 = 350\text{K}$

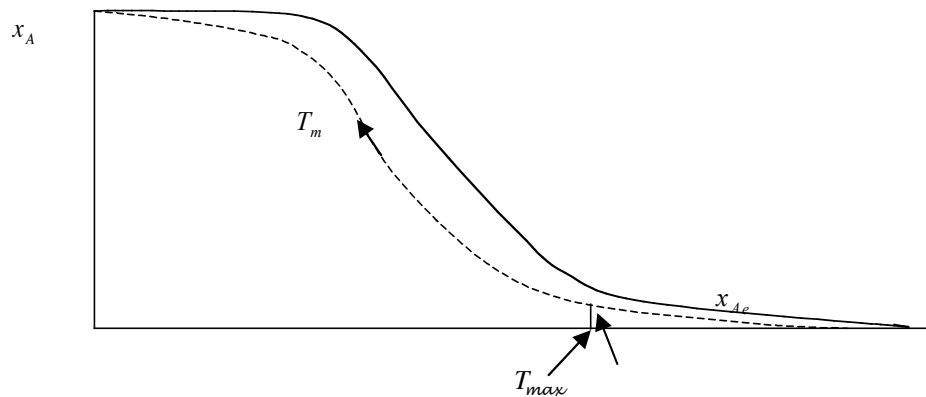
The graphical representation of parts (a-c) has the following form:



- a. Isothermal. Solid lines are operating lines for  $\tau = 15$  min



- b. Adiabatic. Adiabatic line with  $\tau = 15$



- c. Operating along the locus of maximum rates

- d) Permissible temperature range is  $0^\circ\text{C}$  to  $100^\circ\text{C}$ . We want minimum reactor size for  $x_A = 0.85$ . Preheat to  $100^\circ\text{C}$ , run along the locus of maximum rates

$$\tau = \int_0^{x_A=0.85} \frac{dx}{5x10^8 e^{-\frac{12,500}{1.987T_m}} \left[ 5x10^8 e^{-\frac{12,500}{1.987T_m}} + 3.4x10^{21} e^{-\frac{32,500}{1.987T_m}} \right]}$$

with  $T_m = \frac{10,065}{30.51 + \ln\left(\frac{x_A}{1-x_A}\right)}$

$$\tau = 1.8 \text{ min}$$

Thus with Q = 100 lit/min we need only V = 160 liters

The desired temperature profile along the reactor is presented in the enclosed graph. The heat removal per unit volume is

$$\begin{aligned} -\frac{\dot{q}}{Q} &= \rho C_p (T_o - T) + (-\Delta H_r) C_{A_o} x_A \\ &= 2,000(100 - T) + (20,000x2)x_A \end{aligned}$$

This curve is also presented in the figure. The total heat density is:

$$\begin{aligned} -\left(\frac{\dot{q}}{Q}\right)_{tot} &= 2,000(100 - 70) + 40,000x0.85 \\ &= 1.56x10^5 \text{ (cal/lit)} \end{aligned}$$

With Q = 100 lit/min  $-\dot{q}_{tot} = 1.56x10^7 \text{ (cal/min)}$

For comparison, if cooling failed and reactor ran adiabatically with  $T_o = 100^\circ\text{C}$  one would get

$$x_{A_{adiabatic}} = 0.068, T_{exit} = 126^\circ\text{C}$$

The adiabatic temperature profile is shown also on the enclosed figure.

**Extension to Multiple Reactions**

$$\sum_{j=1}^s \nu_{ij} A_j = 0 \quad i = 1, 2, \dots, R \quad (1)$$

$$-\frac{dF_j}{dV} + \sum_{i=1}^R \nu_{ij} r_i = 0 \quad j = 1, 2, \dots, R \quad (2)$$

or

$$-\sum_{i=1}^R \nu_{ij} \frac{d\dot{X}_i}{dV} + \sum_{i=1}^R \nu_{ij} r_i = 0 \quad (2a)$$

$$-\frac{d\dot{X}_i}{dV} + r_i = 0$$

$$-\frac{d(F_j \tilde{H}_j)}{dV} + \dot{q}_v = 0 \quad (3)$$

$$V = 0 \quad ; \quad F_j = F_{j0} (\dot{X}_i = \dot{X}_i^o) \quad ; \quad \tilde{H}_j = \tilde{H}_{j0}$$

