ENVE 301
Environmental Engineering Unit Operations

CHAPTER: 3
Types of reactors

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REACTOR MODELS

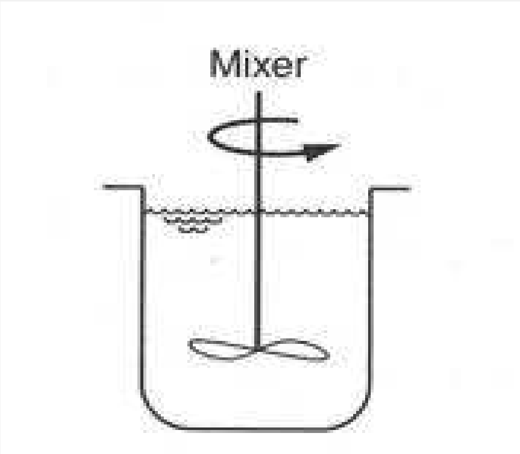
REACTOR:

Containers vessels or tanks in which chemical or biological reactions are carried out.

5 principal reactor models:

1. Batch reactor
2. Complete-mix reactor(continuous–flow stirred tank reactor),(CFSTR)
3. Plug-flow reactor (PFR) (tubular-flow reactor)
4. Cascade of complete mix reactor (complete mix reactors in series)
5. Packed- bed reactor

BATCH REACTORS



Ref: http://www.water-msc.org/e-learning/file.php/40/moddata/scorm/203/Lesson%204_04.htm

The simplest reactor type

Flow is neither entering nor leaving the reactor

The liquid contents are mixed completely and uniformly

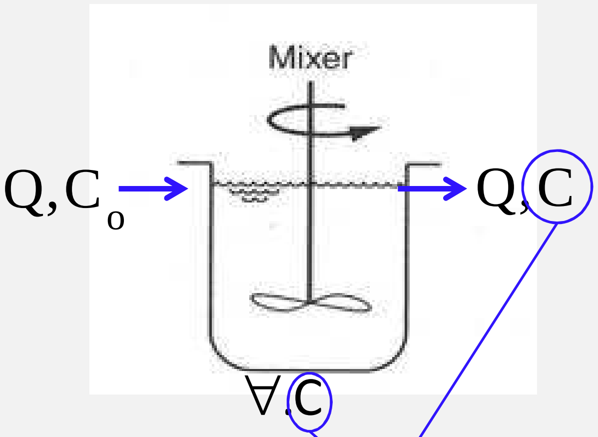
Applications:

Used to model very shallow lake where there is at most no flow

Used to estimate reaction coefficients

BOD test

COMPLETE-MIX REACTORS
(CFSTR = Continuous-Flow Stirred Tank Reactor)



- Fluid particles that enter the reactor are instantaneously dispersed throughout the reactor volume

- Fluid particles leave the reactor in proportion to their statistical population

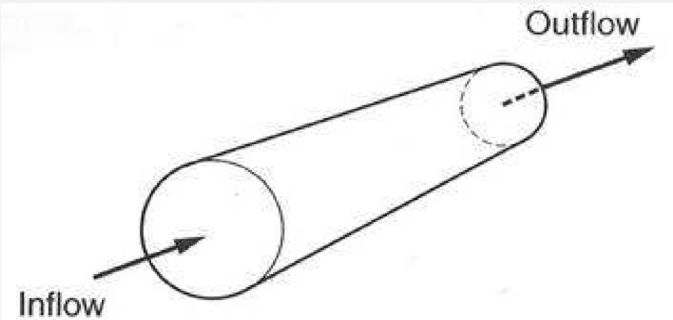
conc of any material leaving = conc. at any point in the reactor (after steady-state conditions are reached)

$$\frac{dc}{dt}\forall = QC_o - QC \pm rV$$

No conc. gradient within the system.

Material entering is uniformly dispersed throughout the reactor

PLUG FLOW REACTOR-(PFR)



Ref: http://www.water-msc.org/e-learning/file.php/40/moddata/scorm/203/Lesson%204_04.htm

→ Fluid particles pass through the reactor and are discharged in the same sequence in which they entered the reactor.

→ Each fluid particle remains in the reactor for a time period equal to the theoretical detention time.

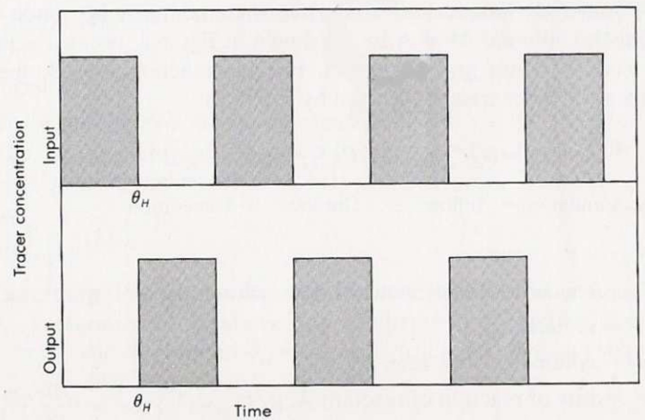


FIGURE 6.7
Tracer input and output response curves for an ideal PFR.

