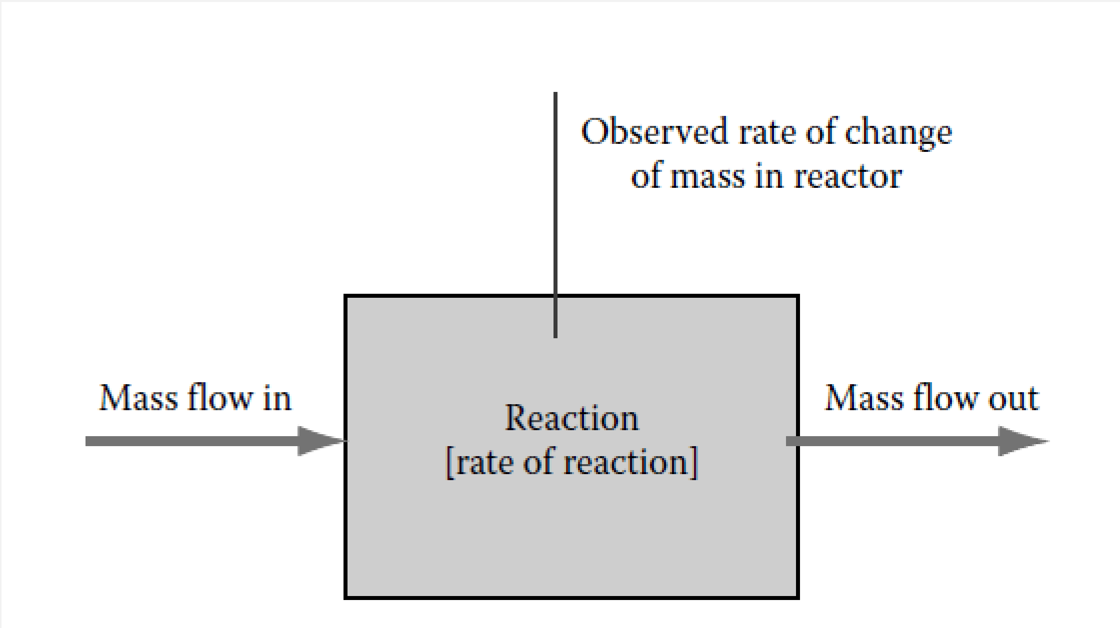
Reactor Models

REACTOR

A reactor is the place where the desired reaction takes place that is, the removal of a selected contaminant.

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



Source: Fundamentals of Water Treatment: Unit Processes Physical, Chemical, and Biological

MATHEMATICS OF REACTORS

Reactor mathematics is based upon two principles:

(1) Materials balance and

(2) reaction kinetics.

Materials Balance: Concept

The basic idea of a reactor model is quite simple and is embodied in the following equation.

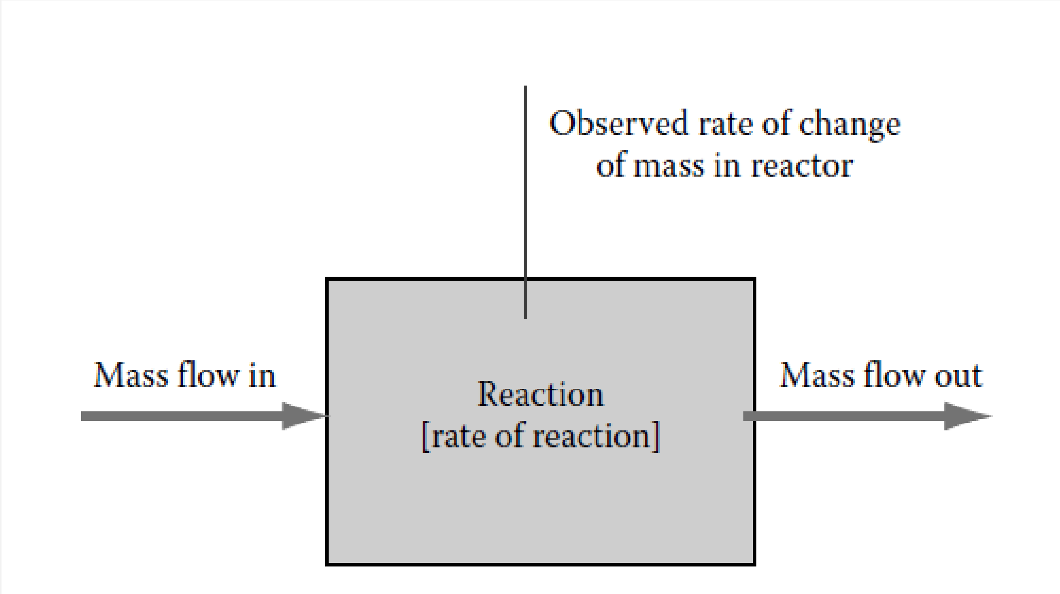
accumulation	=	Σ(inputs)	−	Σ(outputs)	+	Σ(generation)
rate at which component i accumulates within the reactor (mass/time)	=	total rate at which component i enters the reactor (mass/time)	−	total rate at which component i exits the reactor (mass/time)	+	total rate at which component i is transformed within the reactor (mass/time)

FIGURE 7.1 *Word statement of the mass balance upon a targeted substance (component* i*) for an arbitrary reactor.*

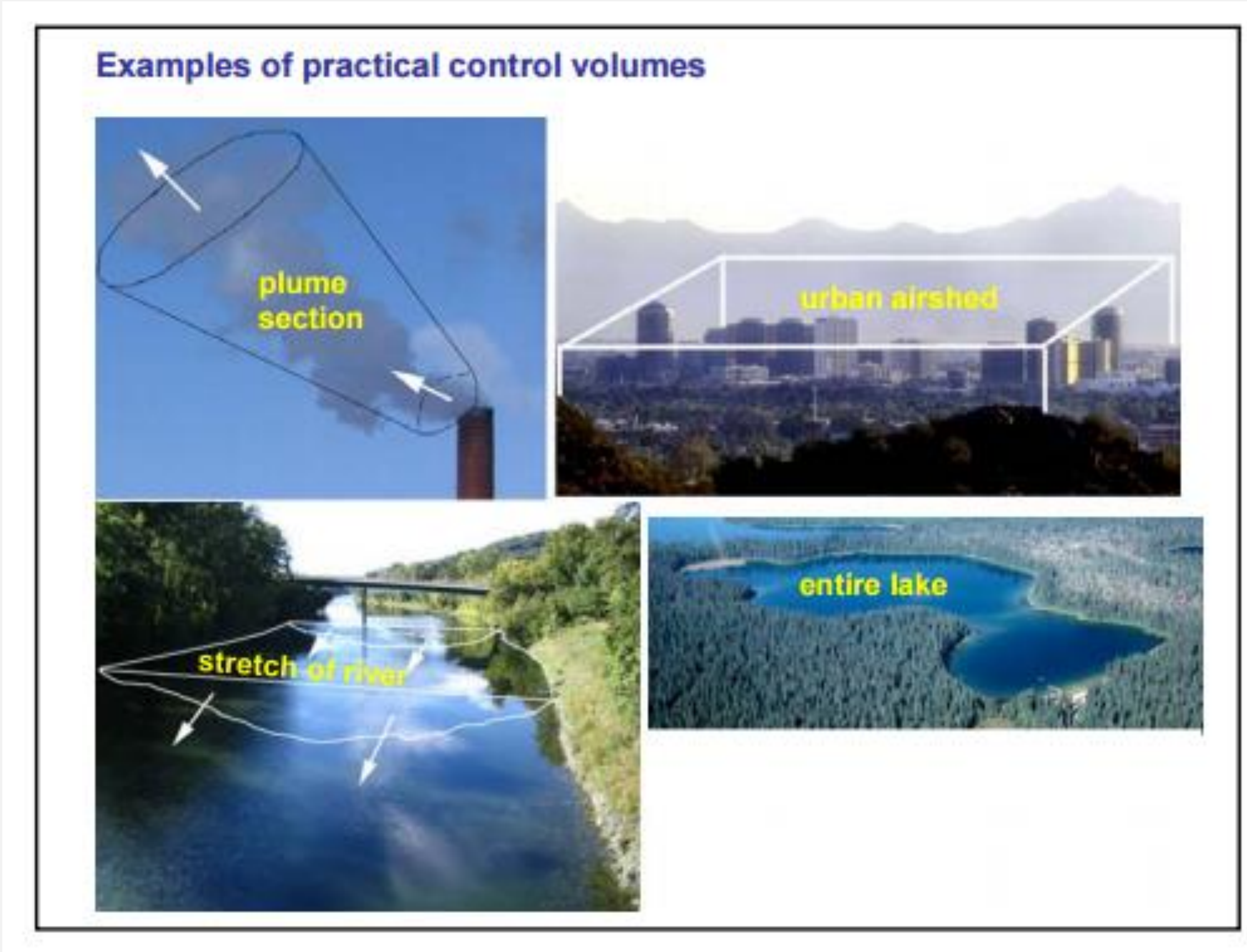
Materials Balance

(mass balance)

The first step involved in preparing a mass balance is to define the **system boundary** so that all the flows of mass into and out of the system boundary can be identified.



Source: Fundamentals of Water Treatment: Unit Processes
Physical, Chemical, and Biological



http://engineering.dartmouth.edu/~d30345d/courses/engs37/massbalance.pdf

Materials Balance

Materials Balance
(mass balance)

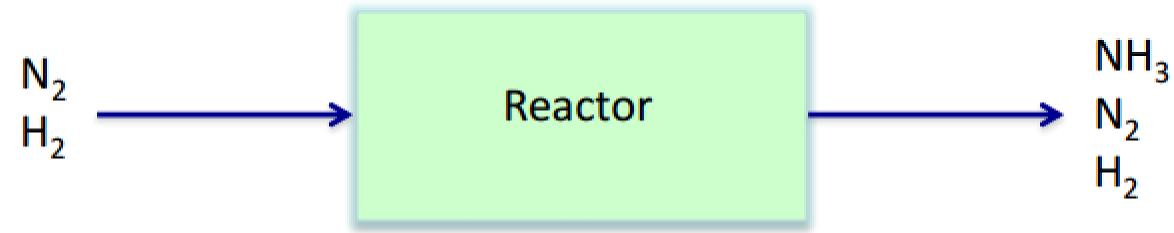
→ quantitative description of all materials that **enter, leave and accumulate** in a system with defined boundaries.

