

5.1 By the definition of Eq 7 or 8 we have

$$\tau = \frac{1}{5} = \frac{1}{1 \text{ min}^{-1}} = 1 \text{ min} \leftarrow$$

From the discussion following Eq 24 \bar{t} is somewhat less than 1 min because the density decreases with conversion. Therefore $\bar{t} > 1 \text{ min} \leftarrow$

Discussion If we really needed it we could derive \bar{t} as follows. For a differential section of plug flow reactor

$$\left. \begin{aligned} dt &= \frac{dV}{v} \\ dV &= \frac{F_{A0} dX_A}{(-r_A)} \end{aligned} \right\} \begin{aligned} &\text{combining and integrating gives} \\ &\text{the expression for } \bar{t}, \text{ or with} \\ &(F_{A0}, \text{ mol/s}) = (C_{A0}, \text{ mol/m}^3)(v_0, \text{ m}^3/\text{s}) \end{aligned}$$

$$\bar{t} = C_{A0} \int_0^{X_{Af}} \frac{dX_A}{(-r_A) \frac{v}{v_0}} \quad \leftarrow \quad C_{A0} \int_0^{X_{Af}} \frac{dX_A}{(-r_A)(1 + \epsilon_A X_A)} \quad \dots \quad (24)$$

changes with conversion for linear expansion

Note that knowing $\tau = \int \frac{dX_A}{-r_A}$ does not allow us to find \bar{t} unless $-r_A = f(C_A)$ is known. But anyway I don't see any need to find \bar{t} except in tracer studies.

5.3 For the mixed flow reactor

$$-r_A = \frac{C_{A0} - C_{Af}}{\tau} = \frac{C_{A0} - C_{Af}}{V/v} = \frac{1 - 0.01}{2/4} = 1.98 \frac{\text{mol}}{\text{lit} \cdot \text{min}} \leftarrow$$

and

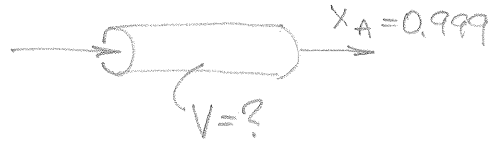
$$r_W = \frac{C_{WF} - C_{W0}}{\tau} = \frac{0.0002 - 0}{2/4} = 0.0004 \frac{\text{mol}}{\text{lit} \cdot \text{min}} \leftarrow$$

5.5

$$C_{A0} = 100 \text{ mmol/lit}$$

$$C_{B0} = 200 \text{ mmol/lit}$$

$$v = 400 \text{ lit/min}$$



$$-r_A = 200 C_A C_B$$

mol/lit·min

For a 2nd order reaction, Eq 3.14 gives

$$k \tau C_{A0} (M-1) = \ln \left[\frac{M-X_A}{M(1-X_A)} \right] \quad \text{where } M = \frac{C_{B0}}{C_{A0}} \neq 1$$

Thus $M = \frac{200}{100} = 2$

Replacing all values

$$200(\tau)(0.1)(2-1) = \ln \left[\frac{2-0.999}{2(1-0.999)} \right] = 6.2156$$

or

$$\tau = 0.31 \text{ min}$$

Therefore

$$V = \tau v = (0.31)(400) = 124 \text{ lit}$$

5.7

First find the rate constant: $k = \frac{\ln 2}{t_{1/2}} = \frac{\ln 2}{5.2} = 0.1333 \text{ day}^{-1}$

Then for mixed flow, Eq 14a gives

$$\frac{a}{a_0} = \frac{1}{1+k\bar{E}} = \frac{1}{1+(0.1333)30} = 0.2$$

$$\therefore \text{Fraction of activity removed} = 1 - 0.2 = 0.8 = 80\%$$

5.9

From Eq 3.58a, for this M-M type reaction,

$$k_1 \frac{V}{v} = \ln \frac{C_{A0}}{C_A} + k_2 (C_{A0} - C_A)$$

Inserting $k_1 = 0.1$, $k_2 = 0.5$, $v = 25$, $C_{A0} = 2$ and $C_A = 0.1$ we get

$$V = \frac{25}{0.1} \left[\ln \frac{2}{0.1} + 0.5(2-0.1) \right]$$

$$= 986 \text{ lit} \approx 1 \text{ m}^3$$

5.11



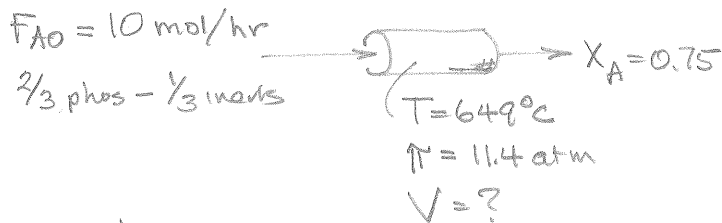
$$-r_A = \frac{0.1 C_A}{1 + 0.5 C_A} \text{ mol/lit} \cdot \text{min}$$

