Variable Volume Reaction Part-II (Flow Reactors)

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Flow reactors

- There are two types of Flow reactors

1. Continuous Stirred Tank Reactors(CSTR) or Ideal mixed Reactor.
2. Plug Flow Reactor(PFR)

There are the two extreme flow conditions from no-mixing in PFR to complete mixing in CSTR

Their performances are evaluated by two parameters

1. Space time and
2. Space volume

Space time: It is the time required to process one reactor volume of the feed at specified conditions. It is denoted by τ and has a unit sec or min.

Space time is obtained by dividing reactor volume 'V' with the volumetric flow rate of feed entering the reactor

$$\tau = \frac{V}{v_0}$$

If reactor volume= 10 liters and feed flow rate=5 liter/min, then space time= 2 min.

Space volume: It is the number reactor volumes of feed at specified conditions which can be processed in unit time. It is denoted by 's'. It has a unit of time^{-1} Where,

$$s = \frac{v_0}{V} = \frac{1}{\tau}$$

τ is used as the main design parameter for flow reactors.

- A reactor with a space time of 2min means every 2 mins one reactor volume can be processed. In 6 min 3 reactor volume can be treated.

- A space velocity of 5 hr^{-1} means five reactor volume of feed at specified conditions are being fed into the reactor per hr.

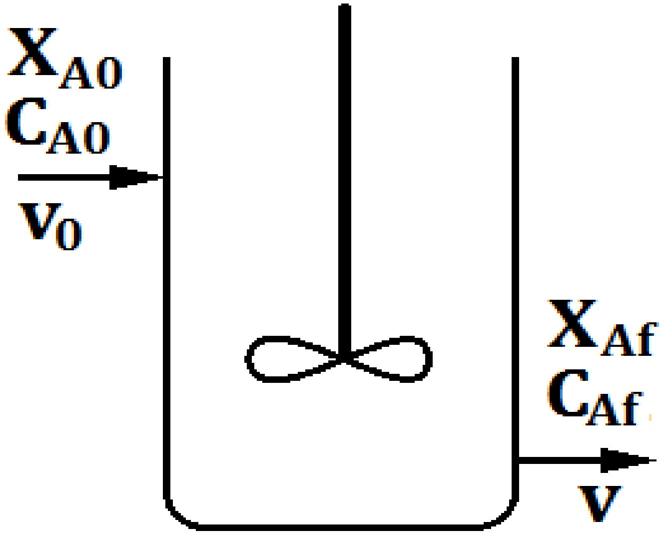
$$\tau = \frac{V}{v_0} or \qquad \frac{\tau}{C_{A0}} = \frac{V}{v_0 C_{A0}} = \frac{V}{F_{A0}}$$

For catalytic reactor we use

$$\frac{W}{F_{A0}} \quad is\ called\ 'TimeFactor'$$

W = weight of catalyst in a packed bed reactor

Ideal CSTR or Mixed Flow Reactor



$$F_{A0}(1 - X_{A0}) = F_{A0}(1 - X_A) + (-r_A)V$$

$$At \;\; X_{A0} = 0, \qquad F_{A0}X_A = (-r_A)V$$

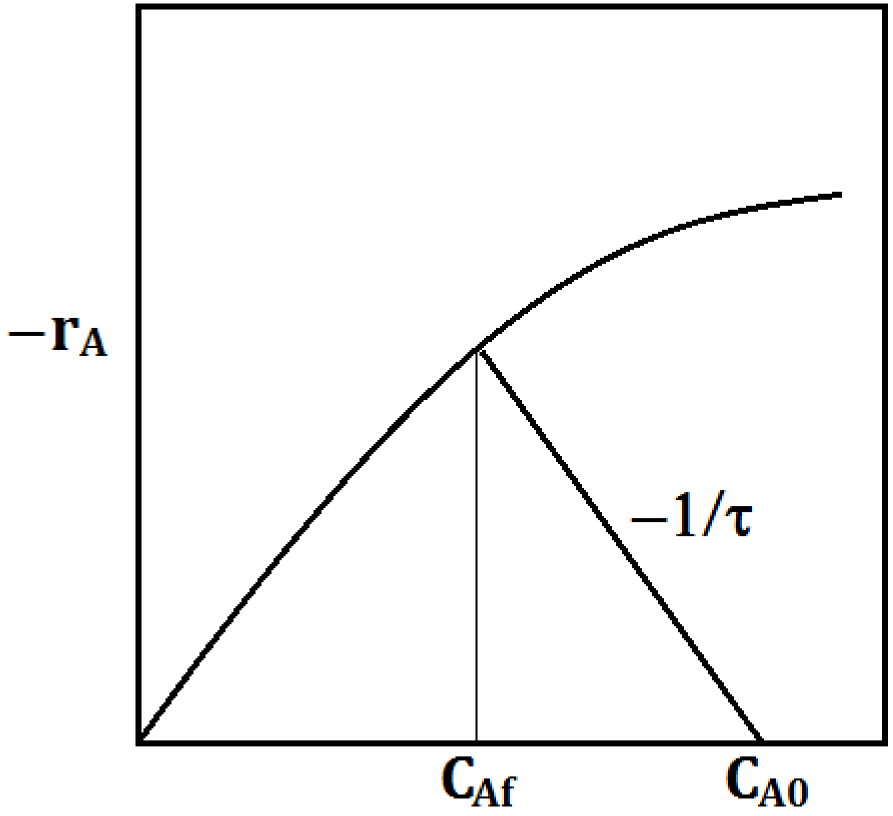
$$\frac{V}{F_{A0}} = \frac{X_A}{-r_A} = \frac{C_{A0} - C_{Af}}{C_{A0}(-r_A)}$$

