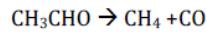


1. Mass Balance for a Mixture with Chemical Reaction

At high temperatures acetaldehyde (CH_3CHO) dissociates into methane and carbon monoxide by the following reaction



At 520°C the rate at which acetaldehyde dissociates is

$$\frac{dC_{\text{CH}_3\text{CHO}}}{dt} = -0.48 C_{\text{CH}_3\text{CHO}}^2 \frac{\text{m}^3}{\text{kmol s}}$$

where C is the concentration in kmol/m^3 . The reaction occurs in a constant-volume, 1-L vessel, and the initial concentration of acetaldehyde is $10 \text{ kmol}/\text{m}^3$

- a. If 5 mols of the acetaldehyde reacts, how much methane and carbon monoxide is produced?

First identify V_B (the stoichiometric coefficient) for each species.



From that form the stoichiometric coefficient is readily identifiable

$$V_{\text{CH}_4} = +1 \quad V_{\text{CO}} = +1 \quad V_{\text{CH}_3\text{CHO}} = -1$$

at this point expressions for their present value can be obtained using the form:

$$N_{a,i} = N_{a,0} + V_a \cdot X$$

where $N_{a,i}$ is the quantity of species a @ time t	V_a is the stoichiometric coefficient of species a
$N_{a,0}$ is the quantity of species a @ time 0	X is the extent of reaction.

Specifically we get the following expressions

$$N_{\text{CH}_3\text{CHO}} = 10 - X \quad N_{\text{CH}_4} = X \quad N_{\text{CHO}} = X$$

- A) 5 mols of CH_3CHO is used, this means $X = 5$. Using the above equations

$$N_{\text{CH}_3\text{CHO}} = 10 - X \quad N_{\text{CH}_4} = X \quad N_{\text{CHO}} = X$$

$$N_{\text{CH}_3\text{CHO}} = 5 \text{ mols} \quad N_{\text{CH}_4} = 5 \text{ mols} \quad N_{\text{CHO}} = 5 \text{ mols}$$

- B) Develop expressions for the amounts of acetaldehyde, methane, and carbon monoxide present at any time, and determine how long it would take for 5 mol of acetaldehyde to have reacted.

The first part of the question asks for expressions for each species at any time. These expressions were formulated above.

$$N_{\text{CH}_3\text{CHO}} = 10 - X \quad N_{\text{CH}_4} = X \quad N_{\text{CHO}} = X$$

X is the extent of reaction at time t . you can substitute from the latter half of this problem to put each species in terms of time directly.

The 2nd part wants the time for 5 mol acetaldehyde to have reacted.

The problem provides a rate law for acetaldehyde

$$\frac{dC_{CH_3CHO}}{dt} = -.48C_{CH_3CHO}^2$$

C is concentration.

The question asks for time. So you can integrate to introduce a variable T and then solve for T. There are many ways to do this. I will demonstrate what we feel is the simplest.

First how can you relate C_{CH_3CHO} to N_{CH_3CHO} ?

$C = N/V$ or in this case $C_{CH_3CHO} = N_{CH_3CHO} / \text{Volume}$

Because we have information about mols of CH_3CHO being used – lets use that form (you could instead convert the expression we have into Concentration if you insisted)

If we substitute as appropriate we find that the rate law becomes

$$\frac{dC_{CH_3CHO}}{dt} = -.48C_{CH_3CHO}^2 \rightarrow \frac{d N_{CH_3CHO} / \text{Volume}}{dt} = -.48 \frac{N_{CH_3CHO}^2}{\text{Volume}^2}$$

Let's rearrange so that we have some components we're familiar with.

$$\frac{1}{\text{Volume}} \frac{dN_{CH_3CHO}}{dt} = -.48 \frac{N_{CH_3CHO}^2}{\text{Volume}^2}$$

Hopefully you can recognize that earlier we determined $N_{CH_3CHO} = 10 - X$

$$\frac{1}{\text{Volume}} \frac{dN_{CH_3CHO}}{dt} = -.48 \frac{(10 - X)^2}{\text{Volume}^2}$$

The first “tricky” part we’ve got to get rid of the dN_{CH_3CHO} .