→ based on the law of conservation of mass *(mass is neither created nor destroyed)*

→ is developed on a chosen control volume.

There may be mass generation in the control volume also.

Chemical reaction: $N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)}$



https://www.princeton.edu/~asme/uploads/2/2/6/7/22674800/chemical_engineering_study_guide.pdf

http://www.seas.ucla.edu/stenstro/Reactor.pdf

http://ocw.mit.edu/courses/civil-and-environmental-engineering/1-77-water-quality-control-spring-2006/lecture-notes/chapter5lecture.pdf

Please find these pdf documents and read!!!

Wastewater Treatment Plants

Primary settling

Secondary settling

Waste stabilization

http://ocw.mit.edu/courses/civil-and-environmental-engineering/1-77-water-quality-control-spring-2006/lecture-notes/chapter5lecture.pdf

Rate of **accumulation** of mass within the system boundary	=	Rate of flow of mass **into the system** boundary	—	Rate of flow of mass **out of the system** boundary	±	Rate of mass **generation/elimination** within the system
Accumulation	=	Inflow	-	Outflow	±	Generation/Elimination

Accumulation = Inflow - Outflow + Generation/Elimination

Generation/Elimination term. can be "+" or "-"

[Most of the materials of interest disappear and therefore generation term is "-" in most cases.]

Symbolic Representation:

Accumulation = Inflow - Outflow + Generation/Elimination

$$\forall \frac{dC}{dt} = (QC_o) - QC \pm r\forall$$

$\forall$ = volume of the reactor, m^3

$\frac{dC}{dt}$ = rate of change of reactant concentration within the reactor (g / m^3 sec)

Q = flow into and out of the reactor (m^3 /sec)

C_0=concentration of reactant in the reactor and effluent (g/ m^3)

r = rate of generation (g/ m^3 sec)

Operational states that must be considered in the application of materials balances:

→ **Steady state:**

There is no accumulation in the system.

Rates and concentration do not vary with time.

$$\frac{\partial C_A}{\partial t} = 0$$

Example: Pump discharging constant volume of water within time.

→ **Unsteady (transient) State:**

Rate of accumulation is changing with time

$$\frac{\partial C_A}{\partial t} \neq 0$$

Example: Filling a reservoir pumping of the contents of a tank.

Types of reactors

REACTOR MODELS

Common reactor configurations include (a) completely mixed batch reactors, (b) completely mixed flow reactors (CMFRs), and (3) plug flow reactors (PFRs).

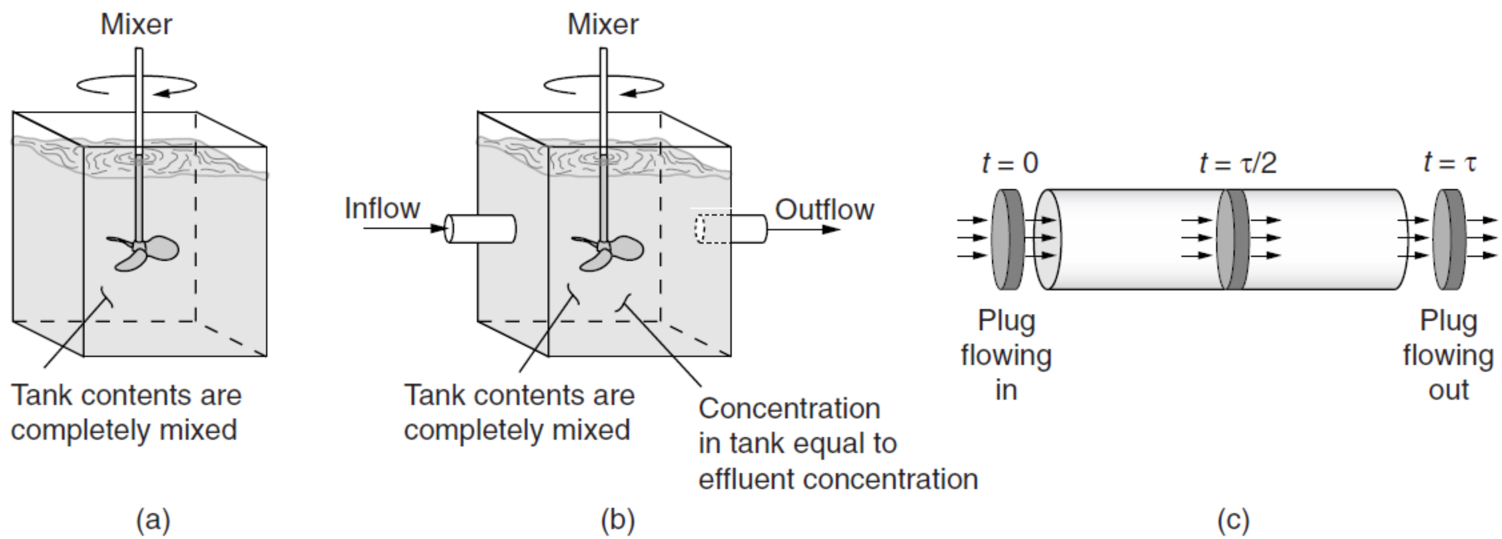


Figure 4-3
Diagrams of three ideal reactors: (a) batch reactor, (b) completely mixed flow reactor, and (c) plug flow reactor.

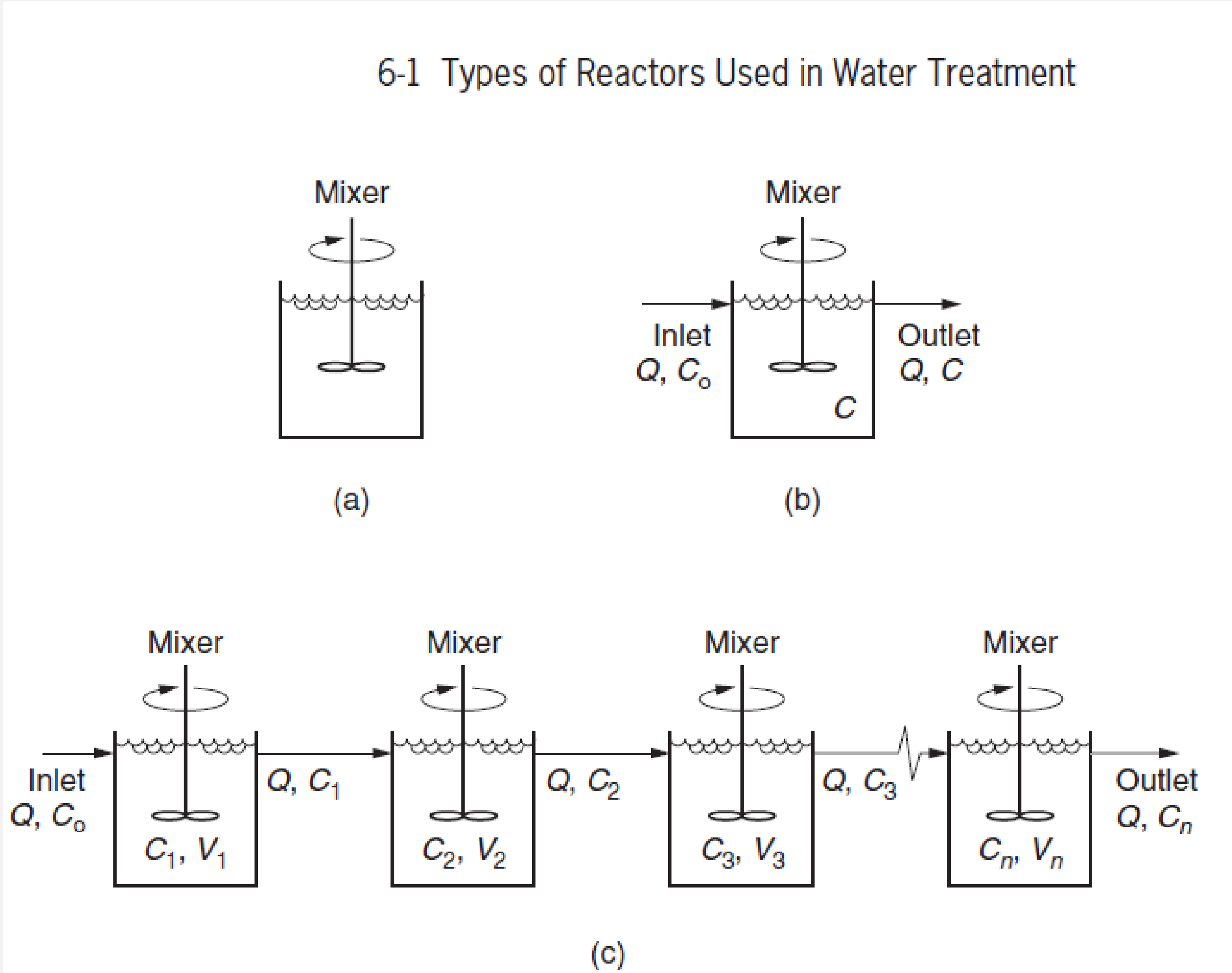
Source: *MWH's Principles of Water Treatment , Third Edition, Ch4*
Kerry J. Howe, David W. Hand, John C. Crittenden, R. Rhodes Trussel and George Tchobanoglous, 2012 John Wiley & Sons, Inc.

REACTOR MODELS

5 principal reactor models used in Environmental Engineering operations:

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

Types of Reactors Used in Water Treatment



Source: *MWH's Water Treatment: Principles and Design, Third Edition, Ch6*
John C. Crittenden, R. Rhodes Trussell, David W. Hand, Kerry J. Howe and George Tchobanoglous, 2012 John Wiley & Sons, Inc.