First of all $C_A = C_{A0}(1 - X_A) = 2(1 - 0.95) = 0.1$

Then for mixed flow

$$V = \frac{v(C_{A0} - C_A)}{-r_A} = \frac{25(2 - 0.1)}{\frac{(0.1)(0.1)}{1 + 0.5(0.1)}} = 4987.5 \text{ lit} \approx 5 \text{ m}^3 \leftarrow$$

5.13



$$-r_{\text{phos}} = (10 \text{ hr}^{-1}) C_{\text{phos}}$$

For a 1st order reaction.

$$k \frac{C_{A0} V}{F_{A0}} = (1 + \epsilon_A) \ln \frac{1}{1 - X_A} - \epsilon_A X_A \quad \text{--- (i)}$$

Evaluate terms

$$C_{A0} = \frac{P_{A0}}{RT} = \frac{11.4 \times \frac{2}{3}}{(0.08206)(649 + 273)} = 0.1 \frac{\text{mol}}{\text{lit}}$$

$$k = 10 \text{ hr}^{-1}$$

$$F_{A0} = 10 \text{ mol/hr}$$

$$\epsilon_A = 0.5 \leftarrow$$

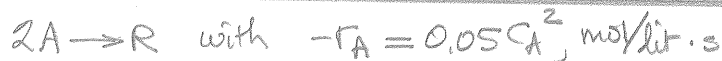
$4A \rightarrow 7R$
 reactants: $40 \rightarrow 70$
 inerts: $20 \rightarrow 20$

$\therefore \epsilon_A = \frac{90 - 60}{60} = \frac{1}{2}$

Replacing in (i) gives

$$V = \frac{10}{10(0.1)} \left[(1 + 0.5) \ln \frac{1}{0.25} - (0.5)(0.75) \right] = 17 \text{ lit} \leftarrow$$

5.15



Evaluate terms $\epsilon_A = \frac{1 - 2}{2} = -0.5$

$$X_A = \frac{C_{A0} - C_A}{C_{A0} + \epsilon_A C_A} = \frac{1 - 0.5}{1 + (-0.5)(0.5)} = \frac{2}{3}$$

So for mixed flow

$$v = \frac{V(-r_A)}{C_{A0} X_A} = \frac{(2)(0.05 \times 0.5^2)}{1(2/3)} = 0.0375 \text{ lit/s} = 2.25 \text{ lit/min} \leftarrow$$

5.17

20% oxone (A)

80% air

 $v = 1 \text{ lit/s}$ $V = ?$

1.5 atm

93°C

 $X_A = 0.5$

ozone

 $2O_3 \rightarrow 3O_2$ $-r_A = kC_A^2$ $k = 0.05 \text{ lit/mol}\cdot\text{s}$

For a 2nd order reaction with expansion, Eq 23 gives:

$$V = \frac{v}{C_{A0}k} \left[2\varepsilon_A(1+\varepsilon_A)\ln(1-X_A) + \varepsilon_A^2 X_A + (\varepsilon_A+1)^2 \frac{X_A}{1-X_A} \right] \quad \text{--- (i)}$$

Evaluate terms

$$C_{A0} = \frac{P_{A0}}{RT} = \frac{(1.5)(0.2)}{(0.08206)(366)} = 0.01 \frac{\text{mol}}{\text{lit}}$$

$$\varepsilon_A = \frac{11-10}{10} = 0.1$$

Replacing in (i) gives

$$V = \frac{1}{(0.01)(0.05)} \left[2(0.1)(1+0.1)\ln(1-0.5) + (0.1)^2(0.5) + (0.1+1)^2 \frac{0.5}{(1-0.5)} \right]$$