Strategy #1 Theory based substitution

dN_{CH_3CHO}/dt is **by definition** the rate of change of N_{CH_3CHO} over time. How can we get that in terms of X to make this equation solvable?

Recall that $N_{a,i} = N_{a,o} + V_a \cdot X$ gives us quantity of N_a at any given time.

If you have a formula for a species at time T you can take the derivative to obtain the rate of change of that species over time.

$$N_{a,i} = N_{a,o} + V_a \cdot X \rightarrow dN/dt = V_a (dx/dt)$$

↓

$$dN_{CH_3CHO}/dt = V_{CH_3CHO} (dx/dt)$$

If you take that substitution into the equation you get

$$\frac{1}{Vol.} \frac{dN_{CH_3CHO}}{dt} = -.48 \frac{(10 - X)^2}{Volume^2} \rightarrow \frac{1}{Vol.} V_{CH_3CHO} \frac{dX}{dt} = -.48 \frac{(10 - X)^2}{Volume^2}$$

Now let's plug in: $V_{CH_3CHO} = -1$ and $Volume = 1$ L

$$-\frac{dX}{dt} = -.48 (10 - X)^2$$

From here its just math.

Strategy #2 Plug and chug

$$\frac{1}{Volume} \frac{dN_{CH_3CHO}}{dt} = -.48 \frac{(10 - X)^2}{Volume^2}$$

To get rid of the dN_{CH_3CHO} just plug in $10-X$ again.

$$\frac{1}{Volume} \frac{d(10 - X)}{dt} = -.48 \frac{(10 - X)^2}{Volume^2}$$

You can't just divide $(10-X)$ to get rid of it in the numerator of the left side of the equation.

You have to take the derivative of $d(10-X) \rightarrow -dx$

$$\frac{1}{Vol.} \frac{-dx}{dt} = -.48 \frac{(10 - X)^2}{Volume^2}$$

Input $Volume = 1$ L and you get

$$-\frac{dX}{dt} = -.48 (10 - X)^2$$

And it's just math from here

MATH:

$$\begin{aligned} -\frac{dX}{dt} &= -.48 (10 - X)^2 \rightarrow -\frac{1}{(10 - X)^2} \frac{dX}{dt} = -.48 \\ -\frac{1}{(10 - X)^2} \frac{dX}{dt} &= -.48 \rightarrow \frac{1}{(10 - X)^2} dx = .48 dt \end{aligned}$$

Now we integrate. We have to take the definite integral of Molar extent at time 0 to time t

$$\int_{X(0)}^{X(t)} \frac{1}{(10 - X)^2} dx = \int_0^t .48 dt$$

So this results in $\frac{1}{10-X} \Big|_0^{X(t)} = .48t \Big|_0^t$

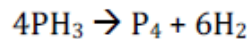
$$\frac{1}{(10 - X(t))} - \frac{1}{(10 - 0)} = .48t - .48(0)$$

X(t) for the t we are interested in is = 5 mols so plug that in

$$\frac{1}{(10 - 5)} - \frac{1}{(10)} = .48t$$

So **t = 0.208**

2. At high temperatures phosphine (PH₃) dissociates into phosphorus and hydrogen by the following reaction:



At 800°C the rate at which phosphine dissociates is

$$\frac{dC_{\text{PH}_3}}{dt} = -3.715 \times 10^{-6} C_{\text{PH}_3}$$

for t in seconds. The reaction occurs in a constant-volume, 2-L vessel, and the initial concentration of phosphine is 5 kmol/m³

- a. If 3 mol of the phosphine reacts, how much phosphorus and hydrogen is produced?



$$V_{\text{PH}_3} = -4 \quad V_{\text{P}_4} = +1 \quad V_{\text{H}_2} = +6$$

$$N_{\text{PH}_3,0} = 5 \text{ kmol/m}^3 \cdot 2 \text{ L} = 10 \text{ Mol}$$

$$N_{\text{PH}_3} = 10 - 4X \quad N_{\text{P}_4} = X \quad N_{\text{H}_2} = 6X$$

- A) To find how much P₄ and H are produced find the molar extent of rxn so you can use the above expressions.