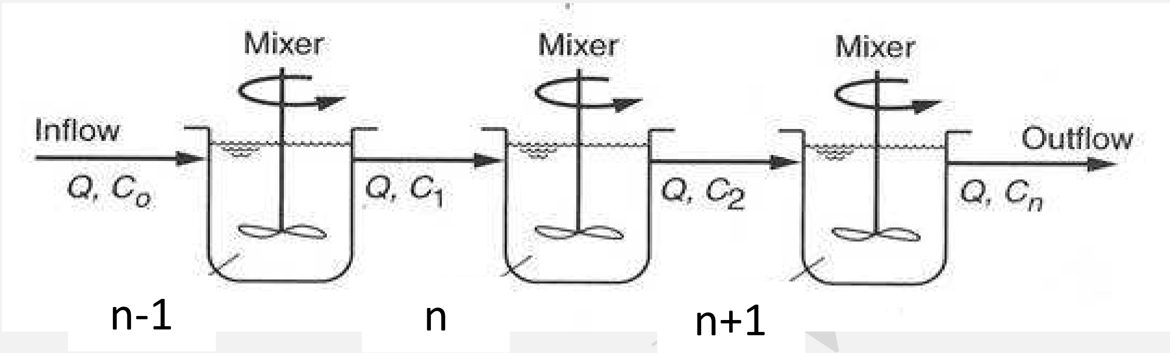
Ref: Tchobanoglous and Scroeder, 1985, Addison-Wesley Publishing Company

→ This type of flow is approximated in long tanks with a high length/width ratio in which longitudinal dispersion is minimal or absent.

Application:

→ Used to study river systems

CASCADE of COMPLETE MIX REACTORS
(Complete Mix Reactor in Series)



is used to model the flow regime that exists between the hydraulic flow patterns corresponding to the complete and plug flow reactors.

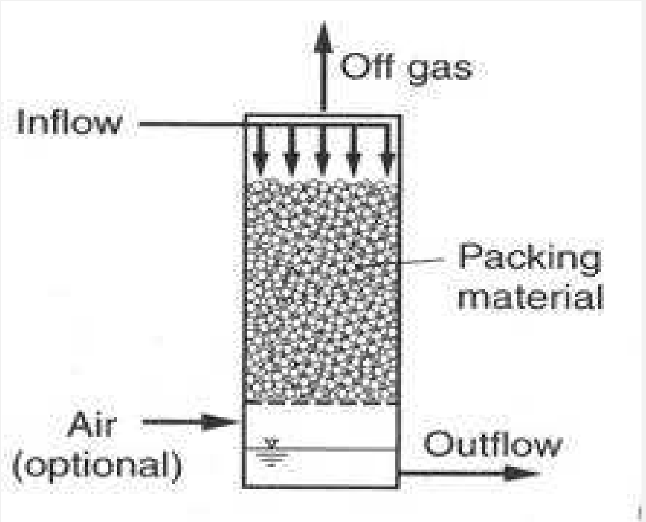
If the series is composed of one reactor → complete mix regime prevails

If the series consists of an infinite number of reactors in series → plug-low regime prevails

Application:

→ In modeling rivers within small increments (segments)

PACKED BED REACTORS



Ref: http://www.water-msc.org/e-learning/file.php/40/moddata/scorm/203/Lesson%204_04.htm

→ These reactors are filled with some type of packing medium (e.g.rock, slag, ceramic or plastic)

→ With respect to flow,
completely filled (anaerobic filter)
intermittently dosed (trickling filter)

When the pore volume of the medium is filled with a liquid → flow is said to be SATURATED

When the pore volume is partially filled → flow is said to be UNSATURATED

PACKED BED REACTORS (continue)

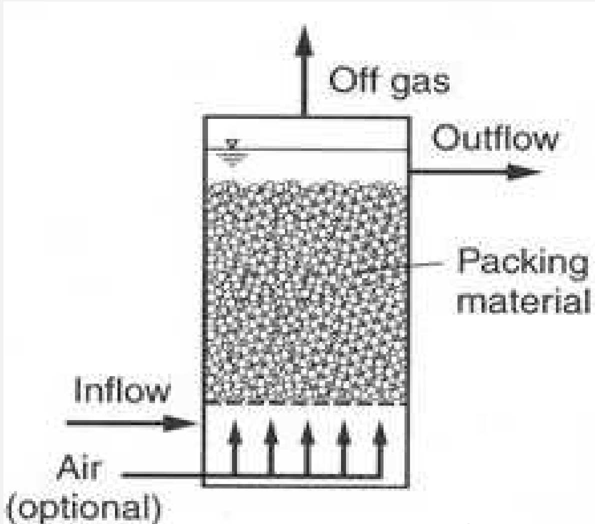
Application:

→ Used to study the movement of water and contaminants in groundwater systems.

FLUIDIZED-BED reactors

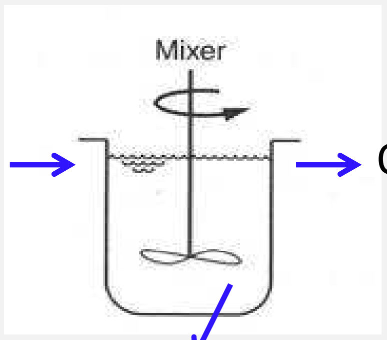
→ Packed bed reactors in which the packing medium is expanded by the upward movement of fluid (air or water) through the bed.