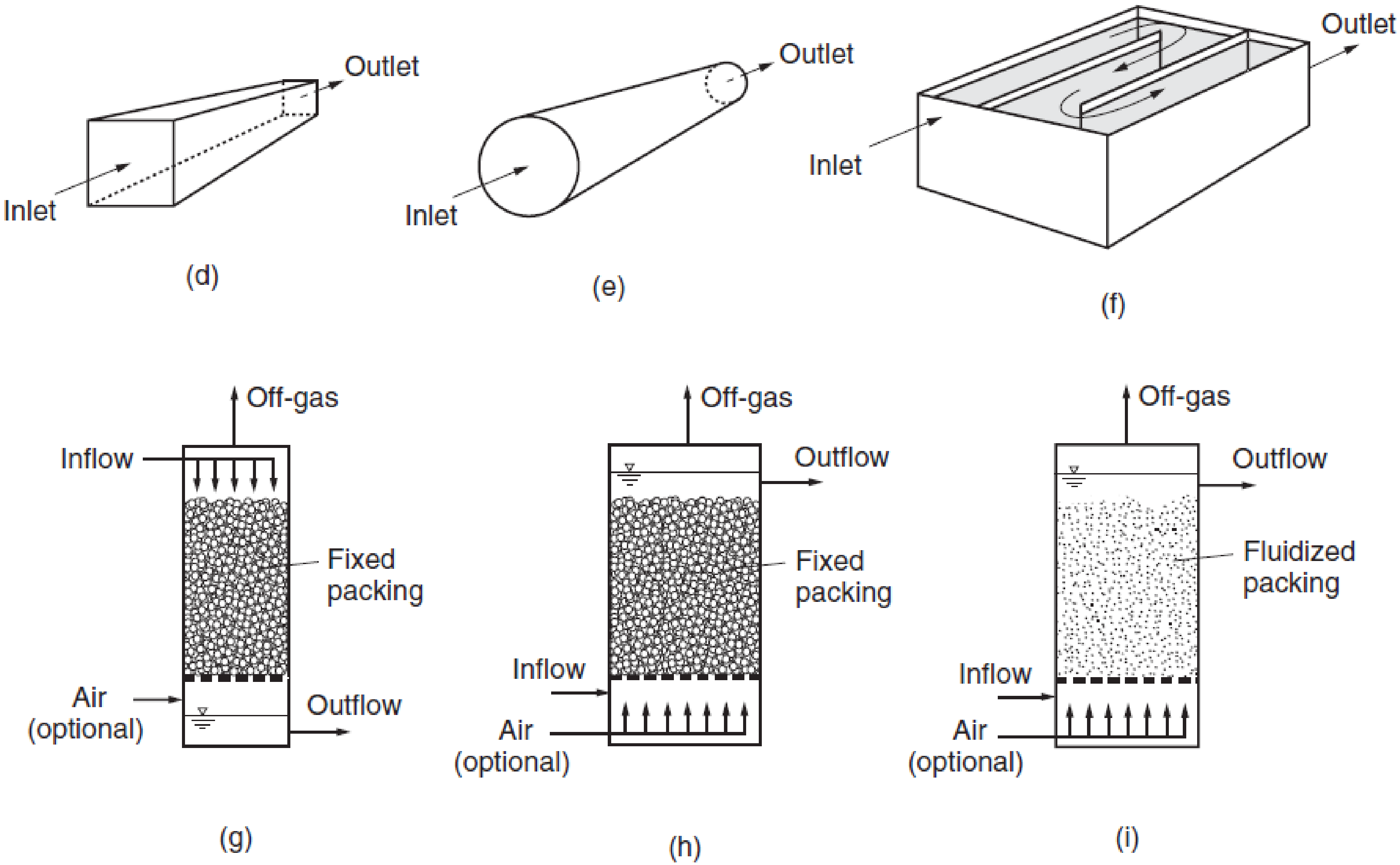
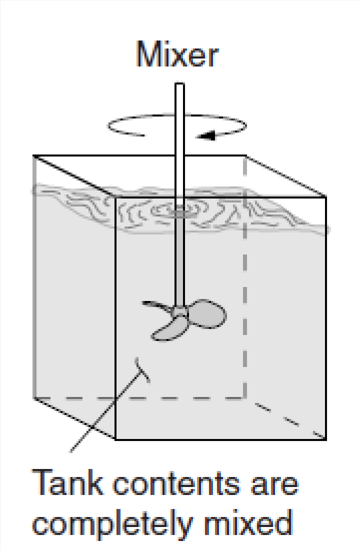


Figure 6-1
Typical reactors used in water treatment processes: (a) batch reactor; (b) continuous-flow mixed reactor; (c) continuous-flow mixed reactors in series, also known as tanks in series; (d) rectangular channel plug flow reactor; (e) circular pipe plug flow reactor; (f) serpentine configuration plug flow reactor; (g) packed-bed downflow reactor; (h) packed-bed upflow reactor; and (i) expanded-bed upflow reactor. (Adapted from Tchobanoglous et al., 2003.)

Source: *MWH's Water Treatment: Principles and Design, Third Edition , Ch6*
John C. Crittenden, R. Rhodes Trussell, David W. Hand, Kerry J. Howe and George Tchobanoglous, 2012 John Wiley & Sons, Inc.

BATCH REACTORS



The simplest reactor type

Flow is neither entering nor leaving the reactor

The liquid contents are mixed completely and uniformly

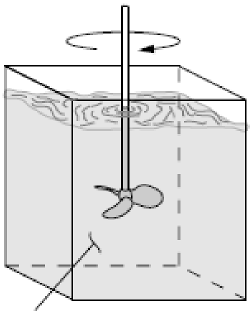
Ref: http://www.water-msc.org/e-learning/file.php/40/moddata/scorm/203/Lesson%204_04.htm

Applications:

Is a non-continuous and perfectly mixed closed vessel where a reaction takes place.

A common use of batch reactors in laboratories is to determine the reaction equation and rate constant for a chemical reaction.

The kinetic information determined in a batch reactor can be used to design other types of reactors and full-scale treatment facilities.



$$[\text{accum}] = [\text{mass in}] - [\text{mass out}] + [\text{rxn}]$$

Batch reactors have no inputs or outputs.

$$[\text{accum}] = [\sout{\text{mass in}}] - [\sout{\text{mass out}}] + [\text{rxn}]$$

$$V\frac{dC}{dt} = Vr \tag{4-63}$$

where V = reactor volume, L
C = concentration of reactant, mg/L

t = time, s
r = reaction rate, mg/L·s

Equation 4-63 can be simplified to

$$\frac{dC}{dt} = r \tag{4-64}$$

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

The reaction rate equation can be substituted for r and Eq. 4-64 can be integrated to yield an equation for C as a function of t.

For a first-order reaction, **r = - kC**

$$\frac{dC}{dt} = -kC \qquad (4\text{-}65)$$

Rearranging and setting up an integration of both sides yields

$$\int_{C_0}^{C} \frac{dC}{C} = -k \int_0^t dt \qquad (4\text{-}66)$$

where C_0 = initial reactant concentration, mol/L

Integration yields

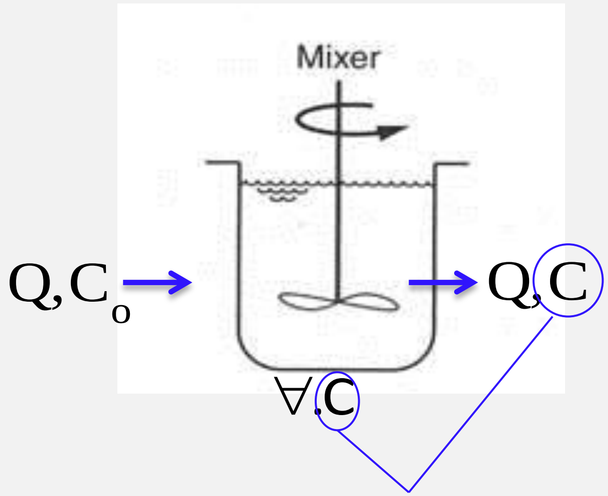
$$C = C_0 e^{-kt} \qquad (4\text{-}67)$$

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

For a second-order reaction, **r = - kC²**

$$\frac{1}{C} = \frac{1}{C_0} + kt \qquad (4\text{-}68)$$

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

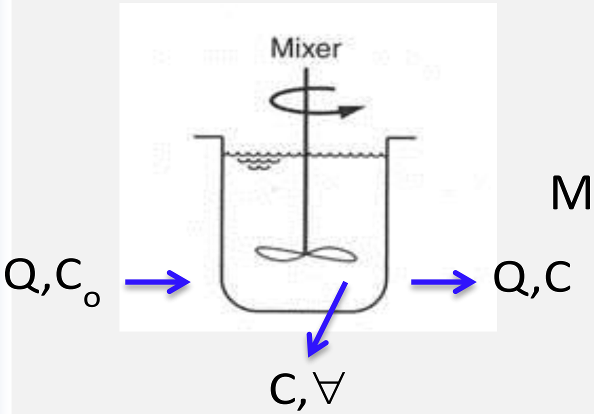
conc of any material leaving = conc. at any point in the reactor

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

No concentration gradient within the system.

Material entering is uniformly dispersed throughout the reactor.

CONTINOUS FLOW STIRRED TANK (CFSTR) REACTOR MODELS



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

Conservative (non-reactive) = Tracer tests

Some reactor analyses are conducted with conservative (or nonreactive) constituents.

It may seem that conservative chemicals would be of little interest in reactor analysis.

However, they provide a mechanism for understanding the hydraulic characteristics of a reactor.

Since conservative constituents do not react, they flow with the water and stay in a reactor as long as the water stays in the reactor.

Thus, a curve of effluent concentration of a conservative constituent reveals the residence time distribution of the water in the reactor.

Conservative constituents are commonly called ***tracers***, and tests to determine the **residence time distribution** of a reactor are called tracer tests.

Source: *MWH's Principles of Water Treatment , Third Edition, Ch4*
Kerry J. Howe, David W. Hand, John C. Crittenden, R. Rhodes Trussel and George Tchobanoglous,
2012 John Wiley & Sons, Inc.

Tracers

→ 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 liquid flow pattern.

Tracer tests

Two types of techniques are used for tracer tests:

- *Pulse input*: At the beginning of the testing period (i.e., time = 0), a known mass of tracer is added to the reactor influent instantaneously (i.e., added as a pulse or slug) and then flows through the reactor. Measurement of the effluent concentration continues until the pulse has completely passed through the reactor.

- *Step input*: At time = 0, a feed pump is turned on and feeds a tracer into the reactor influent. The concentration of the tracer in the influent stays constant over the duration of the test. Measurement of the effluent concentration continues until it is the same as the new influent concentration.