$$\tau = \frac{C_{A0} - C_{Af}}{(-r_A)} \qquad or, \qquad \tau = \frac{C_{A0}(X_{Af} - X_{A0})}{(-r_A)}$$

$$(-r_A) = (C_{Af} - C_{A0})(-1/\tau)$$

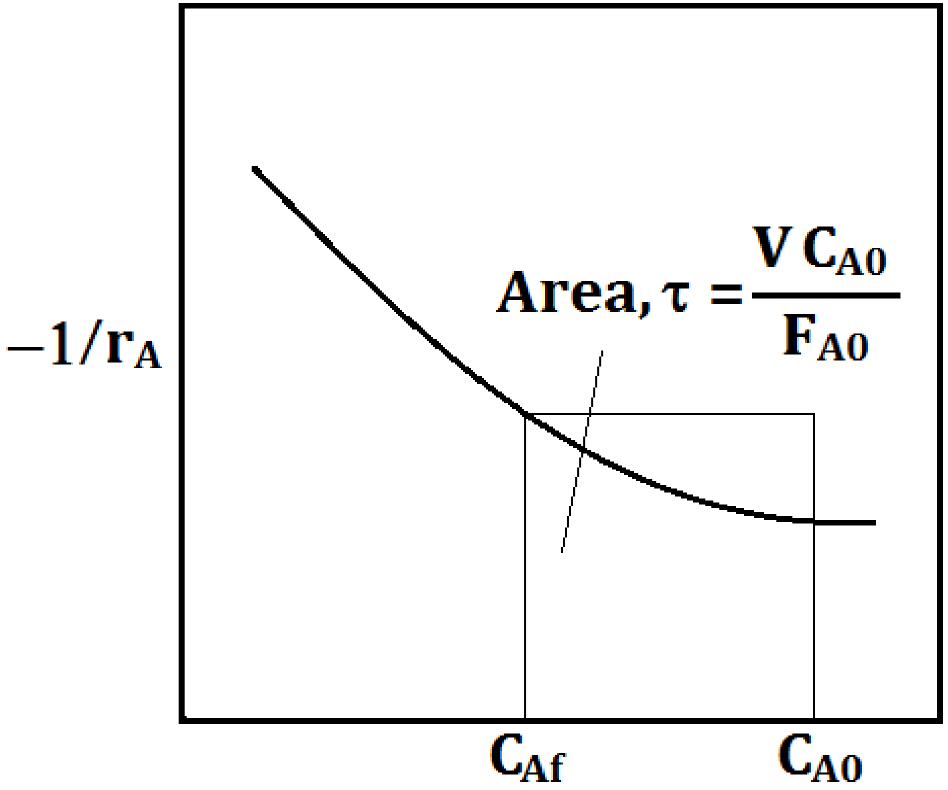
Ideal CSTR or Mixed Flow Reactor

$$\tau = \frac{C_{A0} - C_{Af}}{(-r_A)} \qquad (-r_A) = (C_{Af} - C_{A0})(-1/\tau)$$