$$= 2125 \text{ lit} = 2.1 \text{ m}^3$$

5.19

 $C_{A0} = 120 \text{ mmol/lit}$

3 atm

30°C

Various v_0 Various C_A $A \rightarrow 3R$

Find a rate equation

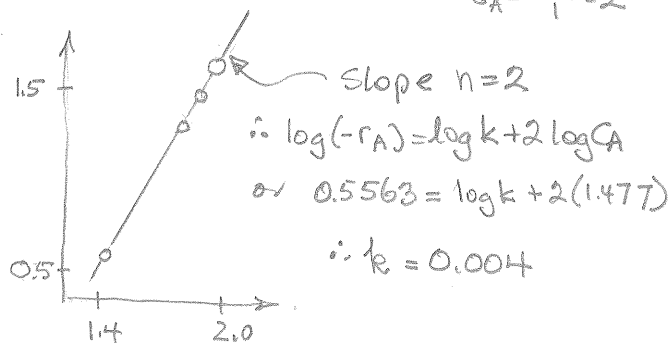
For each run

$$-r_A = \frac{C_{A0} X_A v_0}{V} = \frac{C_{A0} (C_{A0} - C_A) v_0}{(C_{A0} + \varepsilon_A C_A) V} = \frac{120(120 - C_A) v_0}{(120 + 2C_A)}$$

Now tabulate

| v_0 | C_A | $-r_A$ | $\log(-r_A)$ | $\log C_A$ |
|-------|-------|--------|--------------|------------|
| 0.06 | 30 | 3.6 | 0.5563 | 1.477 |
| 0.48 | 60 | 14.4 | 1.1584 | 1.778 |
| 1.5 | 80 | 25.7 | 1.41 | 1.903 |
| 8.1 | 105 | 44.2 | 1.6452 | 2.07 |

given data

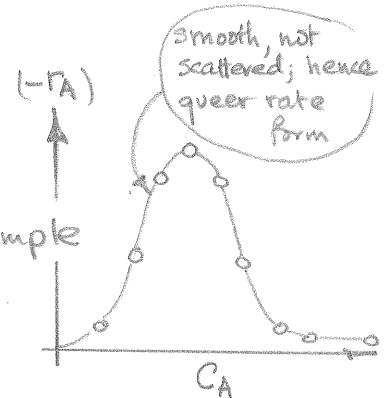


$$\therefore -r_A = 0.004 C_A^2, \text{ mmol/lit}\cdot\text{min}$$

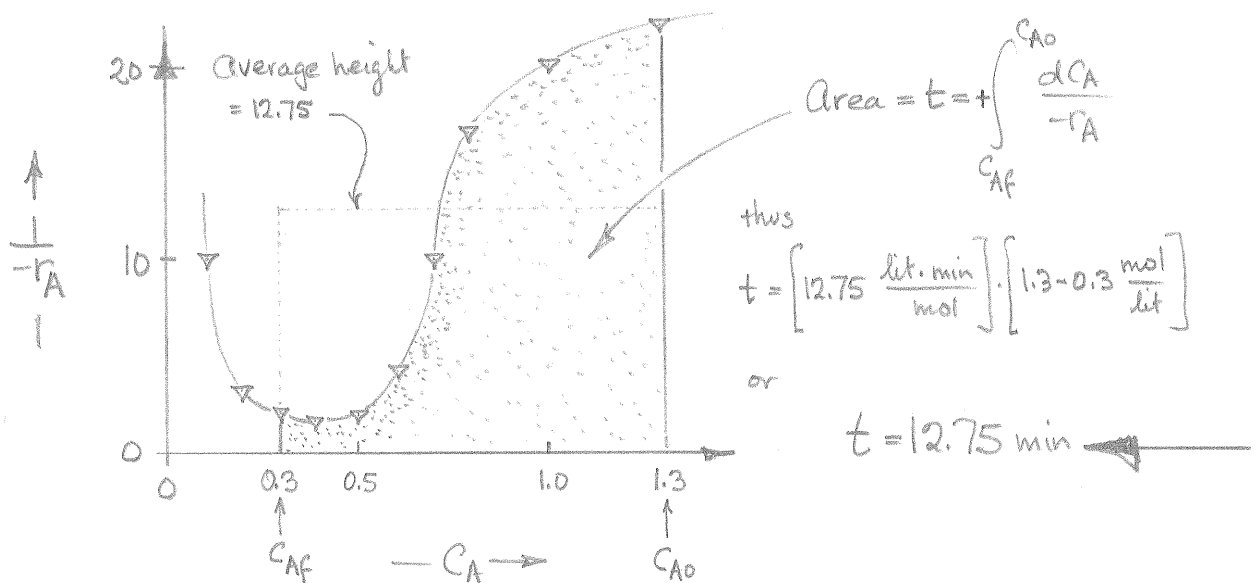
5.21 The approach which probably first comes to mind is to find a rate equation to represent the data, first order, second, etc., and then integrate it to give the time; thus

$$t = - \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A} \quad \text{--- Eq 4, since } \varepsilon_A = 0$$

But a quick plot of the data shows that no simple rate form of chapter 3 will fit the data, so it looks like this approach won't work.



