9.1 Figure E46 presents the solution to this problem.

From Fig. E46, we find:

\[ T_{X=0.4} = 0.24 \quad (T_{X=0.8}) = 0.34 \ (J/J_s) \]

This can be written as:

\[ T_{X=0.4} = 0.24 \quad (T_{X=0.8}) = 0.34 \ (J/J_s) \]

\[ = 0.36 \text{ min} = 22^\circ C \]

Also:

\[ T_{out} = 75^\circ C \]

9.2 From Fig. E46 we can see:

\[ \frac{250}{T_1} \quad \frac{95}{T_2} \quad \frac{62}{T_3} \quad \frac{25}{T_4} \]

For \( \Delta H = 1000 \text{ cal/mol A} + \) \( = 250 \text{ cal/mol A} \)

The heat added to the flowing stream is

\[ Q_1 = C \Delta T \]

\[ = 250 \cdot (95 - 25) = + 17500 \text{ cal} \]

\[ Q_2 = C \cdot \Delta H \cdot \Delta \nu \]

\[ = 250 \cdot (62 - 95) \cdot (18300) = -22650 \text{ cal} \]

\[ Q_3 = C_\rho \Delta T \]

\[ = 250 \cdot (62 - 42) = + 9250 \text{ cal} \]
From the figure above it can be seen that the "law of optimality" should intersect the 0.05 conversion line at a reaction rate value given by

\[-\frac{V_r}{T} = 0.2 \times 4 \text{ mol L}^{-1} \text{ s}^{-1}\]

\[\text{Size of the smallest heater} = V = \frac{F_{\text{in}} \times X_p}{-\frac{V_r}{T}} = \frac{1000 \times 0.05}{0.2} = 875 \text{ liters}\]

If both \(T_{\text{in}} = T_{\text{out}} = 25^\circ C\), then:

\[
\text{there must be a}\ \frac{\text{preheater}}{\text{rectangular}} \text{ as well as a post-cooler for the CSTR, line the reactor would proceed with temperature of 67^\circ C \text{ as shown in the figure.}}
\]
9.7 Look at Fig. 8.3 which is drawn for $C_A = 1$ mol/l and $X_A = 0$. At $X_A = 0.95$, the highest reaction rate occurs at 45°C with a rate between 0.0075 and 0.0085 mol/lite.min.

So for $C_A = 10$, we have $-\Omega = 0.075$ to 0.08 and for mixed flow

$$ q = \frac{V}{A} = \frac{C_m - C_A}{\Omega q} $$

or

$$ V = 0.25(C_m - C_A) = 100 \left( 0.8 \right) \frac{100}{0.075} = 1266 \approx 1167 \text{ m}^3 $$

10.7 From Example 1

$$ \frac{q}{\Omega} = \frac{0.25 C_A}{0.025 + 0.25 C_A + 0.025 C_A^2} \quad \text{and} \quad \begin{cases} \frac{C_A}{C_m} = 0.25^2 \\ \frac{C_B}{C_m} = 0.075^2 \\ \frac{C_A}{C_m} \left( 1 - 0.25 \right) = 0.5 \end{cases} $$

The $q$ vs $C_A$ curve is

For MFR: $C_m = \frac{q}{\Omega} (C_m - C_A) = 0.5 \left( 1 - 0.25 \right) = 0.375$

For PFR & $C_p = \int q dC_A = \frac{\int 0.25 dC_A}{1 + 0.25 C_A + 0.025 C_A^2} = 0.5 \frac{C_A}{C_m} \frac{dC_A}{1 + 0.25 C_A + 0.025 C_A^2}$

But from a table of integrals:

$$ \int \frac{x}{(a + bx)^2} dx = \frac{a}{1 + b} \ln(a + bx) + \frac{1}{b} \int \frac{1}{x} dx = \frac{1}{b} \ln|a + bx| + \frac{a}{1 + b} $$

$$ C_p = \frac{1}{150} \left[ \frac{1}{150} + \frac{1}{150} \int \frac{1}{C_A} dC_A \right] = 0.14 $$

So $C_{C_{100}} = C_{C_{100}} + C_p = 0.375 + 0.14 \approx 0.5175$
10.9  Since $C_A = C_B = 1$ for all $C_A$, the maximum rate is at $C_A = C_B = 0.5$.
Check this if you don't believe it. Thus

![Graph showing rate of reaction vs. feed composition]

Plug flow is best. Do not use recycle as recommended in Fig P9.