Source: *MWH's Principles of Water Treatment , Third Edition, Ch4*
Kerry J. Howe, David W. Hand, John C. Crittenden, R. Rhodes Trussel and George Tchobanoglous,
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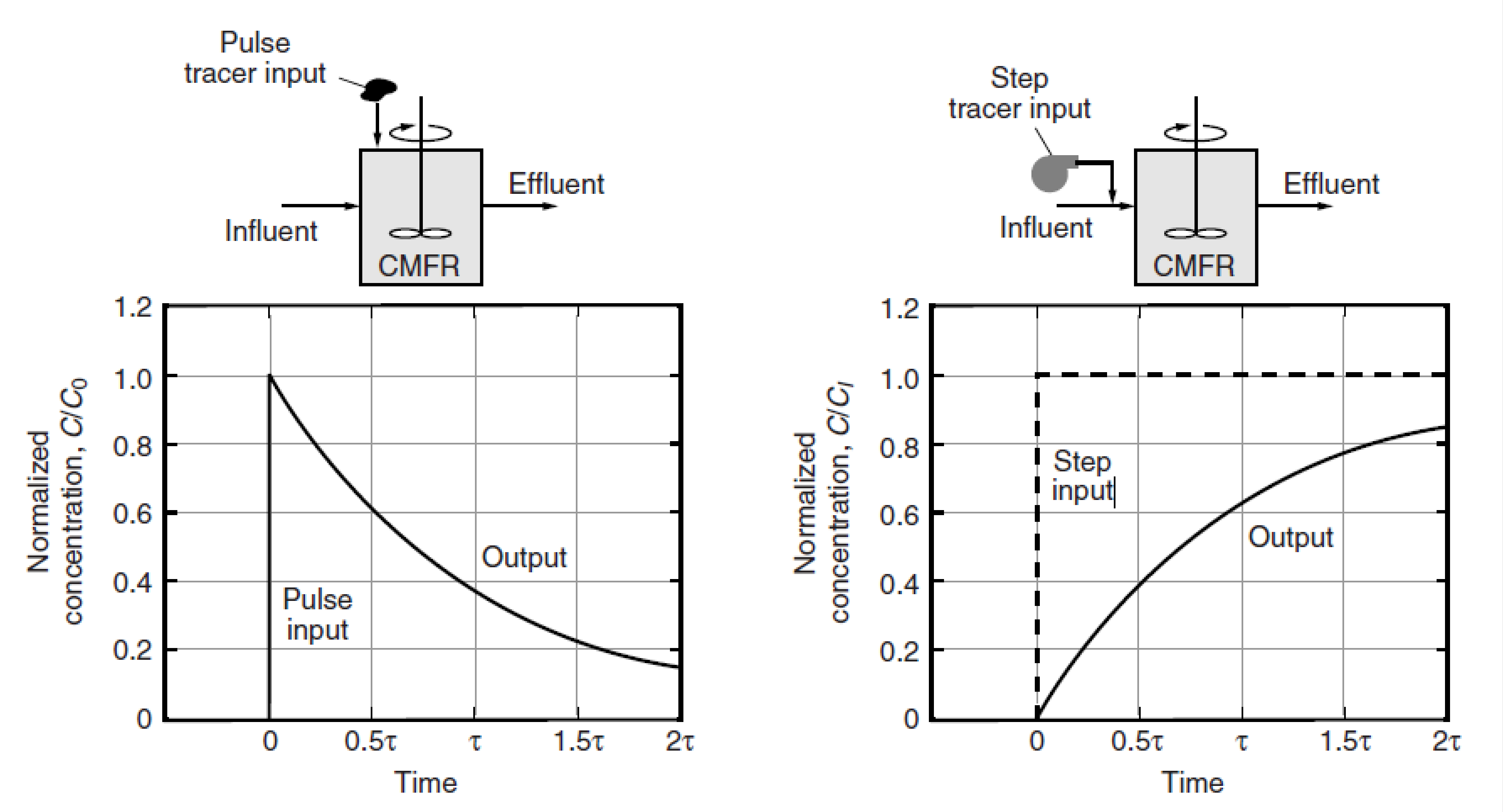
Tracer tests



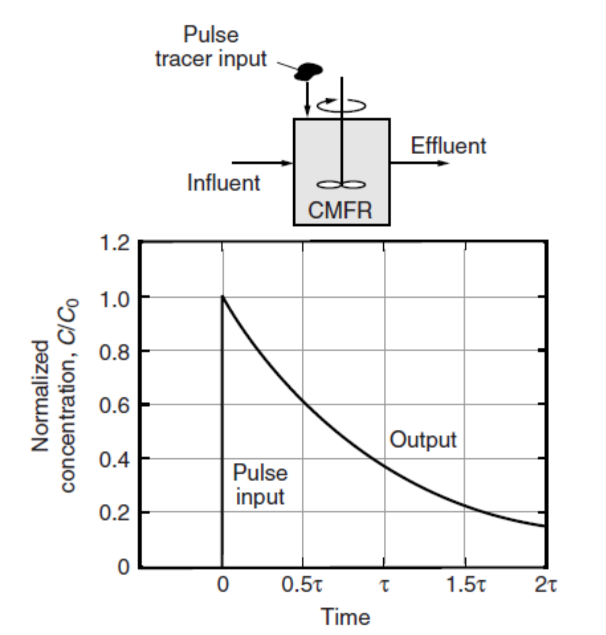
Source: *MWH's Principles of Water Treatment , Third Edition, Ch4*
Kerry J. Howe, David W. Hand, John C. Crittenden, R. Rhodes Trussel and George Tchobanoglous, 2012 John Wiley & Sons, Inc.

Response of CFSTR to Pulse Tracer Input

When a pulse input is introduced into a CFSTR, the effluent tracer concentration instantly reaches a maximum as the tracer is uniformly distributed throughout the reactor.

As clean water (containing no tracer) continues to enter the reactor after time = 0, the tracer gradually dissipates in an exponential manner as the tracer material leaves the effluent.

The exponential shape of the tracer curve can be demonstrated using a mass balance analysis of a CMFR.



Response of CFSTR to Pulse Tracer Input

$$[\text{accum}] = [\sout{\text{mass in}}] - [\text{mass out}] + [\sout{\text{rxn}}]$$

$$\forall \frac{dC}{dt} = -QC \pm r\not\forall$$

since the tracer is non-reactive

$$\forall \frac{dC}{dt} = -QC$$

Divide by V

$$\frac{dC}{C} = -\frac{Q}{V}dt$$

Source: *MWH's Principles of Water Treatment , Third Edition, Ch4*
Kerry J. Howe, David W. Hand, John C. Crittenden, R. Rhodes Trussel and George Tchobanoglous, 2012 John Wiley & Sons, Inc.

Response of CFSTR to Pulse Tracer Input

The hypothetical time, τ, that water stays in a reactor is:

$$\tau = \frac{V}{Q} \tag{4-73}$$

where τ = hydraulic residence time, s
V = reactor volume, m^3
Q = flow rate through the reactor, m^3/s

V/Q is defined as the hydraulic residence time (HRT). It is the time that the influent feed spends inside the reactor. Every molecule entering the reactor will have the exact same amount of time in the reactor

V/Q may be denoted with the symbols , t_R, t_D , HRT, τ.

HRT is an important design parameter. Process efficiency is dependent on hydraulic residence (detention) time.

HRT affects the operational and investment costs and energy requirements, and in general, higher HRTs will lead greater investment costs.

$$\frac{dC}{C} = -\frac{Q}{V} dt$$

At t=0+ (time immediately after tracer is added), the tracer is uniformly dispersed within the CFSTR. Thus, integrate for CFSTR with C_0 beginning at t=0, and C at t=t

$$\int_{C_o}^{C} \frac{dC}{C} = -\frac{Q}{V} \int_{t=0}^{t} dt$$

$$LnC - LnC_0 = -\frac{Q}{V} t$$

$$Ln\frac{C}{C_o} = -\frac{Q}{V} t$$

$$Ln\frac{C}{C_o} = -\frac{Q}{V} t$$

Response of CFSTR to Pulse Tracer Input

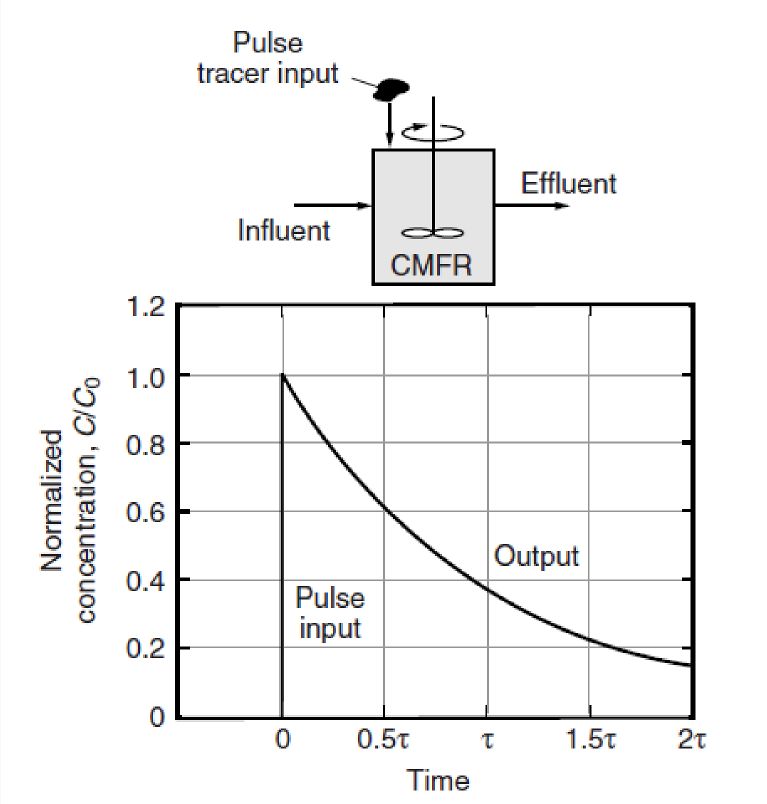
$$\frac{C}{C_0} = e^{-(Q/\forall)t}$$

$$\frac{Q}{V} = \frac{1}{\tau}$$

$$\frac{C}{C_0} = e^{-t/\tau}$$

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

This equation demonstrates that the effluent concentration from a CFSTR will be $C = C_0$ at t =0, C =0 at infinite time, and decay exponentially between those extremes.



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Kerry J. Howe, David W. Hand, John C. Crittenden, R. Rhodes Trussel and George Tchobanoglous, 2012 John Wiley & Sons, Inc.