With a bit more thought we see that we were not asked to find a rate equation, we were just asked for t , and that this could be done by solving the general design equation, Eq 4 directly by graphical procedures. let us do this



This is the more general way of solving this problem since it does not require that we describe the rate by an equation.

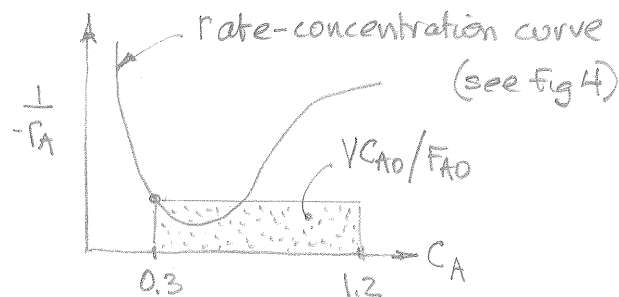
5.23 a) Given

$$C_{A0} = 1.2 \text{ mol/lit} \\ F_{A0} = 1000 \text{ mol/hr} \rightarrow \text{CSTR} \rightarrow X_A = 0.75$$

Since this is a liquid reaction $\varepsilon_A = 0$, so $\frac{C_{Af}}{C_{A0}} = 1 - X_A$
 or $C_{Af} = C_{A0}(1 - X_A) = 1.2(1 - 0.75) = 0.3 \text{ mol/lit}$

From the performance equation for mixed flow, Eq 13,

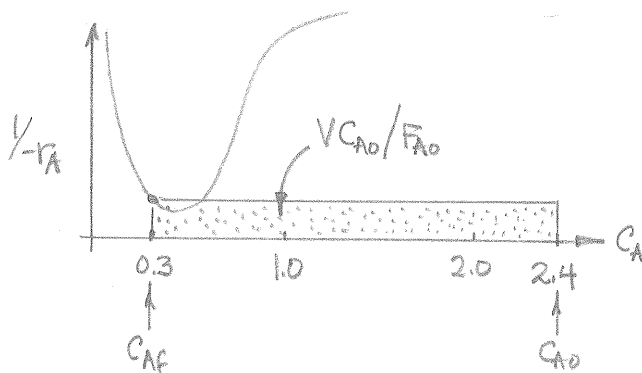
$$V = \frac{F_{A0} \cdot C_{A0} - C_{Af}}{C_{A0} \cdot -r_{Af}} \\ = \frac{1000 \frac{\text{mol}}{\text{hr}} \cdot (1.2 - 0.3 \frac{\text{mol}}{\text{lit}})}{1.2 \frac{\text{mol}}{\text{lit}} \cdot (0.5 \frac{\text{mol}}{\text{lit} \cdot \text{min}})} \cdot \frac{1 \text{ hr}}{60 \text{ min}} = 25 \text{ lit} \quad \leftarrow \text{a)}$$



b) If F_{A0} is doubled while all else remained unchanged we see from

$$V = \frac{F_{A0} \cdot C_{A0} - C_{Af}}{C_{A0} \cdot -r_{Af}} \quad \dots \text{ that } V \text{ is doubled,}$$

$$\text{or } V = 50 \text{ lit.} \quad \leftarrow \text{b)}$$



In doubling C_{A0} keeping all else the same, including F_{A0} , we get

$$V = \frac{F_{A0} \cdot C_{A0} - C_{Af}}{C_{A0} \cdot -r_{Af}} \\ = \frac{1000 \cdot (2.4 - 0.3) \cdot 1}{2.4 \cdot 0.5 \cdot 60}$$

$$\text{or } V = 29.167 \text{ lit} \quad \leftarrow \text{c)}$$

5.25 For a mixed flow reactor, with $\varepsilon_A = 0$, we find the rate of reaction from Eq 13. Thus we tabulate as follows