10.11

The feed has $C_{R1}/C_{R2} = 0.9$.

(a) To maximize $C_{R1}$, do not react at all. The design of Fig P11 is no good.

(b) To minimize $C_{R2}$, run to completion. All the $C_R$ will disappear.

Next reaction is second order; reaction 2 is first order. Keep $C_R$ low.

On use a large size, you will end up with most $C_{R1}$.
Anaerobic reaction:

\[
\tau_{\text{minimum}} (X_a = 0.1) = 4.22 \times 4 \times \frac{6.33 \text{min}}{(C - T) \text{min}} = 0.54 \text{ min}
\]

1. Volume,

\[
V_{\text{exit}} = \frac{1000 \times 0.7}{0.54} = 1777.78 \text{ m}^3
\]

2. Exit temperature, \( T_m = \frac{(C_2 - C_1) / \rho}{C_0 \left[ \frac{K_a X_a}{C_0 X_a + (C_1 - X_a)} \right]} \)

\[
= \frac{(123900) - 48000) / 8.34}{\ln \left[ \frac{117 \times 10^6 + 1.23 \times 10^6}{34 \times 10^6 + 4.69 \times 10^6 + 0.7} \right]}
\]

\[
= 342 \text{ K} = 69 \text{ °C}
\]
(a) Water is in excess.
Upon a pseudo first order reaction,
\[ C_a = 2.16 \times 10^{-2} \text{ mol/L} \]
\[ C_0 = \frac{1}{16} = 6.25 \times 10^{-2} \text{ mol/L} \]
\[ C_0 >> C_a \]

(b) Determined Batch Reactor
\[
t = C_a \int_{x_0}^{x_f} \frac{dx_a}{\frac{x_0}{x_f} - x_a}
\approx \frac{C_a}{0.0206} \int_{x_0}^{x_f} \frac{dx_a}{C_a(1-x_a)}
\approx \frac{1}{0.0206} \ln \left( \frac{1}{1-e^{-r}} \right)
\approx 14.94 \text{ min.}
\]
\[ q = (\text{-CH}_4) V C_a x_a
\]
\[ = 50,000 \times 2.16 \times 10^{-4} \times 200 \times 10^5 \times 10^{-7}
\]
\[ = 14.12 \text{ kcal (As be removed)}
\]

(c) Arrhenius dependency for \( R \)
\[ \ln R = k \cdot \frac{1}{T} \]
\[ \ln R = \ln k + \frac{E_a}{kT} \]

Upon linear regression of \( \ln R \) and \( \frac{1}{T} \):
\[ \frac{1}{T} = \frac{E_a}{k} \text{ (slope)} \]
\[ \ln k = \text{intercept} \]
\[ R = e^{\ln k} e^{\frac{E_a}{kT}} C_a \]
\[ = 2.448 \times 10^4 e^{\frac{E_a}{kT}} C_a \]
Advective Operation

\[ t = C_a \int \frac{d\theta}{\theta} \]

Adiabatic Equation is

\[ T = T_a + \frac{\left( -\Delta H \right)}{\varepsilon C_p} C_a X_a \]

\[ = 208 + \frac{50,000 \times 2.16 \times 10^{-4}}{1.05 \times 0.9} X_a \]

\[ = 208 + 11.4 X_a \]

\[ \therefore (-R_a)_{\text{ad}} = 2.16 \times 10^{-3} \varepsilon \left( \frac{1}{8} \left( 1 + \frac{11.45}{X_a} \right) \right) C_a \left( 1 - X_a \right) \]

\[ = 4.139 \times 10^{-9} \int_{0}^{1} \frac{e^{-\frac{11.145}{X_a}}}{X_a (1 - X_a)} dX_a \]

Upon numerical integration:

\[ t = 11 \text{ min} \]

\[ T_{\text{final}} = 23^\circ C \]