N_{PH₃} = 10 - 4X 3 mols are used at the time you are interested in so plug in 7 for your final amount

$$7 = 10 - 4X \Rightarrow X = 0.75$$

$$N_{\text{P}_4} = X = 0.75 \text{ mols}$$

$$N_{\text{H}_2} = 6X = 4.5 \text{ mols}$$

- b. Develop expressions for the number of moles of phosphine, phosphorus, and hydrogen present at any time, and determine how long it would take for 3 mol of phosphine to have reacted.

B) The question gives you rate of change of phosphine in terms of concentration.

$$\frac{dC_{PH_3}}{dt} = -3.715 \times 10^{-6} C_{PH_3}$$

Rearrange this in terms of mols so you can use the equation you have for molar extent

$$C_{PH_3} = N_{PH_3}/Volume = \frac{10 - 4X}{2L}$$

Substitute back into the given rate

$$d\left(\frac{10 - 4X}{2}\right)/dt = -3.715 \times 10^{-6} \left(\frac{10 - 4X}{2}\right)$$

Use either approach explained in question 1

$$-2 \frac{dX}{dt} = -3.75 \times 10^{-6} (5 - 2X)$$

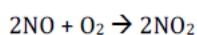
Integrate from the 2 relevant timepoints: when X is 0 (the starting point) and when X = 0.75 (the t you are interested in.

$$\int_{X(0)}^{X(t)} \frac{2}{5 - 2X} dX = 3.75 \times 10^{-6} dt$$

$$-\log(5 - 2X)|_0^{0.75} = (3.75 \times 10^{-6})t$$

$$t = 96000 \text{ seconds}$$

3. The following reaction occurs in air:



at 20°C the rate of this reaction is

$$\frac{dC_{NO}}{dt} = -1.4 \times 10^{-4} C_{NO}^2 C_{O_2}$$

for t in seconds and concentrations in kmol/m³. The reaction occurs in a constant-volume, 2-L vessel, and the initial concentration of NO is 1 kmol/m³ and that of O₂ is 3 kmol/m³

a. If 0.5 mol of NO reacts, how much NO₂ is produced?



$$V_{NO} = -2$$

$$V_{O_2} = -1$$

$$V_{NO_2} = 2$$

Convert given concentrations to mols to find initial conditions

$$N_{NO} = 2 - 2X$$

$$N_{O_2} = 6 - X$$

$$N_{NO_2} = 2X$$

If 0.5 mol of NO has reacted then then 1.5 mol of NO remain. To find molar extent of reaction

$$1.5 = 2 - 2X \text{ so } X = 0.25$$

thus **NO₂ = 0.5 mol**

b. Determine how long it would take for 0.5 mol of NO to have reacted.

$$\frac{dC_{NO}}{dt} = -1.4 \times 10^{-4} C_{NO}^2 C_{O_2}$$

$$C_{NO} = \frac{N_{NO}}{Vol} = \frac{2 - 2X}{2} = 1 - X$$

$$C_{O_2} = \frac{N_{O_2}}{Vol} = \frac{6 - X}{2}$$

$$\frac{dC_{NO}}{dt} = -1.4 \times 10^{-4} C_{NO}^2 C_{O_2} \Rightarrow \frac{d(1 - X)}{dt} = -1.4 \times 10^{-4} (1 - X)^2 \frac{6 - X}{2}$$

$$\frac{-dX}{dt} = -1.4 \times 10^{-4} (1 - X)^2 \frac{6 - X}{2}$$

$$\int_{X(0)}^{X(t)} \frac{1}{(1 - X)^2 \left(\frac{6 - X}{2}\right)} dX = 1.4 \times 10^{-4} dt$$

The relevant $X(t)$ is $X(t) = 0.25$

The integral is very complicated. They will be simpler on the exam.

$$\frac{2}{25} \left(\frac{5}{X - 1} + \log(6 - X) - \log(X - 1) \right) \Big|_0^{.25} = .00014t$$

t=812.311