Example: Filter backwashing



Ref: http://www.water-msc.org/e-learning/file.php/40/moddata/scorm/203/Lesson%204_04.htm

CONTINOUS FLOW STIRRED TANK (CFSTR) REACTOR MODELS

Q, C_o →  → Q, C

$C, \forall$

Material input may be
- conservative (non-reactive)
- non-conservative (reactive)

NOTE

For conservative (non-reactive) material input having C_o conc., eff. conc. is initially C (not C_o) due to unsteady state condition.

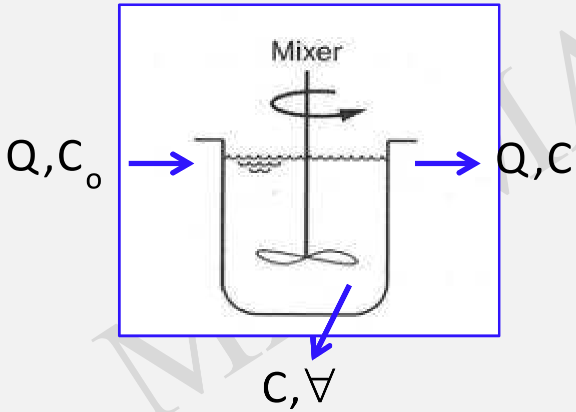
When steady-state is reached effluent conc. (C) = C_o

Response of CFSTR to Conservative (non-reactive) Tracer Input

A conservative (non-reactive) material is injected into the input flow of CFSTR on a continuous basis, beginning at t=0 and resulting in a constant input tracer conc. Determine the reactor output conc. as a function of time and plot the tracer-output response curve.

→ Un-steady-state condition → $C \neq Co$ (although the material is non-reactive)
→ After steady -state condition is reached → $C = Co$

Accumulation = Inflow – Outflow + Generation



$$\frac{dc}{dt}\forall = QC_o - QC + \cancel{r\forall}$$

→ since the tracer is non-reactive

$$\forall \frac{dc}{dt} = Q(C_o - C)$$

$$\longrightarrow \int_{C=0}^{C} \frac{dC}{C_o - C} = \frac{Q}{\forall} \int_{t=0}^{t} dt \longrightarrow \left\{ \int \frac{1}{ax+b} dx = \frac{1}{a} \ln|ax+b| \right\}$$

$$\longrightarrow \frac{1}{-1} \mathrm{Ln}|C_0 - C| \Big|_{C=0}^{C} = \frac{Q}{\forall} t$$

$$\longrightarrow -\mathrm{Ln}|C_0 - C| - \left(-\mathrm{Ln}|C_0 - 0|\right) = \frac{Q}{\forall} t$$

$$\longrightarrow -\mathrm{Ln}(C_0 - C) + \mathrm{Ln}C_0 = \frac{Q}{\forall} t$$

$$\longrightarrow \mathrm{Ln}(C_0 - C) - \mathrm{Ln}C_0 = -\frac{Q}{\forall} t$$

$$\longrightarrow \mathrm{Ln}\frac{C_0 - C}{C_0} = -\frac{Q}{\forall}.t$$

$$\longrightarrow C_0 - C = C_0 e^{-(Q/\forall)t}$$ (Divide both sides to Co)

$$\longrightarrow 1 - \frac{C}{C_0} = e^{-(Q/\forall)t} \longrightarrow \boxed{\frac{C}{C_0} = 1 - e^{-(Q/\forall)t}}$$

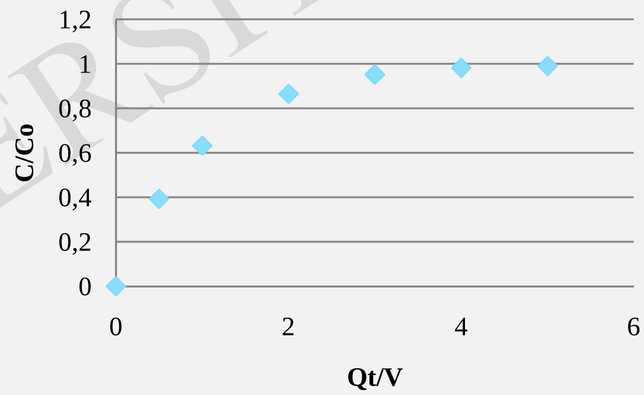
$$\rightarrow \quad \frac{Q}{\forall} = \frac{m^3/\sec}{m^3} = \frac{1}{\sec} = \frac{1}{t_R} \rightarrow$$

Hydraulic retention time (HRT)

$$\frac{C}{C_0} = 1 - e^{-(Q/\forall).t}$$

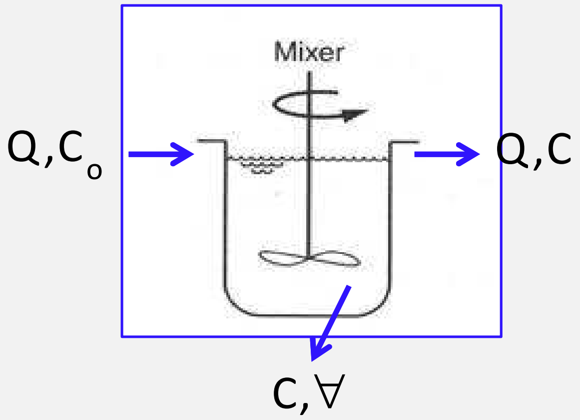
$\left(\frac{Q}{\forall}\right)t$	$\frac{C}{C_0}$
0	0
0,5	$1-e^{-0,5}$ =0,393
1	$1-e^{-1}$ =0,632
2	$1-e^{-2}$ =0,865
3	$1-e^{-3}$ **=0,952**
4	$1-e^{-4}$ **=0,982**
5	$1-e^{-5}$ **=0,99**