* Faster team wins second operation!"
Problem 1

<table>
<thead>
<tr>
<th>T(K)</th>
<th>x(mmol/m³ mol·min)</th>
<th>1/T</th>
<th>ln(k)</th>
</tr>
</thead>
<tbody>
<tr>
<td>291</td>
<td>0.6597</td>
<td>0.0031334</td>
<td>-2.859681</td>
</tr>
<tr>
<td>299</td>
<td>0.3063</td>
<td>0.003472</td>
<td>-2.015257</td>
</tr>
<tr>
<td>298</td>
<td>0.158</td>
<td>0.003368</td>
<td>-1.84516</td>
</tr>
<tr>
<td>313</td>
<td>0.38</td>
<td>0.003188</td>
<td>-2.997594</td>
</tr>
</tbody>
</table>

\[ y = -5621.1x + 17 \]

\[ R^2 = 0.9998 \]
\[ F_{\text{H}_2} = 22 \text{ mol/hr} \]
\[ = 22 \times 454 \text{ Nmol/hr} \]
\[ = 9988 \text{ Nmol/hr} \]
\[ = 11 F_{\text{a}} \]
\[ F_{\text{a}} = 908 \text{ Nmol/hr}. \]

\[ V = F_{\text{a}} \int_0^1 \frac{dX_a}{e_{X_a}} \]
\[ E_a = \frac{Y_a}{1 - Y_a} \left( \frac{1}{11} \right) \]
\[ P_a = \frac{P_a (1 - Y_a)}{1 + E_a Y_a} = \frac{908}{11} \frac{(1 - Y_a)}{(1 + \frac{1}{11} Y_a)} \]

If we neglect an expansion, on the assumption that steam is excess, \( E_a \approx 0 \)

\[ V \approx \frac{F_{\text{a}}}{R P_{\text{a}}} \ln \left( \frac{1}{1 - Y_a} \right) \]
\[ = \frac{908}{11} \cdot \frac{1}{1 - 0.2} \]
\[ = 101 \text{ l/hr}. \]

\[ V = (-441) F_{\text{a}} Y_a = 26,360 
908 \times 0.2 = 4756.98 \text{ kJ/hr. (To be applied)}. \]

The exact solution of \( V \) is,

\[ V = F_{\text{a}} \int_0^1 \frac{dX_a}{E_a} \left( \ln \left( \frac{1 - Y_a}{1 + \frac{1}{11} Y_a} \right) \right) \]
\[ = \frac{908}{22} \int_0^1 \frac{dX_a}{1 - Y_a} \]
\[ = \frac{908}{22} \left[ -X_a + 12 \ln \left( \frac{1}{1 - Y_a} \right) \right] \]
\[ = \frac{908}{22} \left[ -0.2 + 12 \ln \left( \frac{1}{1 - 0.2} \right) \right] \]
\[ = 102 \text{ l/hr}. \]
Problem 2

<table>
<thead>
<tr>
<th>T(K)</th>
<th>%</th>
<th>1/T</th>
<th>ln(x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>832</td>
<td>0.32</td>
<td>0.091282</td>
<td>-1.394634</td>
</tr>
<tr>
<td>856</td>
<td>0.65</td>
<td>0.031173</td>
<td>-0.162519</td>
</tr>
<tr>
<td>877</td>
<td>2.94</td>
<td>0.001144</td>
<td>0.71266</td>
</tr>
<tr>
<td>900</td>
<td>4.9</td>
<td>0.001111</td>
<td>1.662235</td>
</tr>
<tr>
<td>922</td>
<td>11</td>
<td>0.001086</td>
<td>2.337855</td>
</tr>
</tbody>
</table>

![Graph showing a linear regression with equation y = -30106x + 35.049.]

R² = 1
(b) Michaelis

\[ F_{AV} = \frac{2.16 \text{ mol/l} \cdot L}{1} = 90.8 \text{ mol/L} \]

\[ Y = \frac{1}{11} \]

\[ V = F_{AV} \frac{X_A}{E} \frac{dX_A}{(E - X_A) X_A} \]

\[ T = T_0 + \left( \frac{\Delta H_r}{S} \right) \frac{X_A}{V/c_p} \]

\[ C_A = \frac{Y_A e^{P}}{R_T} \quad q = \frac{R}{R_T} \quad \frac{R}{R_T} = \frac{1}{8} \]

\[ T_A = T_0 + \left( \frac{\Delta H_r}{S} \right) \frac{X_A}{M/c_p} \]

\[ = \frac{26.360 \times 1/11}{1/8} \]

\[ = 922 \left( \frac{26.360 \times 1/11}{1/8} \right) \]

\[ = 922 - 225.4 \times X_A \]

\[ k = k_A e^{-E/RT} \]