Response of CFSTR to StepTracer Input

$$[\text{accum}] = [\text{mass in}] - [\text{mass out}] + [\cancel{\text{rxn}}]$$

$$\forall \frac{dC}{dt} = (QC_i) - QC \pm r\cancel{\forall}$$

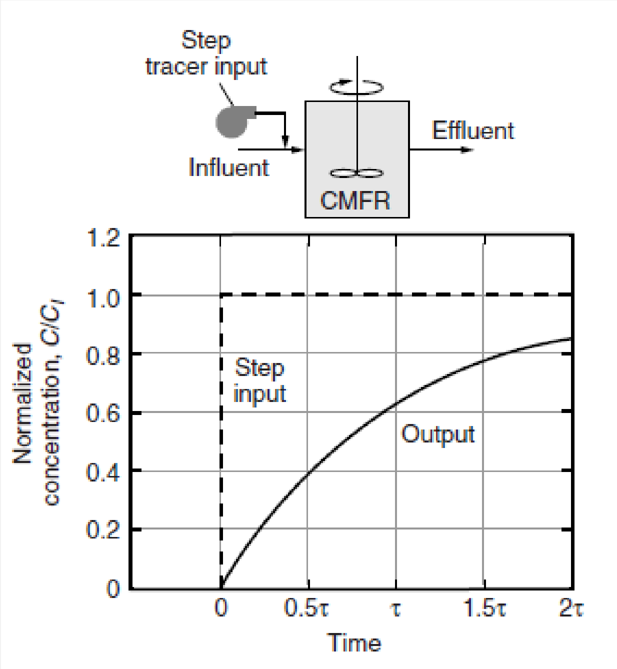
since the tracer is non-reactive

C_i is the influent tracer concentration.

$$\forall \frac{dC}{dt} = (QC_i) - QC$$

Divide by Q

$$\frac{\forall}{Q} \frac{dC}{dt} = C_i - C$$



Response of CFSTR to StepTracer Input

$$\frac{\forall}{Q}\frac{dC}{dt} = C_i - C$$

Integrate for CFSTR with C=0 beginning at t=0, and C at t=t

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

$$\rightarrow \frac{1}{-1}\mathrm{Ln}\left|C_i - C\right|\Big|_{C=0}^{C} = \frac{Q}{\forall}t$$

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

$$\rightarrow -\mathrm{Ln}\left(C_i - C\right) + \mathrm{Ln}C_i = \frac{Q}{\forall}t$$

$$\rightarrow \mathrm{Ln}\left(C_i - C\right) - \mathrm{Ln}C_i = -\frac{Q}{\forall}t$$

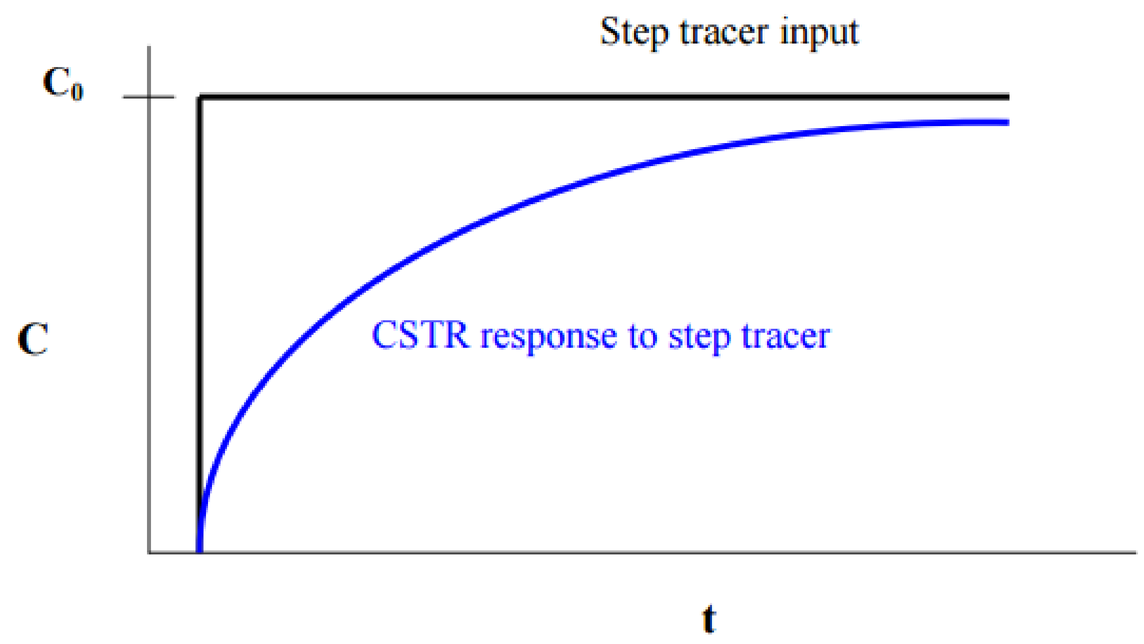
$$\rightarrow \mathrm{Ln}\frac{C_i - C}{Ci} = -\frac{Q}{\forall}.t$$

$$\rightarrow C_i - C = C_i e^{-(Q/\forall)t}$$ (Divide both sides by Ci)

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

$$\rightarrow \boxed{\frac{C}{C_i} = 1 - e^{-(Q/\forall)t}} \rightarrow \boxed{\frac{C}{C_i} = 1 - e^{-t/\tau}}$$

Response of CFSTR to StepTracer Input



Note asymptote, as t → ∞, C → C_0, which is equivalent to dC/dt → 0, which defines the steady state condition (accumulation = 0)

http://ceae.colorado.edu/~silverst/cven5534/IDEAL%20REACTORS.pdf

Response of CFSTR to StepTracer Input

$$\frac{Q}{\forall} = \frac{m^3/sec}{m^3} = \frac{1}{sec} = \frac{1}{t_R}$$ → Hydraulic retention time (HRT)

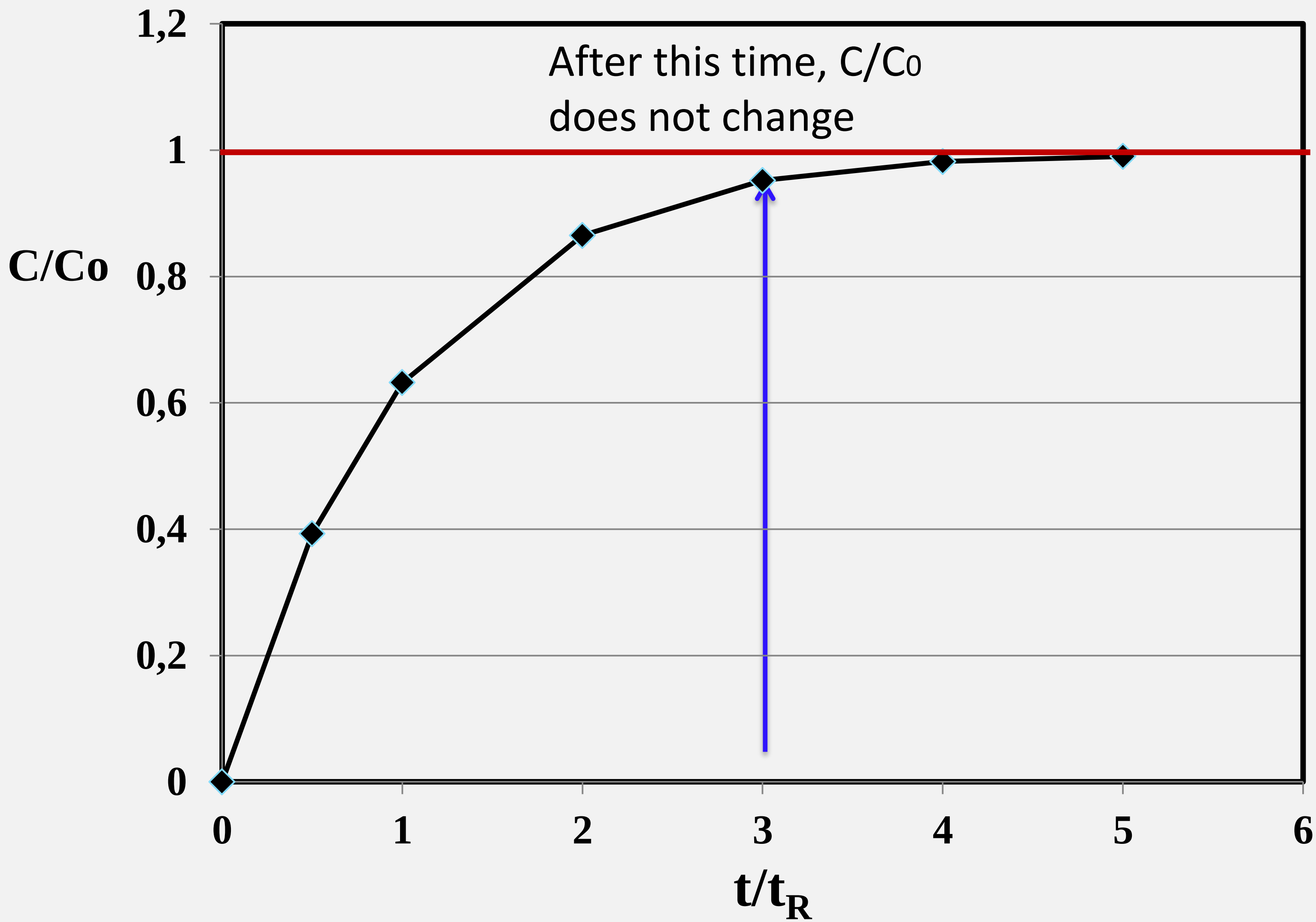
$$\frac{C}{C_0} = 1 - e^{-t/t_R}$$

t/t_R	$\frac{C}{C_0}$
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/C_0 does not change.