→ t=0, C=0



→ After this time, C/Co does not change

Response of CFSTR to Non-Conservative (Reactant) Tracer Input



A reaction A $\longrightarrow$ B , known to be first order, is to be carried out in a CFSTR. Water is run through the reactor at a flow rate Q (m^3/sec) and t=0 the reactant A is added to the input stream on a continuous basis.

Determine the output concentration of A as a function of time and plot reactor-output response curves for reactant A.

Materials balance for the system:

$$\longrightarrow \frac{dc}{dt}\forall = QC_0 - QC + \text{generation}$$

First-order rxn→ r=-kC

∴ generation term =r ∀= -kC ∀

$$\longrightarrow \frac{dc}{dt}\forall = QC_0 - QC - k.C.\forall$$

(Divide both sides to ∀)

$$\rightarrow \frac{dc}{dt} = \frac{Q}{\forall}.(C_0 - C) - k.C \qquad \left(\frac{Q}{\forall} = \frac{1}{t_R}\right)$$

$$\rightarrow \frac{dc}{dt} = \frac{1}{t_R}.(C_0 - C) - k.C$$

$$\rightarrow \frac{dc}{dt} = \frac{C_0 - C - k.C.t_R}{t_R}$$

$$\rightarrow \frac{dc}{dt} = \frac{C_0 - C(1 + k.t_R)}{t_R}$$

$$\rightarrow \frac{dc}{dt} = \frac{C_0}{t_R} - \frac{C(1 + k.t_R)}{t_R}$$

$$\rightarrow \frac{dc}{dt} = \frac{C_0}{t_R} - C.\left(\frac{1}{t_R} + k\right)$$

$$\rightarrow \frac{dc}{dt} + c\left(\frac{1}{t_R} + k\right) = \frac{C_0}{t_R}$$

$$\frac{dy}{dx} + P(x)y = Q(x)$$

Integration factor= $e^{\int P(x).dx}$

Multiply both sides w/integration factor

Left hand side = $\dfrac{d[ye^{\int P(x(/dx}]}{Q(x)}$

$$\left[\frac{1}{t_R} + k = \beta \longrightarrow e^{\int \beta . dt} = e^{\beta . t} \right] \qquad \frac{dc}{dt} + c\left(\frac{1}{t_R} + k\right) = \frac{C_0}{t_R}$$

Multiply both sides with integration factor.

$$\longrightarrow e^{\beta . t} . \frac{dc}{dt} + e^{\beta t} . C . \beta = \frac{1}{t_R} . C_o . e^{\beta . t}$$

$$\longrightarrow \frac{d\left(C . e^{\beta t}\right)}{dt} = \frac{1}{t_R} . C_o . e^{\beta . t}$$

$$\longrightarrow \int_{C_0}^{C_t} d\left(C . e^{\beta t}\right) = \int_{t=0}^{t} \frac{1}{t_R} . C_0 . e^{\beta t} . dt$$

$$\longrightarrow C . e^{\beta . t} \Big|_{C_0}^{C_t} = \frac{1}{t_R} . C_0 . \frac{1}{\beta} . e^{\beta t} \Big|_{t=0}^{t} \left(\int e^{ax} dx = \frac{1}{a} e^{ax} \right)$$

$t=0 \quad e^{\beta t}=1$

$$\rightarrow \quad C_t e^{\beta t} - C_0 e^{\beta t} = \frac{1}{t_R} C_0 \frac{1}{\beta} e^{\beta t} - \frac{1}{t_R} C_0 \frac{1}{\beta}$$

$$\rightarrow \quad C_t e^{\beta t} - C_0 = \frac{1}{t_R} C_0 \frac{1}{\beta} e^{\beta t} - \frac{1}{t_R} C_0 \frac{1}{\beta}$$

$$\rightarrow \quad C_t e^{\beta t} = C_0 + \frac{1}{t_R} C_0 \frac{1}{\beta} e^{\beta t} - \frac{1}{t_R} C_0 \frac{1}{\beta}$$

(Divide both sides to $e^{\beta t}$)