Upon linear regression of \( k_B \) and \( 1/T \), we get:

\[ k_B = 1.666 \times 10^{15} \text{ mol/l} \cdot \text{min} \]

\[ E = 5.9827 \text{ cal/mol} \]

\[ V = F_{AV} \int \frac{X_A}{E} \frac{dX_A}{E(293-293+X_A) P_A} \left( \frac{1-X_A}{14/\pi \cdot X_A} \right) \]

\[ = F_{AV} \frac{X_A}{k_A P_A} \int \frac{(1 + \frac{1}{\pi} X_A) e^{E/293}}{1-X_A} \frac{dX_A}{14/\pi} \]

\[ = 2.9976 \times 10^{-12} \int \frac{(1 + \frac{1}{\pi} X_A) e^{E/293}}{1-X_A} \frac{dX_A}{14/\pi} \]

Upon numerical integration, for \( X_A = 0.1 \):

\[ V = 2.9978 \times 10^{-12} + 2.9978 \times 10^{-12} \]

\[ = 76 \text{ L/min} \]
For $X_e = 0.2$,
\[ V = 270 \text{ Ls} \]

Due to adiabaticity and reaction endothermicity, reactor volume is increased.

For small reactor volume,
(a) Operate不断完善ly
(b) Increase pressure
(c) Increase initial temperature.
Adiabatic CCTR

Mass balance:

\[ F_{in} \cdot x_a + R_i \cdot e^{-E/RT} C_a \cdot V(1-x_a) \]

\[ x_a = \frac{R_i \cdot e^{-E/RT} V/G}{1 + R_i \cdot e^{-E/RT} V/G} \]

\[ = \frac{1.2 \times 10^5 \cdot e^{-12000/1.9877}}{1 + 1.8 \times 10^2 \cdot e^{-12000/1.9877}} \]

\[ = \frac{1.2 \times 10^5 \cdot e^{-11800/1.9877}}{1 + 1.8 \times 10^2 \cdot e^{-11800/1.9877}} \]

Energy balance:

\[ \frac{E_{cpG}(T_i - T) + (-E_{f}) F_{in} x_a}{(-E_{f}) G_a} = 0 \]

\[ \Rightarrow \frac{E_{cp}}{(-E_{f}) G_a} (T - T_i) = x_a = \frac{9 \times 10^4 \cdot e^{-12000/1.9877}}{1 + 9 \times 10^4 \cdot e^{-12000/1.9877}} \]

\[ = \frac{9 \times 10^4 \cdot e^{-11800/1.9877}}{1 + 9 \times 10^4 \cdot e^{-11800/1.9877}} \]

\[ = \frac{9 \times 10^4 \cdot e^{-11800/1.9877}}{1 + 9 \times 10^4 \cdot e^{-11800/1.9877}} \]

This is a non-linear function in \( T \) and can be solved by Newton-Raphson technique.
\[
\frac{d\xi}{dT} = g'(T) = 1 - \frac{9.26 \times 10^{12} e^{-12000/RT}}{T^2(1.91 \times 10^6 e^{-12000/RT})}
\]

Newton Raphson Algorithm:

\[
E_{t+1} = E_t - \frac{g(T_t)}{g'(T_t)}
\]

\[
T_{t+1} = T_t - \frac{g(T_t)}{g'(T_t)}
\]

Iterate till \( T_{t+1} = T_t \)

Initial guess \( T_0 = ? \)

Actually there are three solutions to the problem. Depending on the initial guess of the initial guess to the algorithm, one cannot be obtained from the Newton Raphson Algorithm.

