ENVIRONMENTAL ENGINEERING -1

Lecture 13 – Principles of Process Engineering

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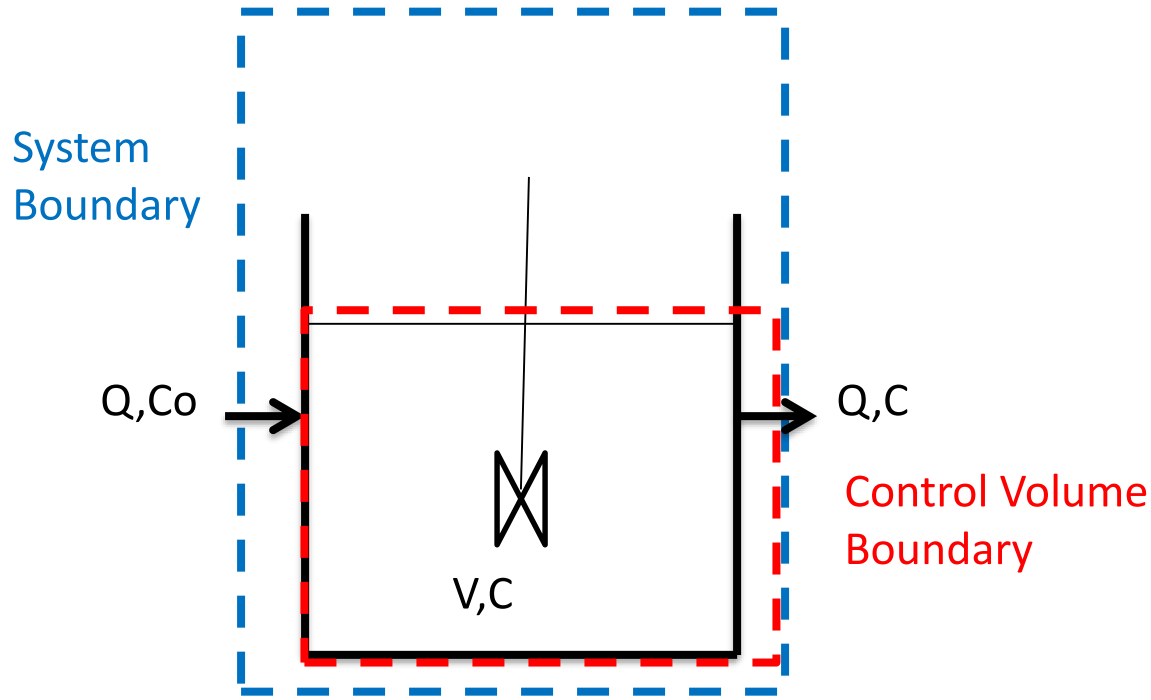
Materials(mass) Balance Approach

Principle:

"Mass can neither be created nor destroy but it can be changed (transformed) in other forms."

Balance(Accumulation)=Deposits(Input)−Withdrawal(Output)±Interest service charges(Transformed material)

Materials(mass) Balance Approach



Accumulation of Material in a system= Input of material – Output of material + Transformed material

Accumulation Rate= Input Rate – Output Rate + Transformation Rate

Conservative substances

“Substances which can not transformed or change with the passage of time are called conservative substances.”