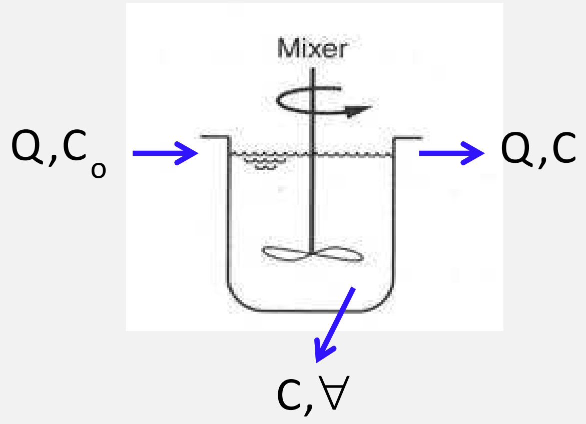
$$\rightarrow \quad C_t = \frac{C_0}{e^{\beta t}} + \frac{1}{t_R} C_0 \frac{1}{\beta} - \frac{1}{t_R} C_0 \frac{1}{\beta} \frac{1}{e^{\beta t}}$$

$$\rightarrow \quad C_t = \frac{C_0}{e^{\beta t}} + \frac{C_0}{t_R \beta}\left(1 - \frac{1}{e^{\beta t}}\right)$$

$$\rightarrow \quad \boxed{C_t = C_0 e^{-\beta t} + \frac{C_0}{t_R \beta}\left(1 - e^{-\beta t}\right)}$$

where $\beta = \frac{1}{t_R} + k$

CFSTR, UNSTEADY-STATE FOR NON-CONSERVATIVE REACTANT HAVING 1ST ORDER REACTION RATE



As t approaches infinity (∞) $\longrightarrow$ steady-state solution is approached $e^{-\beta.t} = 0$

$$C_t = C_0.e^{-\beta.t} + \frac{C_0}{t_R.\beta}.(1 - e^{-\beta.t})$$

$$C_t \cong \frac{C_0}{t_R.\beta} = \frac{C_0}{t_R\left(\frac{1}{t_R} + k\right)} \longrightarrow \boxed{C_t = \frac{C_0}{1 + k.t_R}}$$

CFSTR, steady-state, non-conservative (reactive) reactant having 1st order reaction rate.

For steady-state condition (1st order reaction):

$$\frac{dc}{dt}\forall = QC_0 - QC - kC\forall$$

$$\frac{dc}{dt} = \frac{Q}{\forall}C_0 - \frac{Q}{\forall}C - kC$$

At steady-state

$$\longrightarrow \frac{dc}{dt} = 0$$

$$kC = \frac{1}{t_R}(C_0 - C)$$

$$kCt_R = (C_0 - C)$$

$$kCt_R + C = C_0$$

$$\boxed{C = \frac{C_0}{1 + k.t_R}}$$

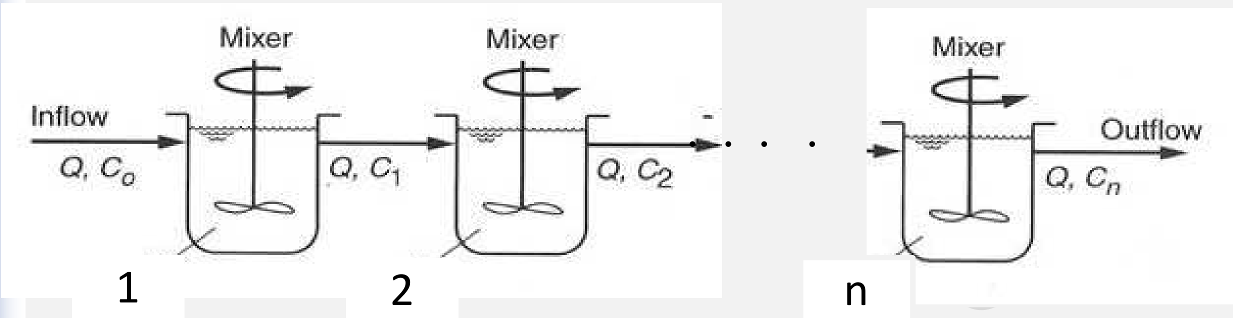
CASCADE OF COMPLETE MIX REACTORS (CFSTR in series)

At steady-state: 1st reactor

$$\frac{dc}{dt}\forall_1 = QC_0 - QC_1 + r\forall_1$$

$$\frac{dc}{dt} = \frac{Q}{\forall_1}C_0 - \frac{Q}{\forall_1}C_1 + r$$

$$0 = \frac{1}{t_{R1}}C_0 - \frac{1}{t_{R1}}C_1 + r$$



For 1st order reaction:

$$0 = \frac{1}{t_{R1}}C_0 - \frac{1}{t_{R1}}C_1 - kC_1 \longrightarrow 0 = \frac{1}{t_{R1}}C_0 - C_1\left(\frac{1}{t_{R1}} + k\right)$$

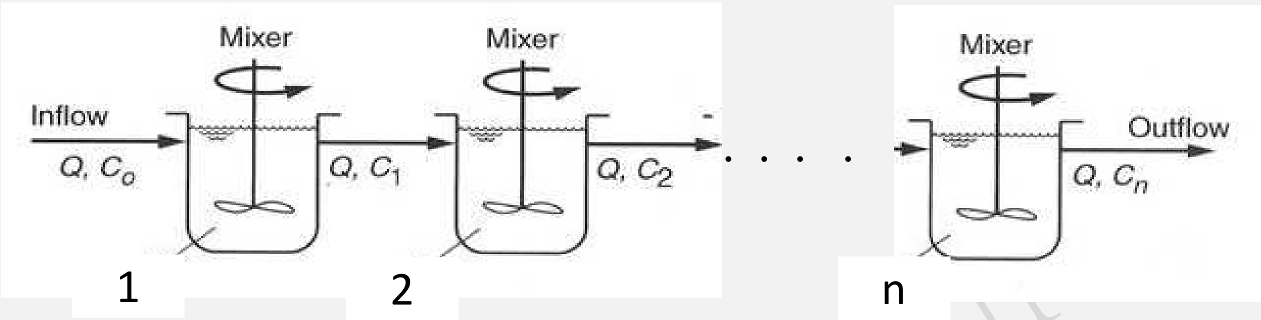
$$\longrightarrow 0 = \frac{1}{t_{R1}}C_0 - C_1\frac{1+kt_{R1}}{t_{R1}} \longrightarrow \boxed{C_1 = \frac{C_0}{1+kt_{R1}}}$$