Design of CSTR (Graphical presentation) in terms of concentration

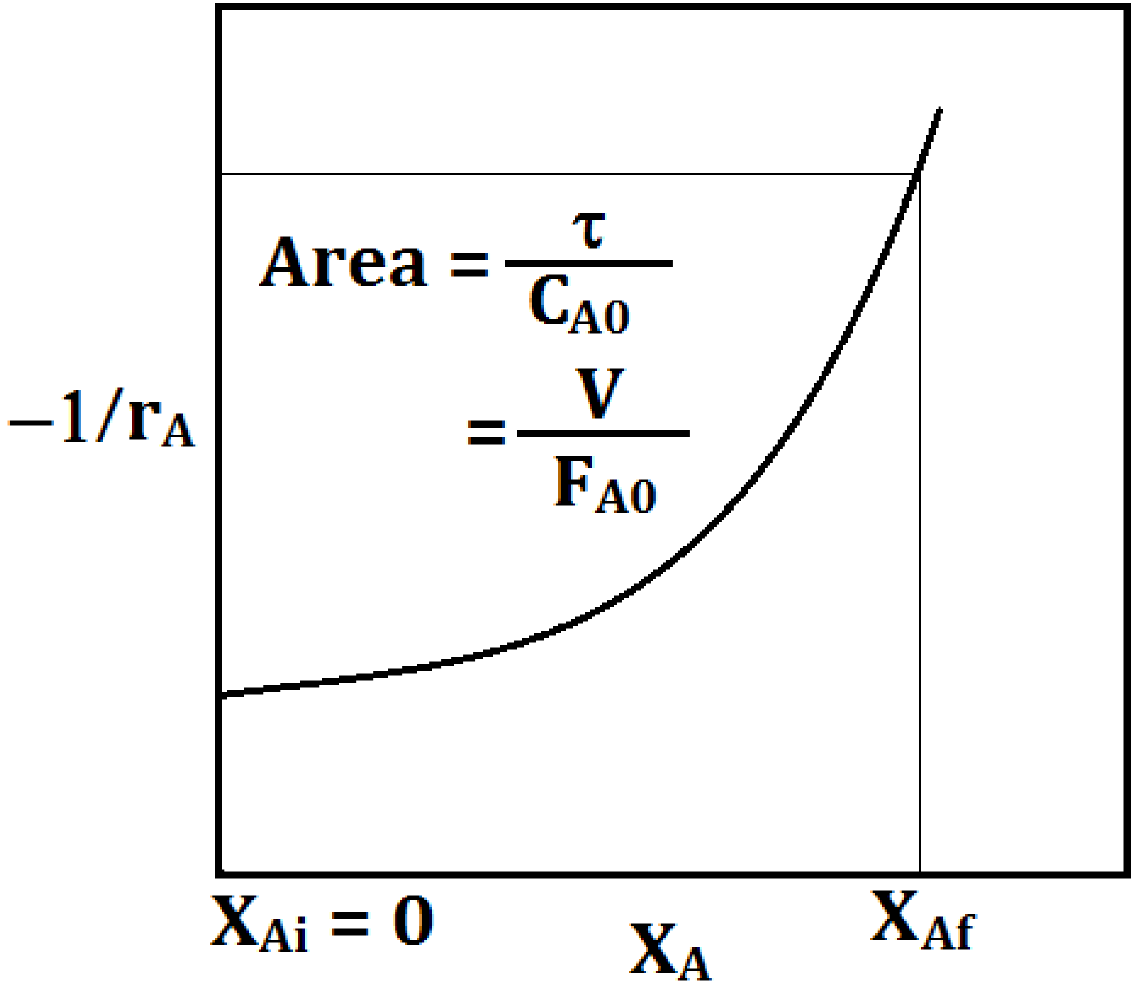
$$Area = \tau = \frac{VC_{A0}}{F_{A0}} = \left(C_{A0} - C_{Af}\right)\frac{1}{-r_A}$$



C_A vs. $-r_A$ plot

Graphical presentation in terms of conversion

$$\tau = C_{A0} \frac{X_{Af} - X_{A0}}{-r_A}$$



Variable density with first-order rate kinetics

$$\frac{\boldsymbol{V}}{\boldsymbol{F_{A0}}} = \frac{\boldsymbol{V_0}(1+\varepsilon_A X_A)}{\boldsymbol{C_{A0}v_0}(1+\varepsilon_A X_A)} = \frac{\boldsymbol{X_A}}{\boldsymbol{kC_{A0}}\frac{\boldsymbol{(1-X_A)}}{(1+\varepsilon_A X_A)}}$$

$$\boldsymbol{k\tau} = \frac{\boldsymbol{X_A}(1+\varepsilon_A X_A)}{\boldsymbol{(1-X_A)}} = f(\boldsymbol{X_A})$$

For various τ values calculate $f(X_A)$ with X_A values and from the slope of the straight line plot k is obtained.