| t, sec | C_{A0} | $C_{A, \text{out}}$ | $-\frac{1}{r_A} = \frac{t}{C_{A0} - C_{A, \text{out}}}$... at $C_{A, \text{out}}$ |
|-----------------|----------|---------------------|--|
| 300 | 2 | 0.65 | $300/(2-0.65) = 222$ |
| 240 | 2 | 0.92 | 222 |
| 250 | 2 | 1.00 | 250 |
| 110 | 1 | 0.56 | 250 |
| 360 | 1 | 0.37 | 572 |
| 24 | 0.48 | 0.42 | 400 |
| 200 | 0.48 | 0.28 | 1000 |
| 560 | 0.48 | 0.20 | 2000 |

Holding time for plug flow.

We may solve this by using conversions as suggested in the text. However since $\varepsilon_A = 0$

the use of concentrations poses no problems.

Let us use this. Then the performance expression is Eq. 19, or

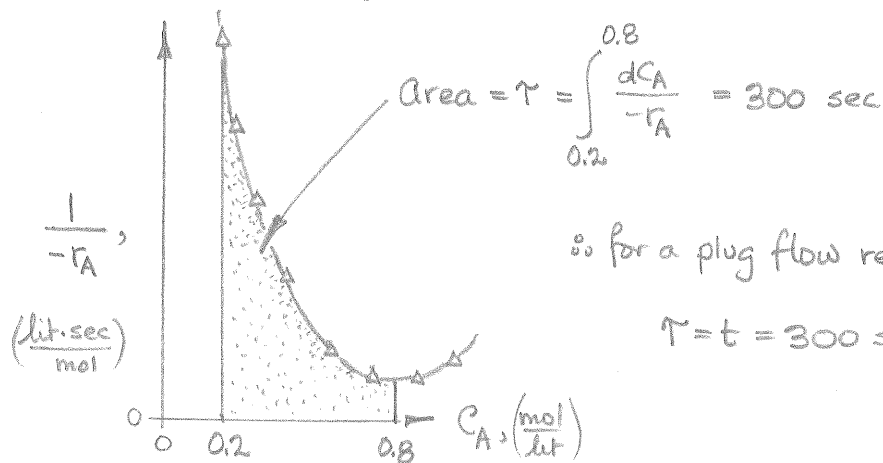
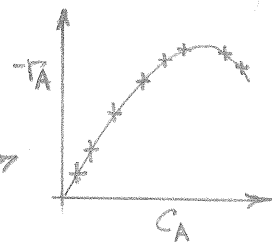
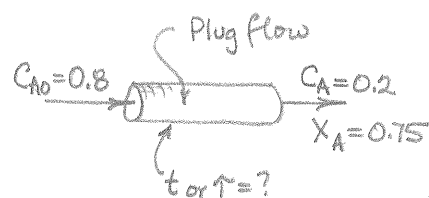
$$\tau = - \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A}$$

So tabulate $-r_A$ as shown in the table above.

Now a plot of C_A vs $-r_A$ gives a figure like this

This indicates that no simple rate expression, say n^{th} order, will fit the data, hence solve graphically.

This is done by plotting C_A vs $1/(-r_A)$ and integrating.



∴ for a plug flow reactor

$$\tau = t = 300 \text{ sec}$$

5.27a) Since the vat contains ~99% ethanol I guess that Imbibit fell-dead drunk - into the vat. This would decrease the volume available for fluid. Let's see if this could account for the decrease in conversion of googlix.

Secondly, since ethanol is in very large excess we can reasonably assume pseudo first order kinetics with respect to googlix (A). So for mixed flow Eq 13 gives, for before & after

$$\left. \begin{aligned} k\tau_1 &= \frac{X_{A1}}{1-X_{A1}} = \frac{0.8}{1-0.8} = 4 \\ k\tau_2 &= \frac{X_{A2}}{1-X_{A2}} = \frac{0.75}{1-0.75} = 3 \end{aligned} \right\}$$

Since $V_2/V_1 = \tau_2/\tau_1$ we have

$$V_2 = 100(3/4) = 75 \text{ Imp gal}$$

So the decrease in volume is $\Delta V = 100 - 75 = 25 \text{ Imp. gal}$

$$\text{or } (25 \text{ Imp. gal}) \left(\frac{10 \# \text{H}_2\text{O}}{1 \text{ Imp. gal}} \right) \left(\frac{1 \text{ ft}^3}{62.4 \# \text{H}_2\text{O}} \right) = 4.01 \text{ ft}^3$$

Let us see if this is Imbibit's volume. With his density being $62.4 \#/\text{ft}^3$

$$\text{Imbibit's volume is } \frac{(18 \text{ stone})(14 \#/\text{stone})}{(62.4 \#/\text{ft}^3)} = 4.04 \text{ ft}^3$$

These volumes agree so Imbibit could well be in the vat. } ←

This hypothesis, or guess does fit the facts

b) Why did Watson never come up with this explanation?