2nd reactor

$$\rightarrow \frac{dc}{dt}\forall_2 = QC_1 - QC_2 + r\forall_2$$

$$\rightarrow \frac{dc}{dt} = \frac{Q}{\forall_2}C_1 - \frac{Q}{\forall_2}C_2 + r$$

$$\rightarrow 0 = \frac{1}{t_{R2}}C_1 - \frac{1}{t_{R2}}C_2 + r$$



For 1st order reaction:

$$\rightarrow 0 = \frac{1}{t_{R2}}C_1 - \frac{1}{t_{R2}}C_2 - kC_2 \rightarrow 0 = \frac{1}{t_{R2}}C_1 - C_2\left(\frac{1}{t_{R2}} + k\right)$$

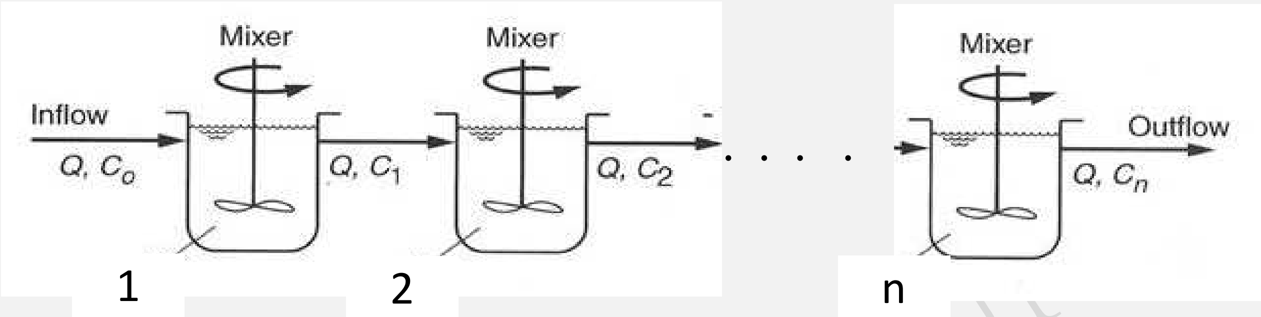
$$\rightarrow 0 = \frac{1}{t_{R2}}C_1 - C_2\frac{1+kt_{R2}}{t_{R2}} \rightarrow \boxed{C_2 = \frac{C_1}{1+kt_{R2}}}$$

$$C_1 = \frac{C_0}{1+kt_{R_1}} \rightarrow \boxed{C_2 = \frac{C_0}{(1+kt_{R1}).(1+kt_{R2})}}$$

3rd reactor $\rightarrow$ $\frac{dc}{dt}\forall_3 = QC_2 - QC_3 + r\forall_3$

$\rightarrow$ $\frac{dc}{dt} = \frac{Q}{\forall_3}C_2 - \frac{Q}{\forall_3}C_3 + r$

$\rightarrow$ $0 = \frac{1}{t_{R3}}C_2 - \frac{1}{t_{R3}}C_3 + r$



For 1st order reaction: $\rightarrow$ $0 = \frac{1}{t_{R3}}C_2 - \frac{1}{t_{R3}}C_3 - kC_3$

$\rightarrow$ $0 = \frac{1}{t_{R3}}C_2 - C_3\left(\frac{1}{t_{R3}} + k\right)$

$$C_2 = \frac{C_0}{(1+kt_{R1})(1+kt_{R2})}$$

$\rightarrow$ $0 = \frac{1}{t_{R3}}C_2 - C_3\frac{1+kt_{R3}}{t_{R3}}$ $\rightarrow$ $\boxed{C_3 = \frac{C_2}{1+kt_{R3}}}$

$$\boxed{C_3 = \frac{C_0}{(1+kt_{R1})(1+kt_{R2})(1+kt_{R3})}}$$

$$C_1 = \frac{C_0}{1+kt_{R1}}$$

$$C_2 = \frac{C_0}{(1+kt_{R1}).(1+kt_{R2})}$$

$$C_3 = \frac{C_0}{(1+kt_{R1})(1+kt_{R2})(1+kt_{R3})}$$

n^{th} reactor $\rightarrow$ $$\boxed{C_n = \frac{C_0}{(1+kt_{R1})(1+kt_{R2})\ldots(1+kt_{Rn})}}$$

CFSTR in series under steady – states and for 1st order rxn.