Response of CFSTR to StepTracer Input



Example:

Calculate time to reach 95% of the steady-state condition in a CSTR:

$$C/C_0 = 0.95 = (1\text{-}\exp(-t/\tau))$$

$$\frac{C}{C_0} = 1 - e^{-t/t_R}$$

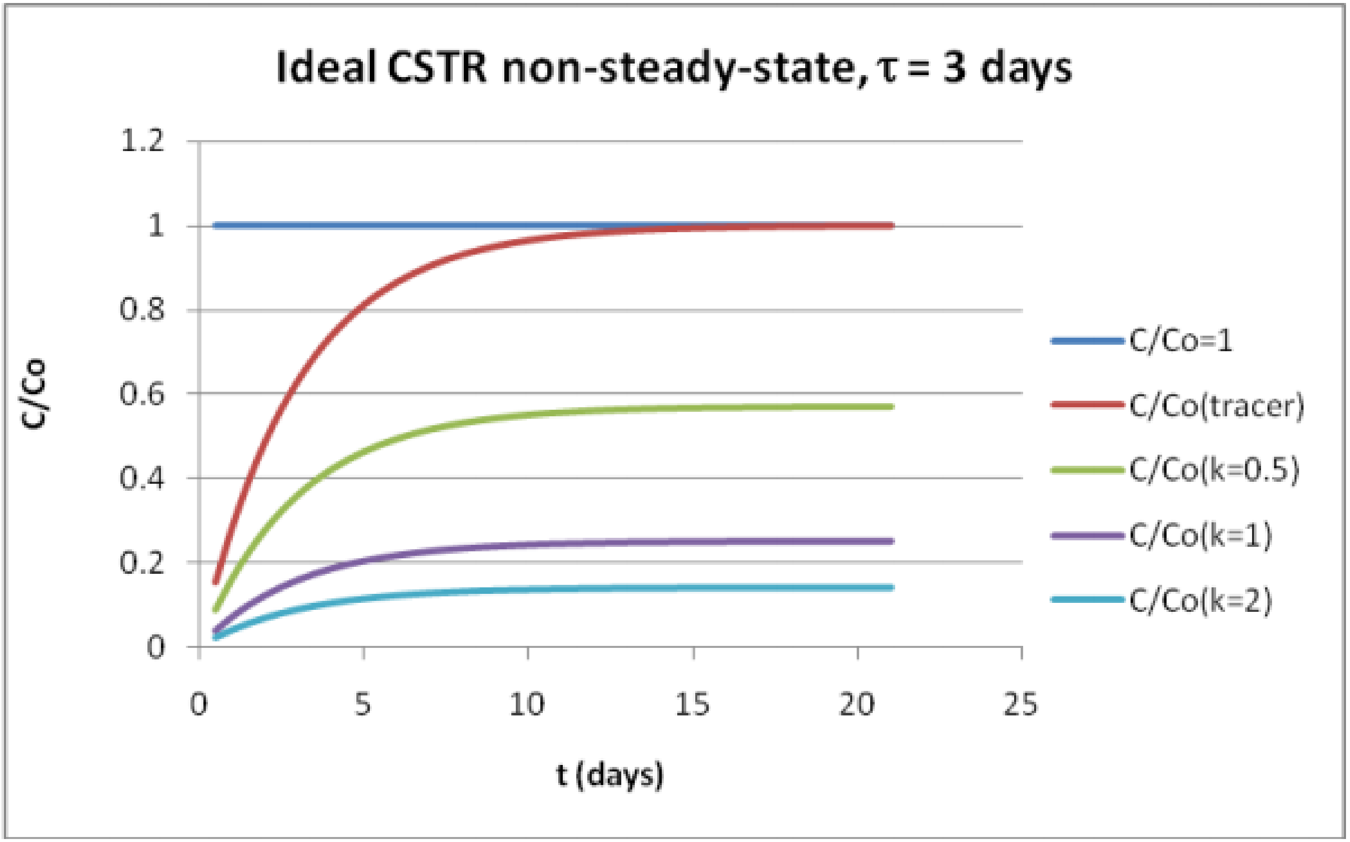
$$\exp(-t/\tau) = 1 - 0.95$$

$$-t/\tau = \ln(0.05) = -3$$

$$t_{95\%} = 3\tau$$

http://ceae.colorado.edu/~silverst/cven5534/IDEAL%20REACTORS.pdf

This is characteristic of CSTR flow, and also can be shown to be true in a CSTR with a reaction.

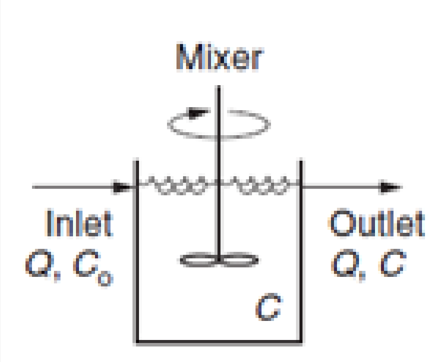


http://ceae.colorado.edu/~silverst/cven5534/IDEAL%20REACTORS.pdf

Response of CFSTR to Non-Conservative (Reactant) Input Unsteady State

Unsteady State Analysis

Reactors of concern in water treatment engineering typically operate at steady-state conditions.



Accumulation = Inflow - Outflow + Generation/Elimination

$$\forall \frac{dC}{dt} = (QC_o) - QC \pm r\forall$$

At steady state the accumulation term is zero. Therefore, there is no change in concentration within the reactor with time.

Response of CFSTR to Non-Conservative (Reactant) Input Unsteady State

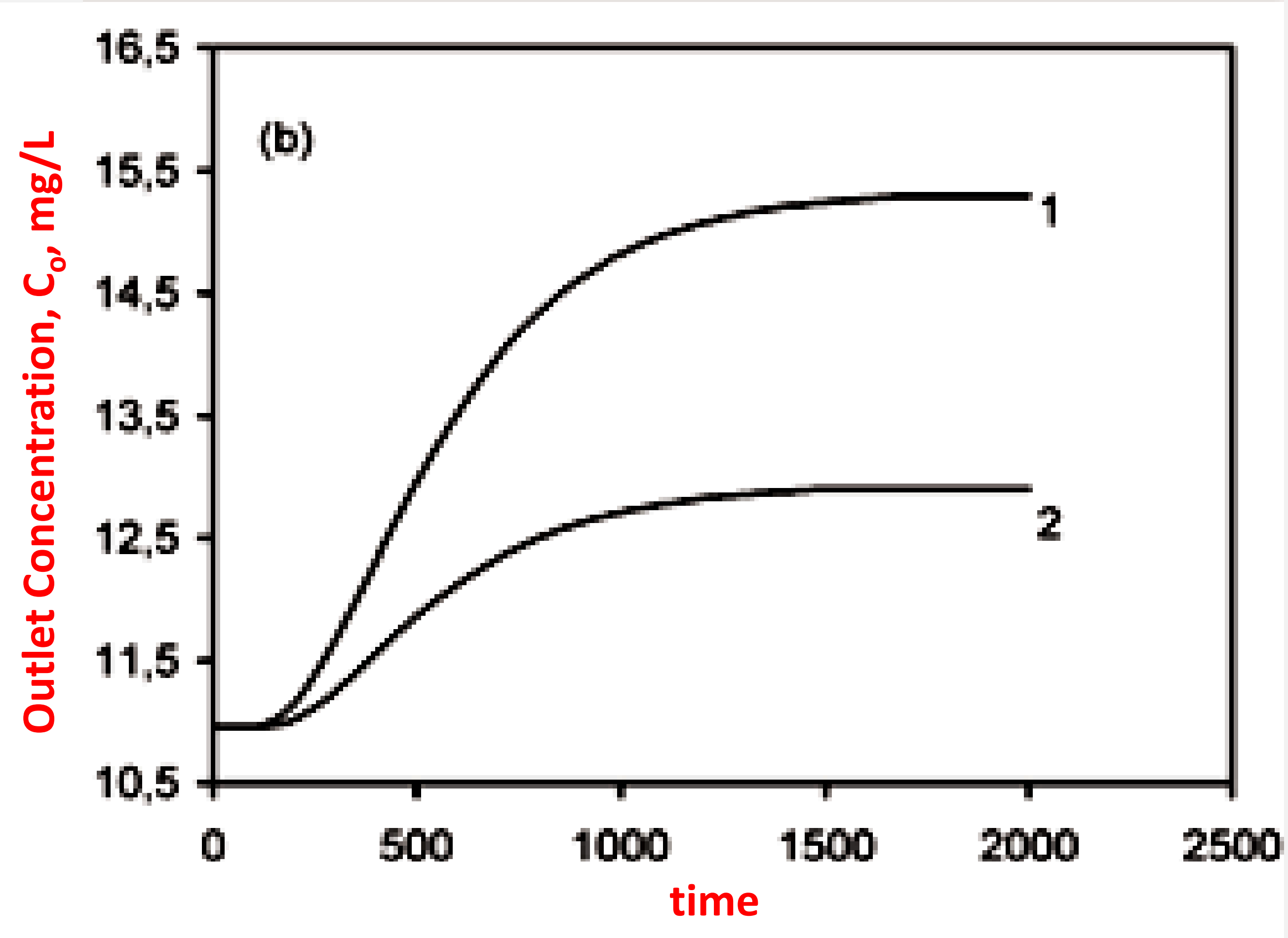
Unsteady State Analysis

However, sometimes the reactors operate at unsteady-state conditions

- When a reactor is first brought online,
- After maintanance or inoperation,
- When the inlet concentration, C_o, changes.

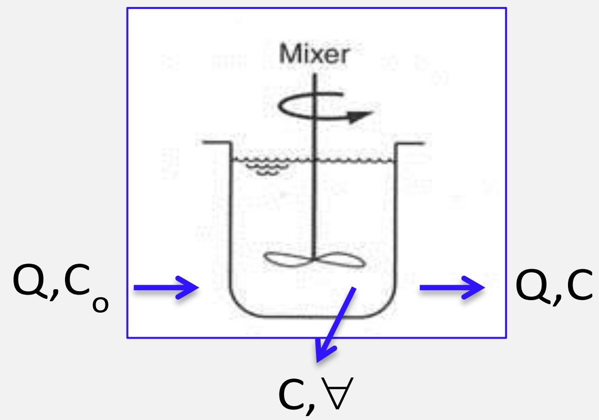
Unsteady state: concentrations vary with time & accumulation is non-zero

The goal of unsteady state analysis is to determine the time necessary to reach steady-state operation.