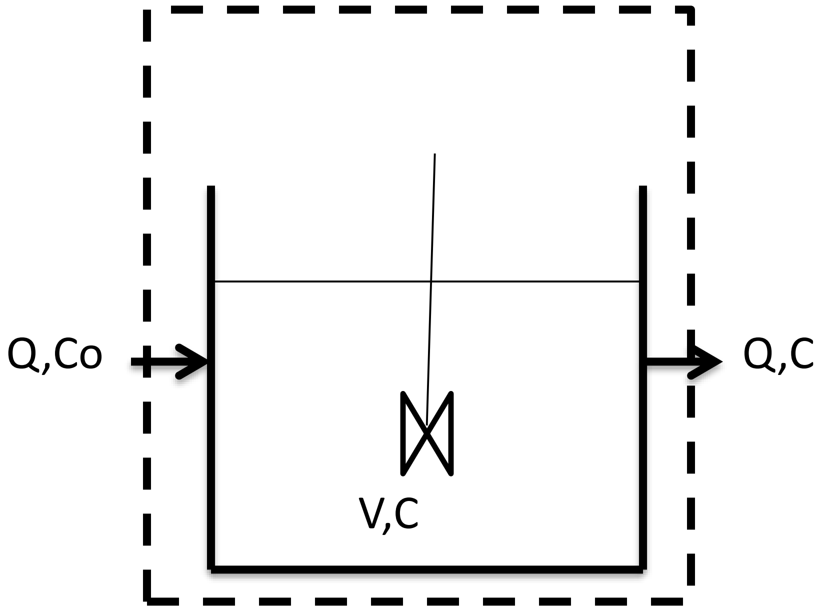
Non Conservative substances

"Substances which can transformed or change with the passage of time are called non-conservative substances."

Materials(mass) Balance Approach

Non Conservative substances

Substance which can be transformed in other forms reacting in a container (reactor), mass balance approach is employed as shown below;



Assumptions:

- Flow in and out of the container is constant,
- Liquid in container is not subjected to evaporation.
- Liquid is completely mixed
- Chemical reaction involving the reactant 'C' is occurring within container

Non Conservative substances

Considering above assumptions, a material balance will be as follow:

Accumulation Rate=Input Rate − Output Rate + Transformation Rate

Symbolic representation:

$$V\,dC/dt = QC_o - QC + Vr$$

V= Volume of reactor , m3

$\frac{dC}{dt}$ =Rate of change of reactant concentration within the reactor , mg/l/day

Q= Rate of flow in and out of the reactor , m3/day

Co = Concentration of the reactant in the inflow , mg/l

C= concentration of the reactant in the outflow , mg/l

r=rate of reaction , per day

Non Conservative substances

Steady State Simplication:

The state at which the concentration of the reactant in the reactor does not change with time.

$$\frac{dC}{dt} = 0$$

So above equation becomes;

$$0 = QC_o - QC + Vr$$

$$0 = Q(C_o - C) + Vr$$

$$-Q(C_o - C)/V = r$$

Reaction Kinetics & Rate Laws

Kinetic Reactions

“Time dependent reactions are called kinetic reactions”

Rate Laws

“The mathematical expression describing the rate at which a reaction proceeds is called the rate law.”

The rate laws are written in terms of concentration of reactants:

$$r = f(C)$$

R= Rate of reaction , per day
C= concentration of the reactant , mg/l

Order of Reaction

- ✓ For many reactions rate law can be written in the form of a simple expression where rate of reaction is proportional to the concentration of the reactant raised to some power .i.e;

$$r = KC^0$$
$$r = KC^1$$
$$r = KC^2$$

- ✓ If the concentration of the reactant is decreasing in the reactor with time, then rate of reaction;

$$r = -KC^0$$
$$r = -KC^1$$
$$r = -KC^2$$

Zero order reaction:

"It is chemical reaction in which the rate of reaction is independent of concentration of pollutant and proceeds at constant rate."

$$r = -KC^0$$

$$r = -K$$

$$r = \frac{dC}{dt}$$

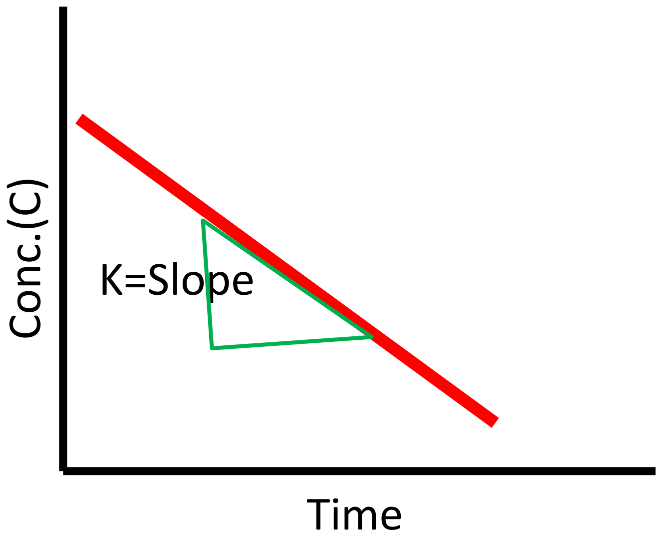
$$\frac{dC}{C} = -\text{Kdt}$$

Integrating:

$$\int_{C_0}^{C} dC = -K\int_{0}^{t} dt$$

$$C - C_o = -Kt$$

$$\boldsymbol{C = Co - Kt}$$



First order reaction:

- In environmental engineering processes, many biochemical reactions proceed as first order reaction
- They are also named as Monomolecular reaction(*it is chemical reaction in which the rate of reaction is proportional to the concentration of the reactant present).*

$$\mathrm{r} = \boldsymbol{KC}$$

First order reaction:

$$\mathbf{r = -KC}$$

$$\frac{dC}{dt} = -\text{KC}$$

$$\frac{dC}{C} = -\text{Kdt}$$

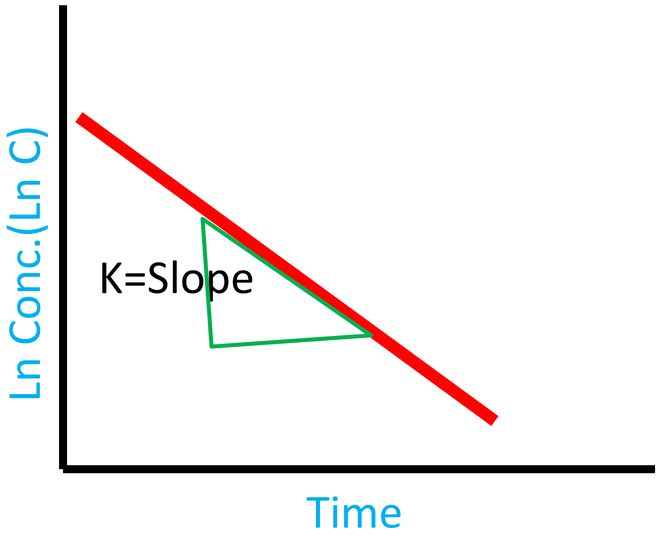
Integrating:

$$\int_{C_0}^{C} \frac{dC}{C} = -K \int_{0}^{t} dt$$

$$ln\frac{C}{C_o} = -Kt$$

$$\frac{C}{C_o} = e^{-Kt}$$

$$\mathbf{C = C_o e^{-Kt}}$$



Reactor Theory

Reactor

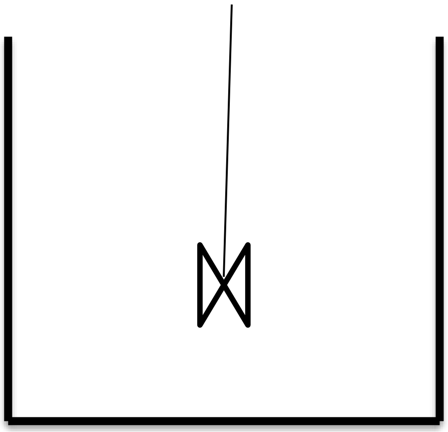
Reactor refers to a vessel(container) in which reaction takes place.

Three types of reactors:

- Completely mixed batch reactor(CMBR)
- Continuous flow stirred tank reactor(CSTR)
- Plug flow reactor(PFR)

Completely mixed batch reactor

- It is a closed system
- Flow neither entering nor leaving the reactor
- The reactants are initially introduced into the container, well mixed, and left for certain period after which they are discharged to empty the reactor and the process is repeated. Concentration of the reactant changes with time. So it is an Unsteady state of operation.
- Used for bench scale experimental studies



First order reaction:

Mathematical Equation(Mass Balance):

$$V\frac{dC}{dt} = QC_O - QC + Vr$$

Since no flow is occurring i.e. Q=0

Therefore;

$$\frac{dC}{dt} = r$$

Considering the first order reaction i.e; r = KC

$$\frac{dC}{dt} = -KC$$

$$\frac{dC}{C} = -Kdt$$

Integrating:

$$\int_{C_0}^{C} \frac{dC}{C} = -K\int_{0}^{t} dt$$

$$ln\frac{C}{C_o} = -Kt$$

$$\frac{C}{C_o} = e^{-Kt}$$

$$C = C_o e^{-Kt}$$

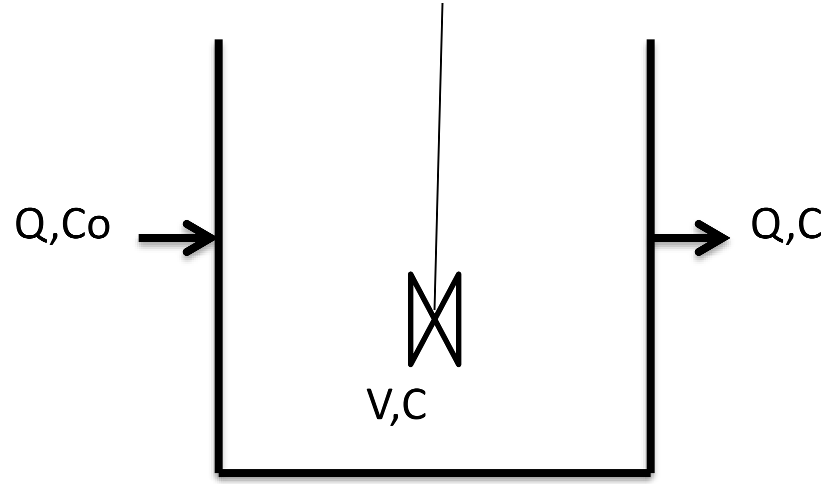
C= Initial concentration of the reactant , mg/l

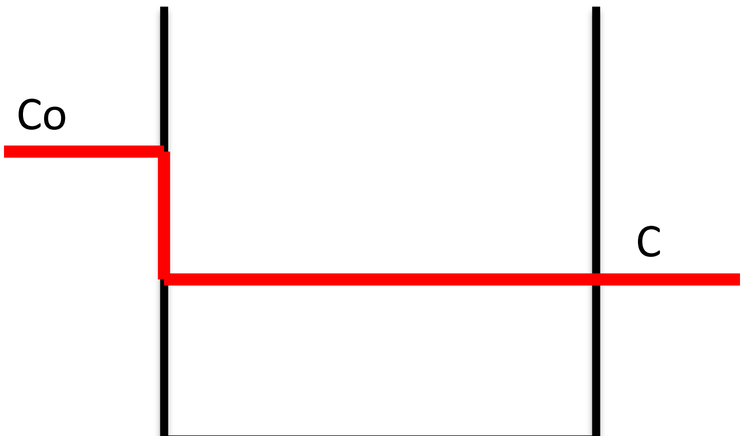
Co= Concentration of reactant at time t

K= Reaction rate constant , per day

Continuous Flow Stirred Tank Reactor (CSTR)

- The inflow and outflow are continuous.
- The contents in the reactor are well mixed, so the concentration of the reactant in the reactor is the same as in the outflow.
- If the influent concentration (Co) remains constant , a steady state will be achieved.





- Mathemtical Equation:

$$V\frac{dC}{dt} = QC_O - QC + Vr$$

Under steady state condition, $\frac{dC}{dt}=0$ and $\frac{V}{Q}=t_{CSTR}$

t_{CSTR} = Detention time in the reactor

Therefore; $0 = \frac{Q}{V}(Co - C) + r$

Or

$$\frac{C_O - C}{t_{CSTR}} = -r$$

First order reaction:

- Considering first order reaction

$$r = -KC$$

$$\frac{C - C_o}{t_{CSTR}} = -KC$$

$$\frac{C - C_o}{C} = -Kt_{CSTR}$$

$$1 - \frac{C_o}{C} = -Kt_{CSTR}$$

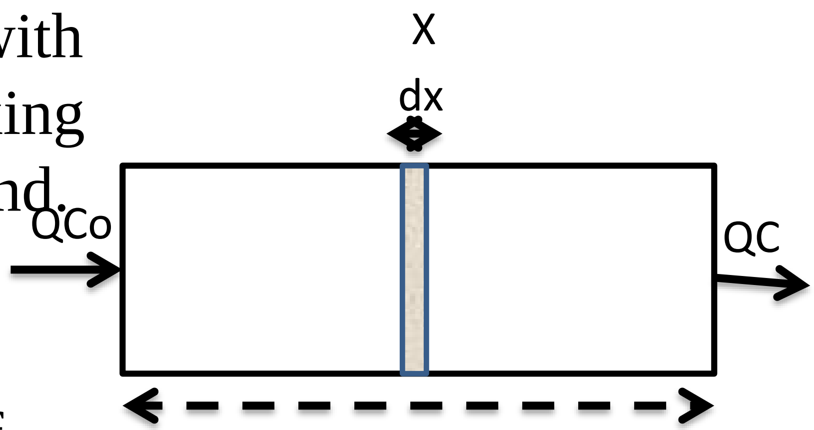
$$\frac{C_o}{C} = 1 + Kt_{CSTR}$$

$$\mathbf{C = \frac{C_o}{1 + Kt_{CSTR}}}$$

Plug Flow Reactor:

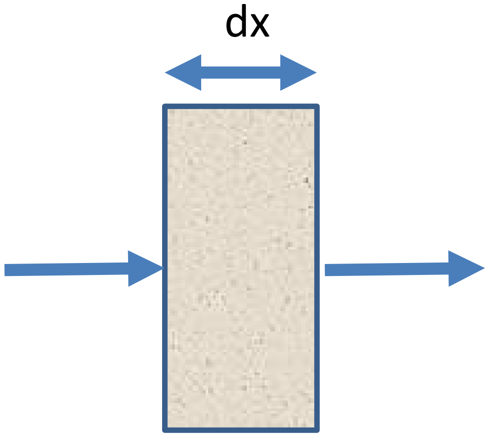
Assumptions:

1. The flow through reactor is orderly, with no element of fluid overtaking or mixing with any other element ahead or behind.
2. The concentration of the reactant C across the X-section of the reactor is same but varies along the direction of flow.
3. All fluid elements remain in the tank for the same time.
4. Steady state can be achieved, if influent concentration remains constant.



Mathematical Equation:

- Consider a strip of fluid , with d_x width moving at a velocity V_x across, the X-section. This strip can be considered as a **Batch Reactor** as no diffusion or mixing is taking place.
- In the start at time=0 ,or x=0, the concentration of the reactant in the strip=C . If t is the time taken by the strip (Batch reactor) to accomplish the reaction , then