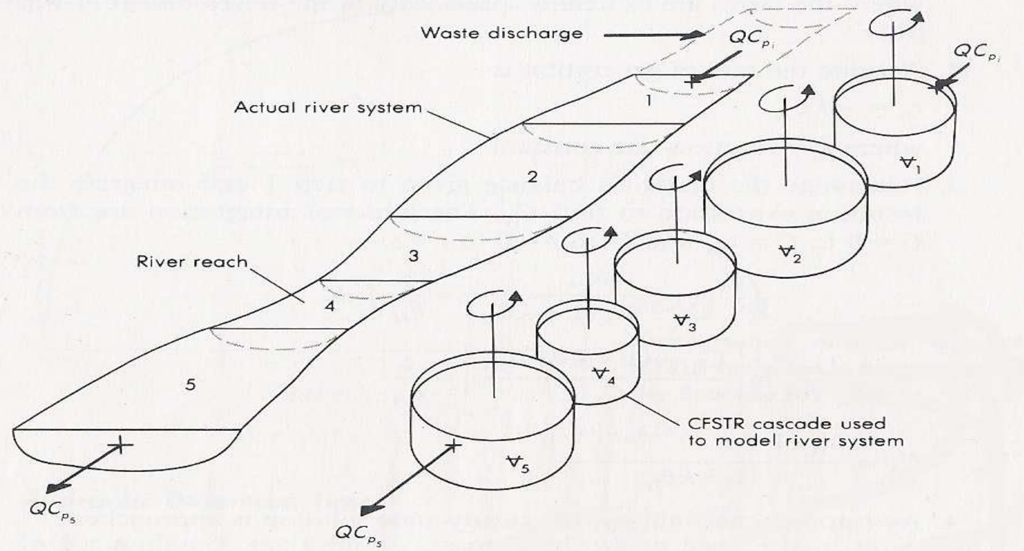


FIGURE 6.5

River reach segmented for analysis as a cascade series of connected reactors for Example 6.3.

V1=8.68 x 10 ^5 m3

V2=25.9x 10 ^5 m3

V3=17.28 x 10 ^5 m3

v4=8.64 x 10 ^5 m3

V5=25.92x 10 ^5 m3

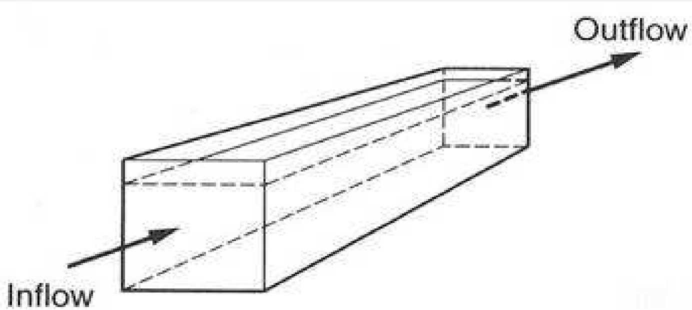
EXAMPLE 1:

Ref: Tchobanoglous and Scroeder, 1985, Addison-Wesley Publishing Company

The river reach shown has been divided into 5 segments based on measured velocities and depths. An industrial facility is planned just upstream of the 1st segment and it is necessary to estimate effect of ww discharge. A series of dye experiments have been run and each of the segments was found to behave as an approximate CFSTR. The pollutant is expected to disappear according to 1st order reaction. For the data given determine the steady-state pollutant con. in each segment.

$$Q_{river} = 5m^3/sec$$
$$k = 0{,}2day^{-1}$$
$$C_0 = 30g/m^3$$

PLUG FLOW REACTORS (PFR)



Ref: http://www.water-msc.org/e-learning/file.php/40/moddata/scorm/203/Lesson%204_04.htm

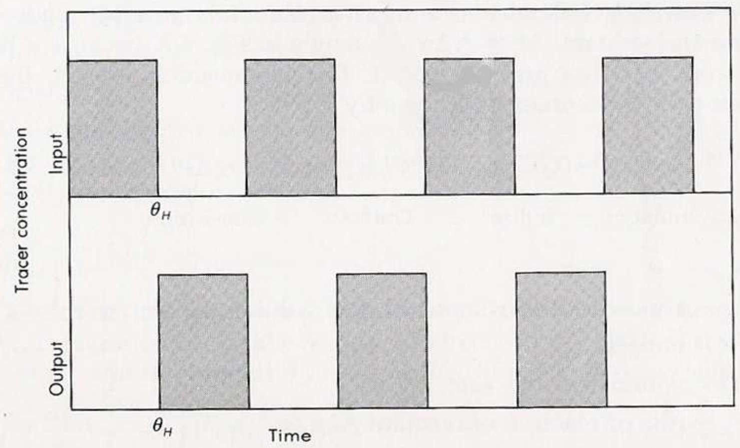


FIGURE 6.7
Tracer input and output response curves for an ideal PFR.
Ref: Tchobanoglous and Scroeder, 1985, Addison-Wesley Publishing Company

- → Are ideally mixed in lateral direction and unmixed longitudinally
- → Unrealistic assumption for most real-world systems but can be approximated closely
- → The mean HRT time = true HRT time

An effluent tracer (conservative) signal is exactly the same as the input , expect that is transposed in time by t_R.

→ Tracers (dyes, electrolytes, radioactive isotopes) are used to characterize the degree of mixing.