- **Variable Density with second-order rate kinetics**
- $\boldsymbol{Rate\ equation:\ -r_A = kC_A^2}$
- $C_A = C_{A0}\frac{(1-X_A)}{(1+\varepsilon_A X_A)}$

Variable Density with second-order rate kinetics

$$\frac{V}{F_{A0}} = \frac{V_0(1+\varepsilon_A X_A)}{C_{A0}v_0(1+\varepsilon_A X_A)} = \frac{X_A}{kC_{A0}{}^2\,\frac{(1-X_A)^2}{(1+\varepsilon_A X_A)^2}}$$

$$\boldsymbol{k\tau = \ (X_A) = \frac{X_A(1+\varepsilon_A X_A)^2}{kC_{A0}(1-X_A)^2}}$$

Problem-1 (mixed reactor)

A high molecular weight hydrocarbon stream A is fed continuously to a heated high temperature mixed reactor where it tharmally cracks (homogeneous gas reaction) into a lower molecular weight product, R by a stoichiometry approximated by $A \rightarrow 5R$. By changing the feed rate different extents of cracking are obtained as follows:

F_{A0}, millimol/hr	300	1000	3000	5000
$C_{A,out}$, millimol/liter	16	30	50	60

The internal void volume is V=0.1 liter, and at the temperature of the reactor the feed concentration is C_{A0} = 100 milimol/liter. Find a rate equation to represent the cracking reaction

Solution to Problem 1

- $A \rightarrow 5R, \epsilon_A \neq 0$
- $\epsilon_A = \frac{5-1}{1} = 4, \quad C_{A0} = 100\,\frac{millimol}{liter},\ V = 0.1\,liter,$
- $C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X_A)}{V_0(1+\varepsilon_A X)} = \frac{C_{A0}(1-X_A)}{(1+\varepsilon_A X)}$
- $X_A = \frac{1-(C_A/C_{A0})}{1+\epsilon_A(C_A/C_{A0})}$
- For C_A= 16millimol/liter, $X_A = \frac{1-(16/100)}{1+4(16/100)} = 0.512$
- $-r_A = \frac{F_{A0}X_A}{V} = \frac{300\times 0.512}{0.1} = 1536$
- Similarly, for all data points calculate C_A and $-r_A$. Also lnC_A and ln$(-r_A)$