Response of a CFSTR to an increase in the inlet concentration from 50 mg/L to 100 mg/L (1) and from 50 mg/L to 75 mg/L (2)

Response of CFSTR to Non-Conservative (Reactant) Input Unsteady State

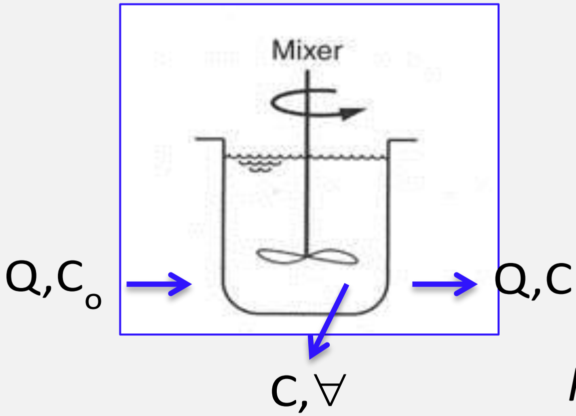


A reaction A $\longrightarrow$ B , known to be first order, is to be carried out in a CFSTR.

Water is run through the reactor at a flow rate Q (m^3/sec) and at 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.

Response of CFSTR to Non-Conservative (Reactant) Input
Unsteady State



The unsteady-state analysis begins with a mass balance equation, which is written for a first-order reaction assuming constant volume and using detention time, τ = *V* /*Q*, as follows:

Materials balance for the system:

$$\frac{dC}{dt}\forall = QC_0 - QC + \text{elimination}$$

First-order rxn→ r=-kC

∴ elimination term =r$_\forall$ = -kC∀

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

(Divide both sides by ∀)

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

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

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

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

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

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

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

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

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

Multiply both sides w/integration factor

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

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

Multiply both sides with integration factor.

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

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

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

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

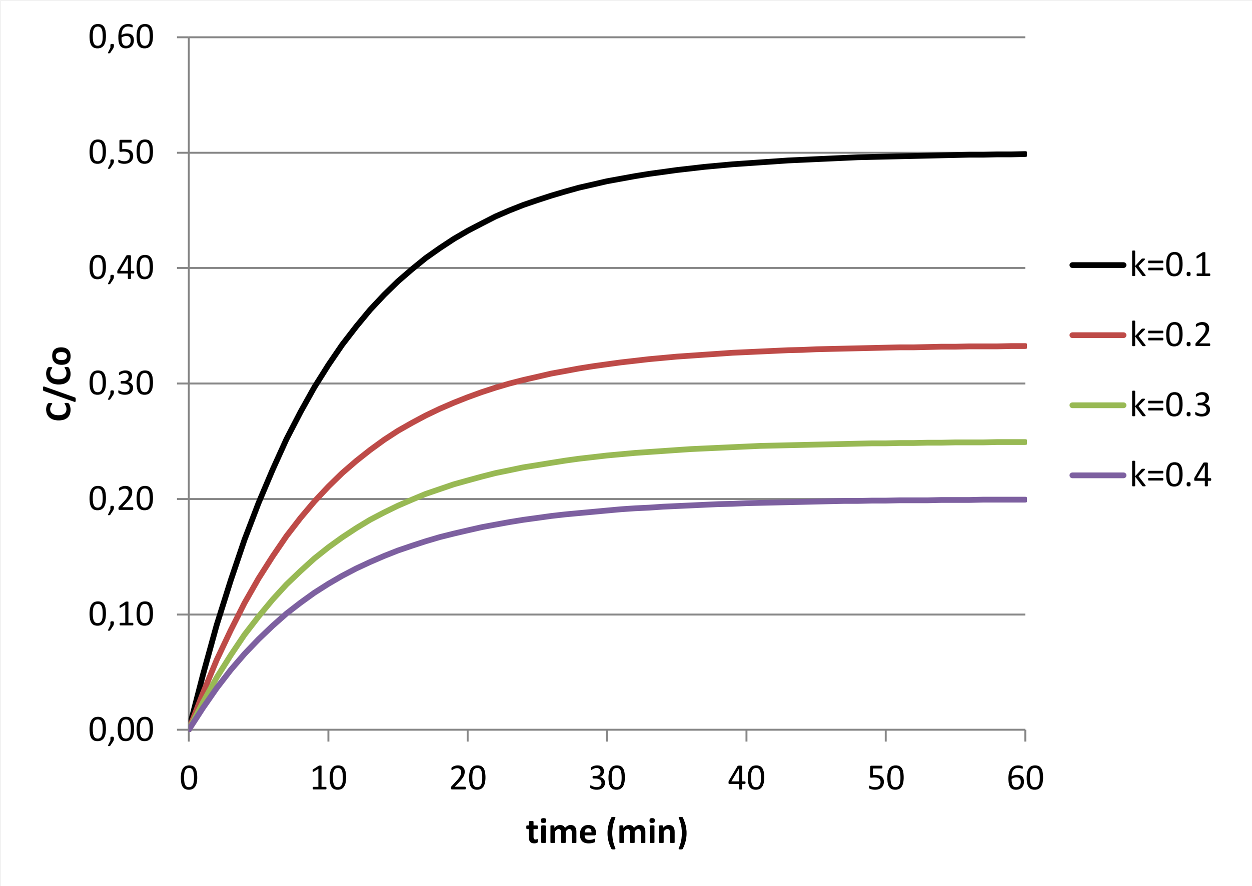
$$C_t = \frac{C_0}{1+kt_R}(1-e^{-t/t_R})$$

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

Start-up of an ideal CFSTR.

C_o=100 mg/L t_R = 10 min

$$C_t = \frac{C_0}{1+kt_R}\left(1-e^{-t/t_R}\right)$$



Start-up of an ideal CFSTR.

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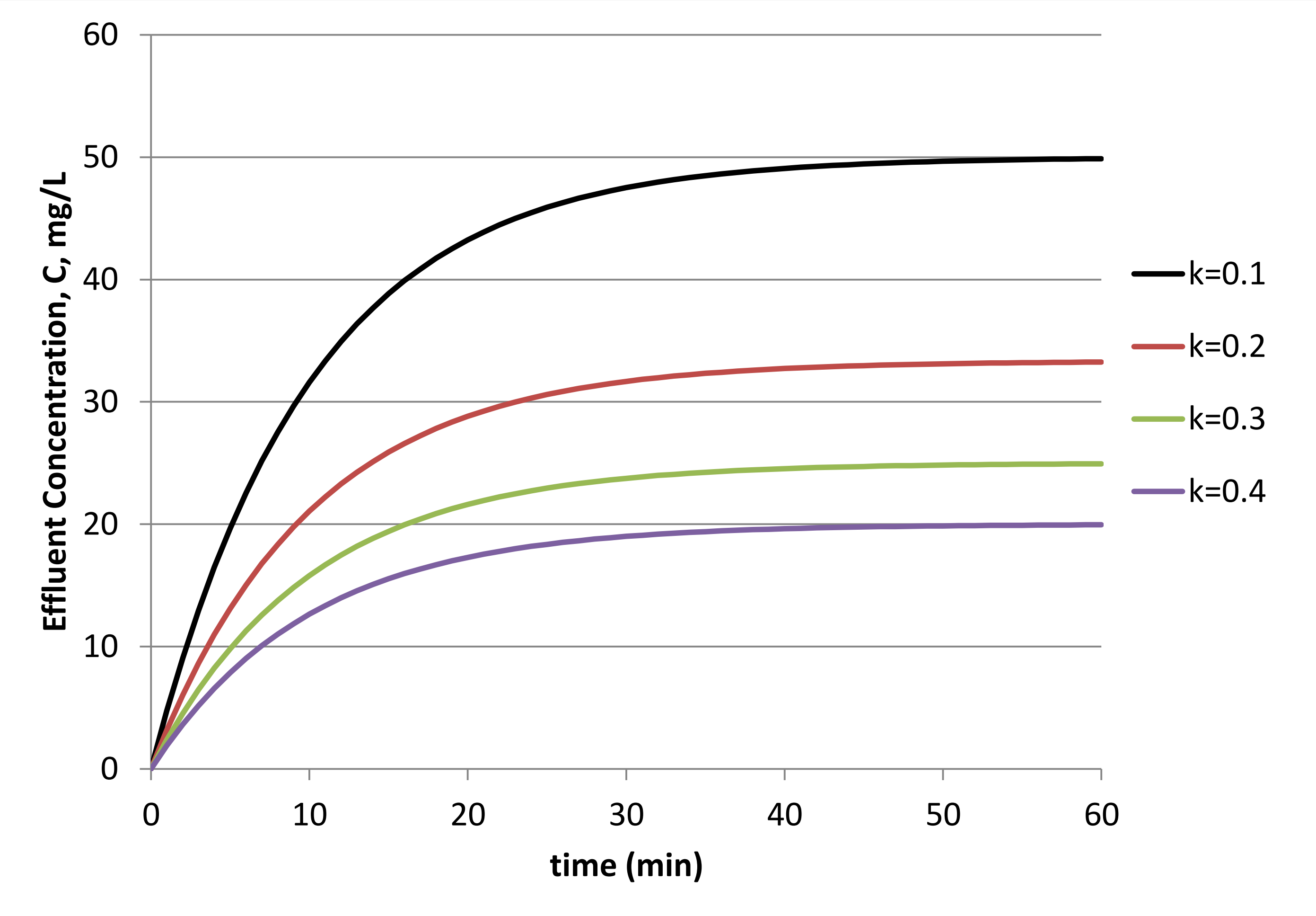
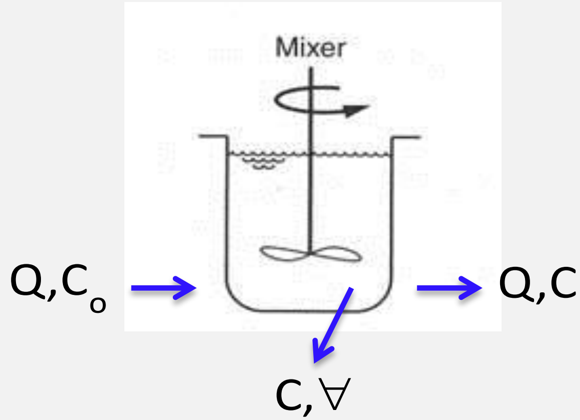


Response of CFSTR to Non-Conservative (Reactant) Input
Steady State



As t approaches infinity (∞) → steady-state solution is approached

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

$$e^{-t/t_R} = 0$$

→

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

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

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

$$\frac{dc}{dt}\forall = QC_0 - QC - kC\forall$$ (Divide both sides by $\forall$)

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

At steady-state

→ $\frac{dc}{dt} = 0$

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

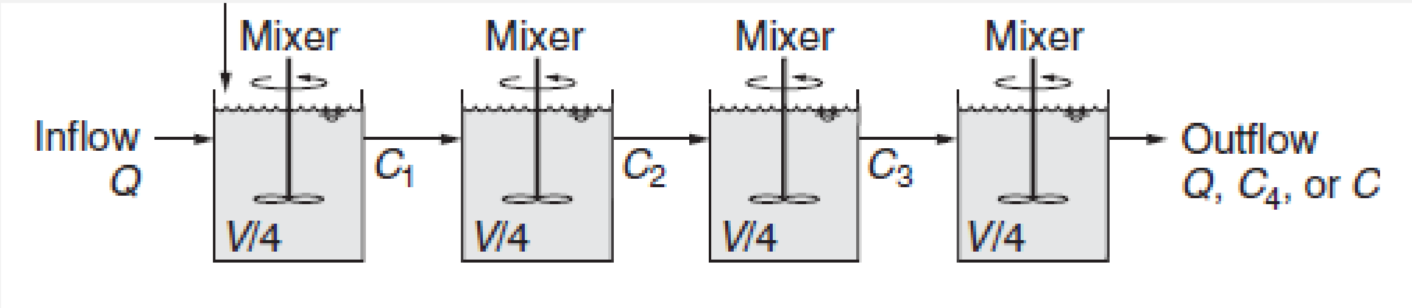
$$kCt_R = (C_0 - C)$$

$$kCt_R + C = C_0$$

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

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

CASCADE OF COMPLETE MIX REACTORS (CFSTR in series)



Output of the first reactor is the input of the second reactor.