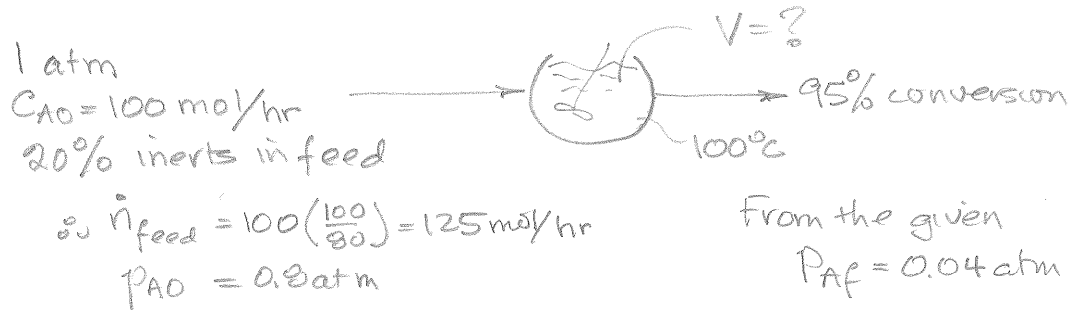
Because smoking near 99% alcohol was not really cool. ←

Note • Watson was not knowledgeable on pickling. You use dill for pickling in brine, not alcohol.

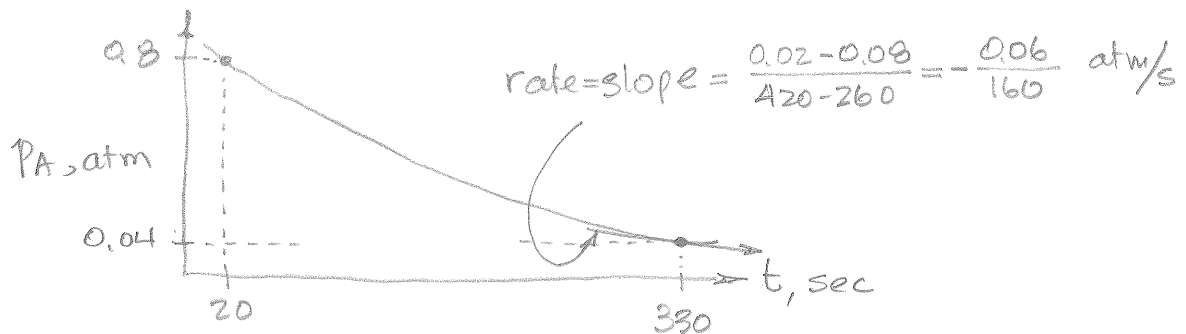
• Of course everyone knows that 1 Imp. gal is the volume of 10 # H₂O, and that 1 stone weighs 14 #.

5.29 (extension of problem 5.28)

Given a gas phase reaction $2A \rightarrow R + S$



For mixed flow we must find the rate at the exit conditions. Then we can proceed to finding the reactor size. So draw an accurate p_A vs t curve and find the slope (hence rate) at $p_A = 0.04 \text{ atm}$



The performance equation for mixed flow, Eq 13, in pressure units is

$$\tau = \frac{V}{v} = \frac{P_{A0} - P_A}{-r_A} = \frac{0.8 - 0.04}{(0.06/160)} = 2026.67 \text{ s}$$

But $\tau = \frac{V}{v}$ so evaluate v from $p v = n R T$. Thus

$$v = \frac{n R T}{P} = \frac{(125)(0.08206)(373)}{(1)} = 3826 \text{ lit/hr}$$

$$\therefore V = \tau v = (2026.67 \text{ s})(3826 \text{ lit/hr}) \left(\frac{1 \text{ hr}}{3600 \text{ s}} \right) = 2150 \text{ lit} = 2.15 \text{ m}^3$$