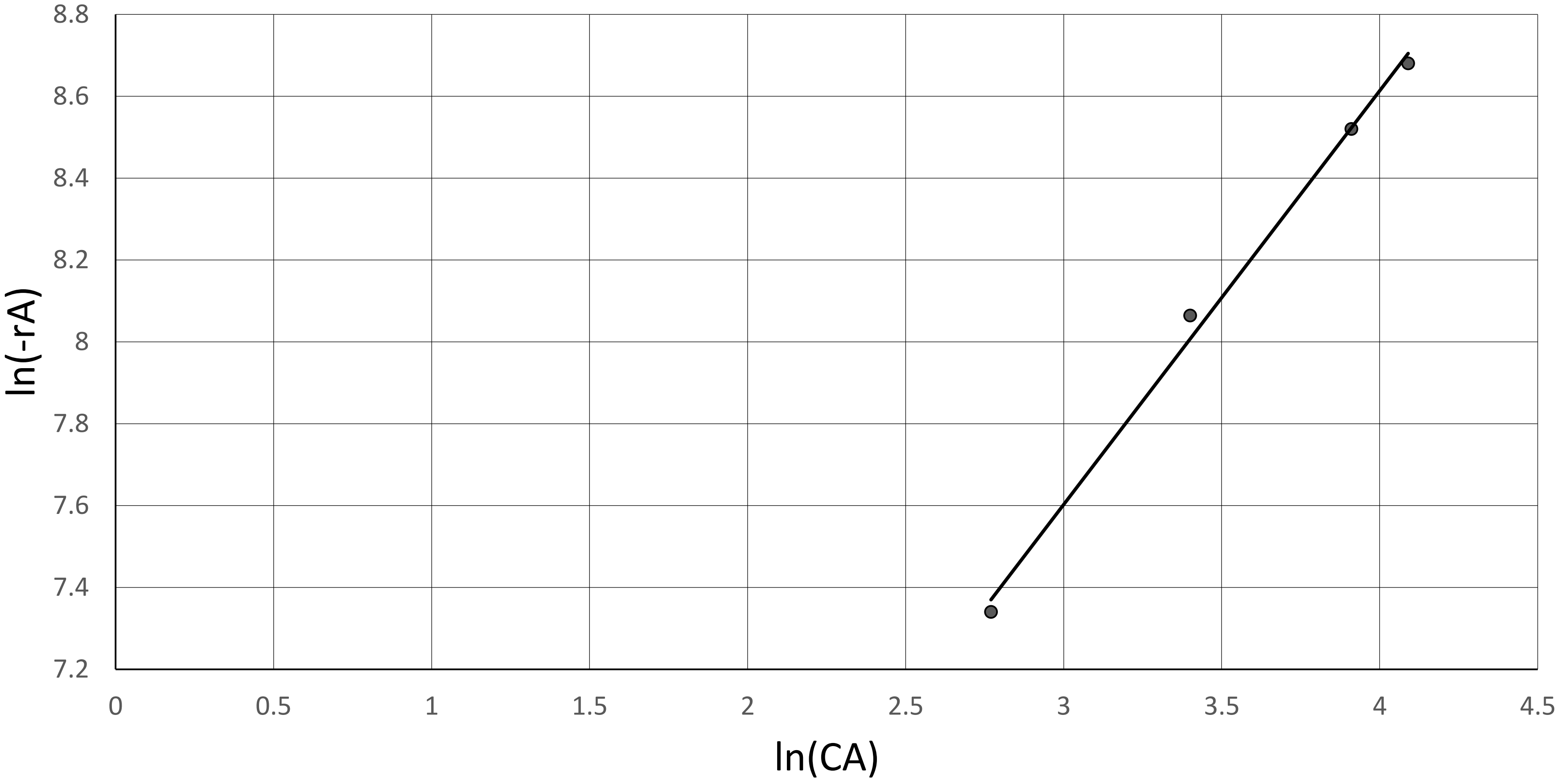
Data Analysis

F_{A0}, millimol/hr	300	1000	3000	5000
$C_{A,out}$, millimol/liter	16	30	50	60
X_A	0.512	0.318	0.166	0.1176
$-r_A$, millimol/liter-hr	1536	3180	5000	5880

$\ln(-r_A)$	7.34	8.064	8.52	8.68
$\ln(C_A)$	2.77	3.4	3.91	4.09

$$\ln(-r_A) = lnk + nln(C_A)$$

Plot of $\ln(C_A)$ vs. $\ln(-r_A)$



$n=1.017$

$\ln k = 4.57$

$K = 96.54\ hr^{-1}$

$-r_A = 96.54\ C_A$

12. From the following data find a satisfactory rate equation for the gas-phase decomposition $A \rightarrow R$ taking place isothermally in a mixed reactor

Run Number	1	2	3	4	5
τ sec	0.423	5.1	13.5	44	192
X_A	0.22	0.63	0.75	0.88	0.96

$C_{A0} = 0.002$ mol / lit

Solution:

gas-phase reaction $A \rightarrow R + S$

$$\epsilon = \frac{2-1}{1} = 1$$

$$C_A = C_{A0}(1 - X_A)/(1 + X_A) \qquad \tau = \frac{C_{A0} X_A}{-r_A}$$

or $$-r_A = \frac{C_{A0} X_A}{\tau}$$

let the rate equation is $-r_A = k C_A^n$

C_A	1.278×10^{-3}	4.54×10^{-4}	2.857×10^{-4}	1.276×10^{-4}	4.08×10^{-5}
$\ln(10000 C_A)$	2.547	1.513	1.049	0.2437	-0.896
$\ln(-r_A 10^5)$	4.644	3.206	2.406	1.386	0.0

from slope, $k = 1.36$

$$1.04 \times 10^{-3} = k\,(1.278 \times 10^{-3})^{1.36}$$

$$k = 8.9567 \qquad \therefore -r_A = 8.956\, C_A^{1.36}$$

$-r_A = 11.692\ C_A^{1.4}$ from computer program

$A \rightarrow R + S$ (gas phase) $C_{A0} = 0.002$ mol/lit.

τ Sec	0.423	5.10	13.5	44.0	192
X_A	0.22	0.63	0.75	0.88	0.96
$-r_A$	1.040×10^{-3}	2.47×10^{-4}	1.11×10^{-4}	4×10^{-5}	1×10^{-5}