$$\frac{dC}{dt} = \mathbf{r}$$

- considering first order reaction

$$r = -\mathrm{KC}$$

$$\frac{dC}{dt} = -\mathrm{KC}$$

$$\int_{C_o}^{C} \frac{dC}{C} = -\mathrm{K} \int_{0}^{t} dt$$

$$\ln \frac{C}{C_o} = -K t_{PFR}$$

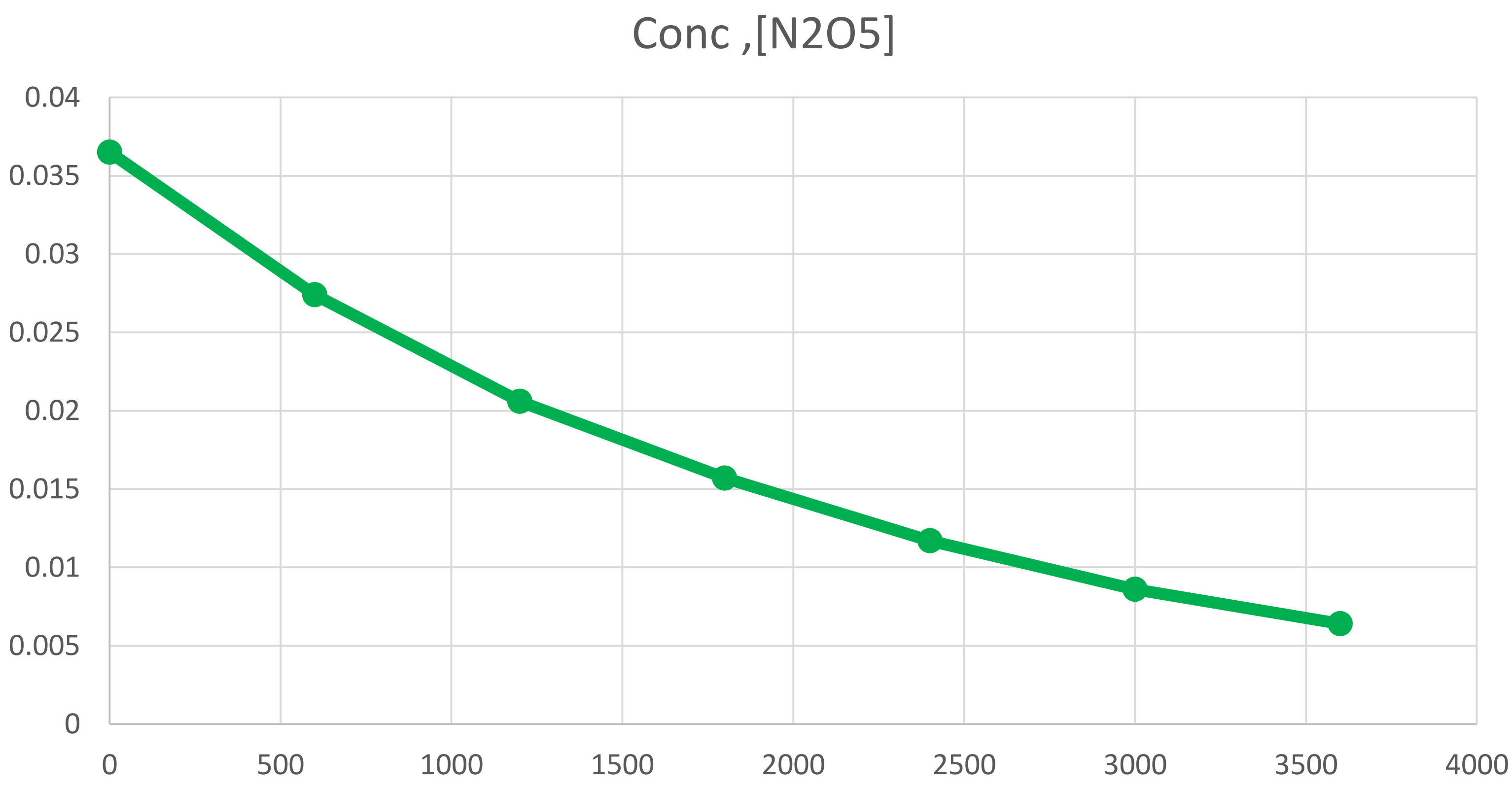
$$\mathbf{C} = C_o \, e^{-K t_{PFR}}$$

Numericals

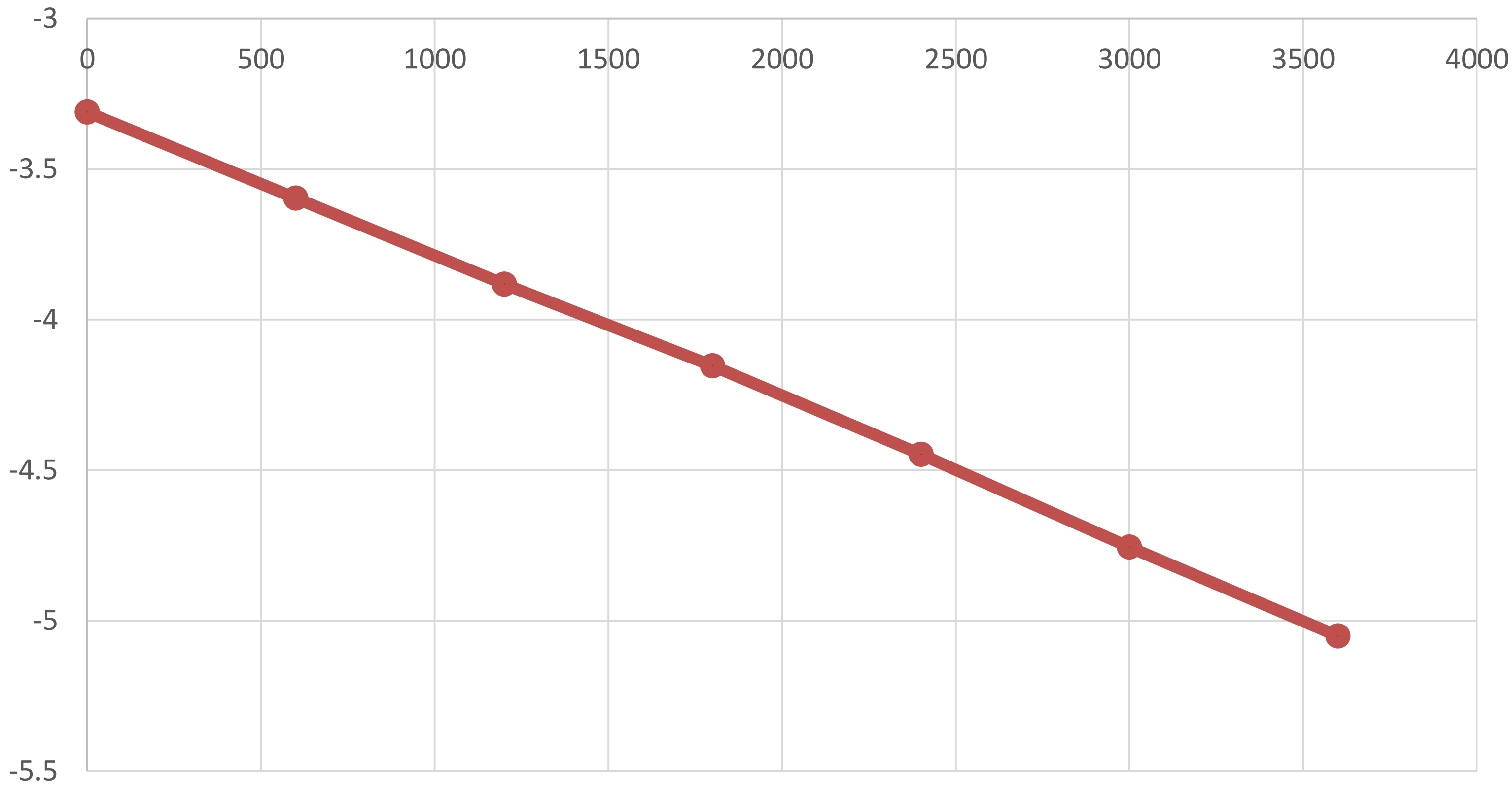
1. A chemical batch reactor achieves a reduction of component A from 100 mg/L to 5 mg/L in one hour. If the reaction is known to follow zero order kinetics, determine the rate constant . Repeat the same thing for first order kinetics.
2. Nitrogen pentoxide (N2O5) decomposes to NO2 and O2 at relatively low temperature . Plot a graph of the concentration versus t, ln concentration versus t, and then determine the rate law(order of reaction) and calculate the rate constant