With the usual assumptions made about the energy balance (see the lecture on CSTR) one gets:

$$-\sum_{j=1}^s F_{j0} C_{p_j} \frac{dT}{dV} + \sum_{i=1}^R (-\Delta H_{r_i}) r_i + \dot{q}_v = 0 \quad (4)$$

The equations to be solved for a set of multiple reactions are:

$$-\frac{d\dot{X}_i}{dV} + r_i = 0 \quad i = 1, 2, \dots, R \quad (A)$$

$$-\rho C_p Q \frac{dT}{dV} + \sum_{i=1}^R (-\Delta H_{r_i}) r_i + \dot{q}_v = 0 \quad (B)$$

$$V = 0 \quad ; \quad \dot{X}_i = \dot{X}_{i0} \quad T = T_o$$

$$\rho Q = \text{const}$$

$$r_i = k_{i10} e^{-E_{i1}/RT} \prod_{j=1}^s C_j^{\alpha_{ij}} - k_{i20} e^{-E_{i2}/RT} \prod_{j=1}^s C_j^{\beta_{ij}} \quad (C)$$

with

$$C_j = C_{jo} \frac{\rho T_o}{\rho_o T} \left( \frac{1 + \frac{\sum_{i=1}^R \nu_{ij} \dot{X}_i}{F_{jo}}}{1 + \frac{\sum_{i=1}^R \sum_{j=1}^S \nu_{ij} \dot{X}_i}{F_{bot o}}} \right) \quad (D)$$

The constitutive relationship for  $\dot{q}_v$  is:

$$\dot{q}_v = U_{a_v} (T_m - T)$$

- a)  $T_m = \text{const}$   
 b)  $T_m$  is governed by another D.E.

$$\mp \rho_m Q_m C_{p_m} \frac{dT_m}{dV} - \dot{q}_v = 0 \quad (E)$$

$$V = 0 \quad T_m = T_{mo} \text{ (cocurrent flow)}$$

$$V = V \quad T_m = T_{mo} \text{ (countercurrent flow)}$$

### Problems

Consider the reaction introduced in the last lecture  $A \xrightleftharpoons[\leftarrow]{\rightarrow} R$ .

$$R = k_1 C_A - k_2 C_R \text{ (mol/lit s)}$$

$$k_1 = \exp\left(7 - \frac{83,700}{RT}\right) \times 10^3 \text{ (s}^{-1}\text{)}$$

$$k_2 = \exp\left(18 - \frac{167,400}{RT}\right) \times 10^3 \text{ (s}^{-1}\text{)}$$

$$\Delta H_r = -80,000 \text{ (J/mol)}$$

$$C_p = 40 \text{ (J/mol K)} \quad (\text{Activation energies given in joules})$$

1. The above reaction occurs in liquid phase! Permissible temp range of operation is  $300 < T < 900$  K.

Feed conditions:

$$Q_o = 100 \text{ (lit/s)} ; \quad T_o = 300 \text{ K} ; \quad C_{Ao} = 1 \text{ (mol/lit)}$$

You have a  $V = 100$  liters PFR. How would you operate this reactor if the only objective is to maximize the production rate of R.

- a) What is maximum  $F_R$ .
- b) What are final  $x_A$  and  $\Delta T$ .
- c) What is the profile of heat addition or removal for every 10% of reactor volume.
- d) What is the overall heat duty for the reactor and any heat exchangers preceding it.
- e) Sketch your system.

2. The above reaction occurs in gas phase.

The gas feed rate is

$$Q_o = 100(\text{lit/s}) \text{ at } T_o = 300\text{K}, P_o = 24.6 \text{ atm}$$

The feed is 50%A, 50% inerts. Permissible temperature range is  $250 < T < 900$  K. Pressure is constant in the reactor. Gases start to condense below 250 K. Desired conversion is 85%.

- a) What reactor volume is needed if you operate along the locus of maximum rates?
  - b) What is the distribution of heat duty along the reactor?
  - c) What is the production rate of R?
3. For the above problem what would  $F_R$  and  $x_A$  be if you had a reactor (PFR) of  $V = 100$  liters available?
  4. Suppose that the reactor can only be operated adiabatically and the desired conversion is 85%. Minimize the required reactor size.
    - a) What reactor type do you recommend?
    - b) What feed temperature would you use?
    - c) What is the heat duty?