And original non-linear equation is

\[
5.87 \times 10^{-3} (T-293) = 7 \times 10^4 e^{-12000/RT} \frac{1 + 9.26 \times 10^6 e^{-12000/RT}}{1 + 9.26 \times 10^6 e^{-12000/RT}}
\]
Another way to solve the problem is to plot $T_{ln} e^{-T}$ separately for each $T$. This gives the following:

![Graph showing $T_{ln} e^{-T}$](image)

The three points of intersection give the results:

<table>
<thead>
<tr>
<th>$T$</th>
<th>$X_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>295 K</td>
<td>0.0114</td>
</tr>
<tr>
<td>395 K</td>
<td>0.48%</td>
</tr>
<tr>
<td>452 K</td>
<td>0.93%</td>
</tr>
</tbody>
</table>
Second order Reaction

Mass balance on A:

\[ F_{in} \Delta X_A = -k_A e^{-\frac{E_A}{RT}} C_A^0 (1-X_A)^n V = 0 \]

\[ \frac{\Delta X_A}{X_A} = \frac{1 + 2k_A C_A^0}{k_A C_A^0} x_a + 1 = 0 \]

\[ X_A = \frac{\frac{1 + 2k_A C_A^0}{k_A C_A^0} x_a + 1}{\sqrt{\left( \frac{1 + 2k_A C_A^0 e^{\frac{E_A}{RT}}}{2k_A C_A^0 e^{\frac{E_A}{RT}}} \right)^n - 1}} \]

This is the G curve.

Energy balance:

\[ \delta Q C_A (T_c - T) + (-\Delta H_e) F_{in} X_A = 0 \]

\[ 2 \times 10^{-2} \times (258 - T) + 131000 \times 14.2 \times 2 \times 10^{-4} x_A = 0 \]

\[ T = 298 + 26.72 \times x_A \]

\[ X_A = 3.74 \times 10^{-3} (T - 298) \]

This is the L curve.

Graphical plot of L and G curves yield Xo solution.

In other approach:\n
\[ X_A = \frac{k_A e^{-\frac{E_A}{RT} X_A + \delta C_A (1-x_A)^n}}{C_A} \]
\[ T = 22^\circ C = 300 K \]

\[ \text{Rin} = \text{Watt} \cdot \text{Ohm} \]

\[ \frac{dU}{dR} = \frac{dU}{dE} \]

\[ \int \frac{dU}{dR} = \frac{dU}{dE} = \frac{V_{10}}{0C} \]

\[ \int \frac{dU}{dX} = \frac{2V_{10}}{0C} \]

\[ X_1 \quad X_2 \quad X_3 \]

\[ X_2 = X_1 / \epsilon \] 10000

\[ -q_1 = (-4 \mu A) \text{ PNE} X_4 \]

\[ \begin{align*}
q_2 &= (4 \mu A) \text{ PNE} (X_2 - X_1) \\
X_1 &= X_2 \\
X_2 &= X_3 \\
X_3 &= X_4 \\
X_4 &= X_5 \\
X_5 &= X_6 \\
X_6 &= X_7 \\
X_7 &= X_8 \\
X_8 &= X_9 \\
X_9 &= X_{10} \\
\end{align*} \]
b) Mary Tmt line

For some value \( T_m = \bar{P} \alpha \eta \)

\( q'_{CR} \frac{dx}{dV} = \left( \frac{1}{\alpha^2} \right) x \)

\( \frac{dx}{dV} = \left( \frac{1}{\alpha^2} \right) \frac{q'_{CR}}{x} \)

\( V > 0 \quad x > 0 \)
\( \int_0^V dV = \int_{x_0}^{x_1} dx \)

\( \frac{dx}{dV} = \left( \frac{1}{\alpha^2} \right) \frac{q'_{CR}}{x} \)

\( V = V_{so} \quad x_1 = x_{AI} \)

Sign of reactant \( x_1 = c + V \)

\( u = \frac{1}{\alpha^2} \)

\( \alpha_x = \alpha_x \quad (x_{AI}) \)

\( \bar{e}_i = \left( -\alpha x_{AI} \right) \bar{F}_{AI} (x_1 - x_{AI}) \)

\( + \rho \alpha x (T_m - \bar{T}_{AI}) \)
\( \phi \rho \left( \overline{f_0 - 1} \right) + \left( -4 \pi m \right) \phi \psi_0 (x) + \psi = 0 \)

\( (4 \pi m) \phi \overline{x} \psi = -\psi^2 \)