Time (sec)	Conc ,$[N_2O_5]$,(mg/L)
0	0.0365
600	0.0274
1200	0.0206
1800	0.0157
2400	0.0117
3000	0.00860
3600	0.00640

Numerical 2 :Zero Oder



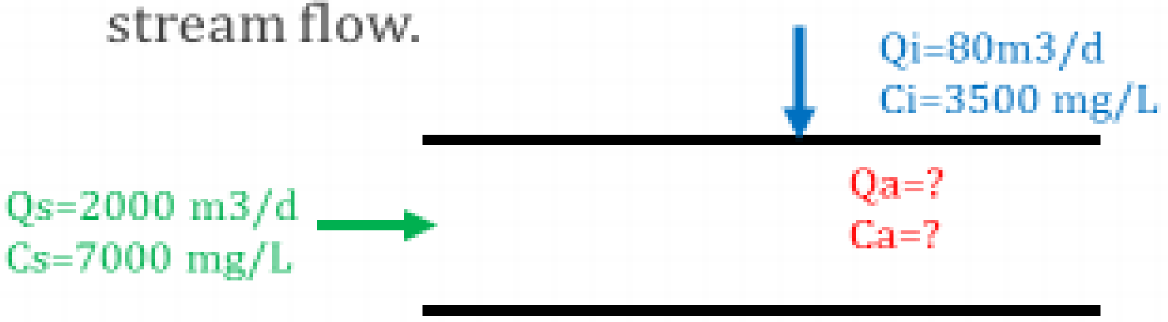
Numerical 2 :First order



3. Considering the first order kinetics with K value of 0.23 per day and the detention time of 5 days , find out the efficiencies achieved in plug flow and completely stirred tank reactor.

Numerical 4

- A stream carries a flow of 2000 m3/day with TDS concentration of 700 mg/l. At a point 80 m3/d of industrial wastewater with a TDS concentration of 3500mg/l is being added to the stream. Find out the resulting TDS concentration in the stream soon after the industrial waste is completely mixed with the stream flow.



5. A CSTR with a volume of 800 m3 is treating 4000 m3/day of water having a pollutant concentration of 10 mg/L. If the first order rate coefficient for the pollutant is 0.8 per hour, calculate the removal efficiency of the pollutant in the reactor. Also determine the concentration in the outflow of the reactor.
6. A PFR with a volume of 800 m3 is treating 4000 m3/day of water having a pollutant concentration of 10 mg/L. If the first order rate coefficient for the pollutant is 0.8 per hour, calculate the removal efficiency of the pollutant in the reactor. Also determine the concentration in the outflow of the reactor