→ must be conservative

does not participate in any reaction
it is not adsorbed or absorbed by reactor or its contents

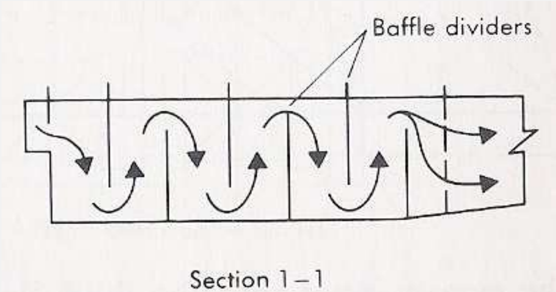
→ are assumed to be moved about in the same manner as the water molecules

their flow pattern will mimic have liquid flow pattern.

→ PF conditions are achieved by

designing long and narrow reactors,

placing baffles in a reactor



Ref: Tchobanoglous and Scroeder, 1985, Addison-Wesley Publishing Company

→ In a PF situation the mass balance must be taken over an incremental volume because a longitudinal concentration gradient exists (since there is no longitudinal mixing.

Materials Balance:

Accumulation = Inflow - Outflow + Generation

→ $\frac{\partial c}{\partial t}\Delta\forall = (QC_0)_x - (QC)_{x+\Delta x} + r\Delta\forall$ (Divide both sides to $\Delta\forall$)

→ $\frac{\partial c}{\partial t} = \frac{Q}{\Delta\forall}(C_x - C_{x+\Delta x}) + r$

→ $\frac{\partial c}{\partial t} = \frac{Q}{A\Delta x}(C_x - C_{x+\Delta x}) + r$

→ $\frac{\partial c}{\partial t} = \frac{Q}{A}\left(\frac{C_x - C_{x+\Delta x}}{\Delta x}\right) + r$

→ $\frac{\partial c}{\partial t} = \frac{Q}{A}\left(-\frac{\partial c}{\partial x}\right) + r$ → $\boxed{\frac{\partial c}{\partial t} = -\frac{Q\partial c}{\partial\forall} + r}$

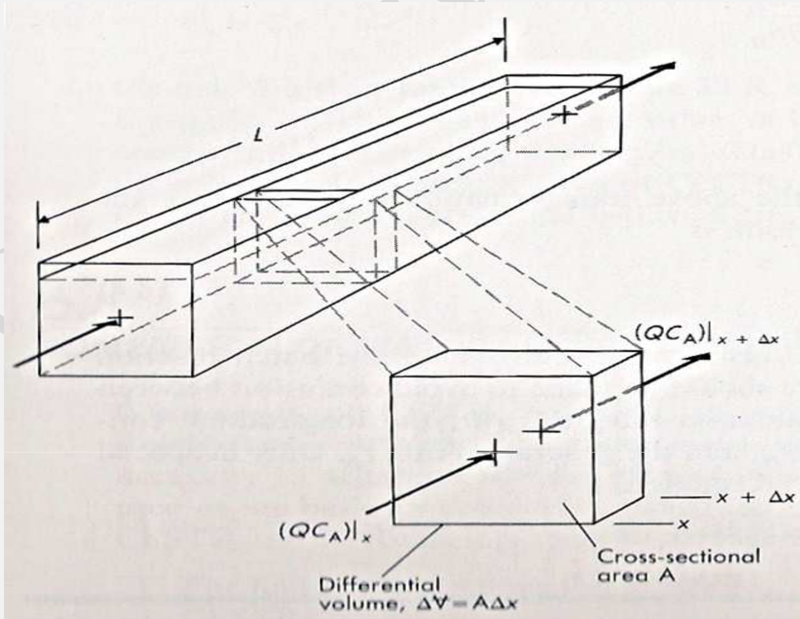


FIGURE 6.8
Definition sketch for the analysis of a PFR.

Ref: Tchobanoglous and Scroeder, 1985, Addison-Wesley Publishing Company

PFR
Unsteady-state conditions

$$\frac{\partial c}{\partial t} = -\frac{Q\partial c}{\partial \forall} + r$$

@ steady-state conditions $\longrightarrow \frac{\partial c}{\partial t} = 0$

$$\frac{\partial c}{\partial t} = 0 \longrightarrow \boxed{r = \frac{Q\partial c}{\partial \forall} = \frac{\partial c}{\partial t_R}}$$

PFR

steady-state conditions

EXAMPLE 2:

A plug flow reactor (PFR) is to be used to carry out the reaction

$A \longrightarrow B$

The reaction is first order and the rate is characterized as r_a=-kC_A

Determine the steady-state eff. conc. as a function of t_R .

EXAMPLE 3:

Determine the volume of a CFSTR required to give a treatment efficiency of 95% for a substance that decay according to half – order kinetics with a rate constant of 0.05 $(mg/L)^{1/2}$.

The flow rate is steady at 300L/hr and the influent concentration is 150mg/L.

EXAMPLE 4:

Determine the volumes of two identical CFSTR reactors in series to provide the same degree of treatment for the conditions given in Example 1.

EXAMPLE 5:

Determine the volume of a PFR to provide same degree of treatment for the conditions given Example 1.

Volume Comparison For Examples 3-5

	Example 1 CFSTR	Example 2 2 CFSTR in series	Example 3 PFR
$\forall(m^3)$	312	180	114

When the same reaction model (except for zero-order rxns) applies, regardless of the mixing regime a **PF system is always the most efficient (less volume requirement)**