In environmental engineering, it is common to employ a series of CMFRs to improve the hydraulic performance of a reactor.

The first CFSTR operates at a higher concentration and, therefore, a higher reaction rate is possible.

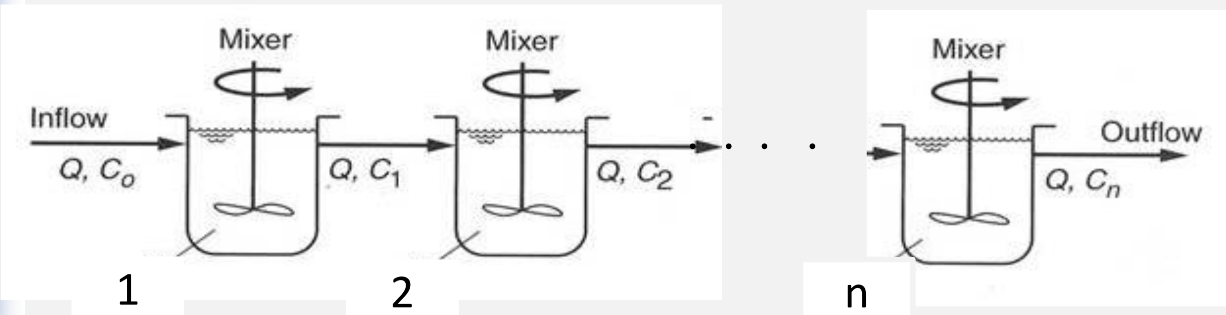
CASCADE OF COMPLETE MIX REACTORS (CFSTR in series)

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:

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

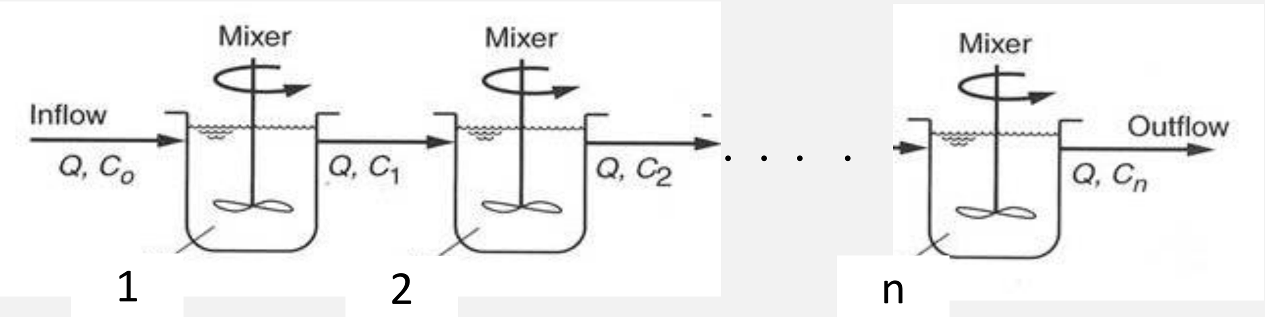
$$\rightarrow 0 = \frac{1}{t_{R1}}C_0 - C_1\frac{1+kt_{R1}}{t_{R1}} \rightarrow C_1 = \frac{C_0}{1+kt_{R1}}$$

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:

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

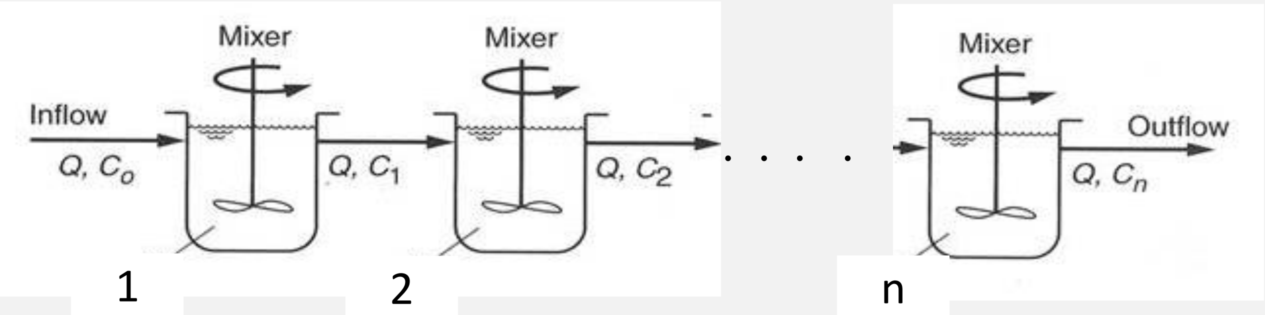
$$\rightarrow 0 = \frac{1}{t_{R2}}C_1 - C_2\frac{1+kt_{R2}}{t_{R2}} \rightarrow \boxed{C_2 = \frac{C_1}{1+kt_{R2}}}$$

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

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

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

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



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

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

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

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

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

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

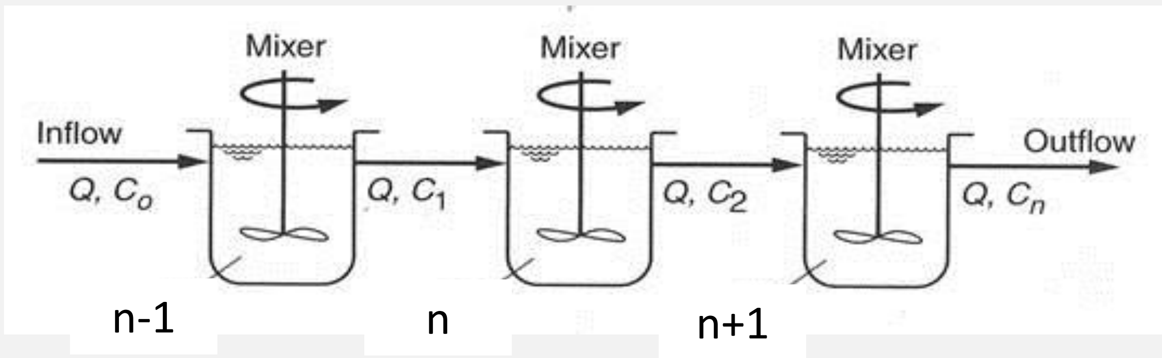
$$C_2 = \frac{C_0}{(1+kt_{R1}).(1+kt_{R2})}$$

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

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

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

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)

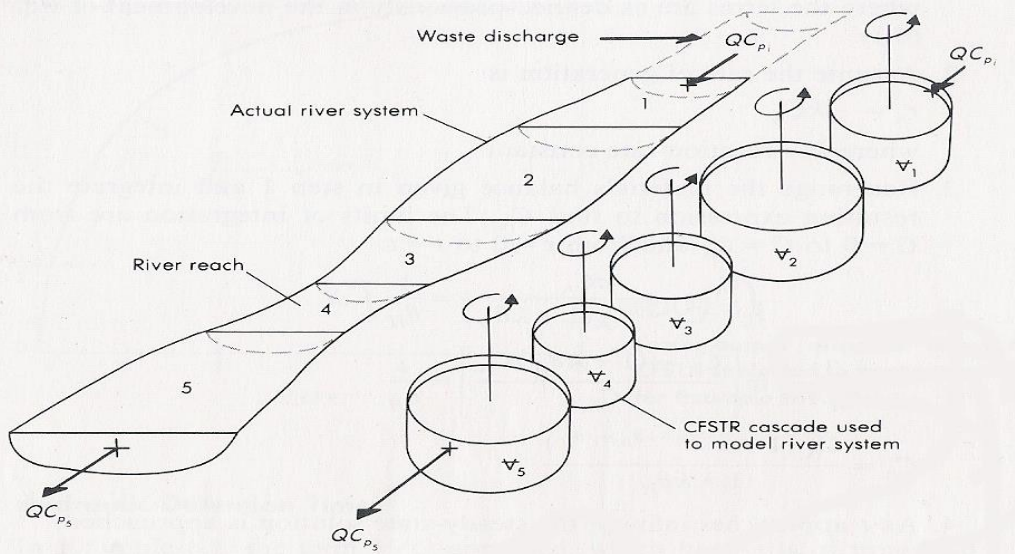


FIGURE 6.5

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

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

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:

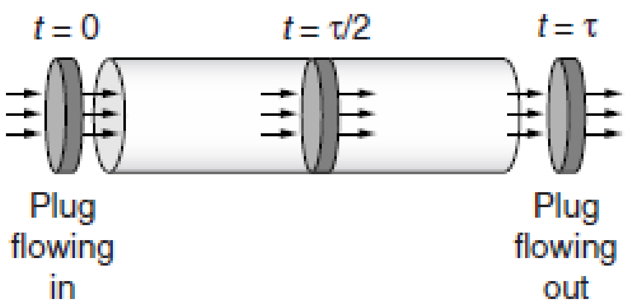
The river reach shown has been divided into 5 segments based on measured velocities and depths. An industrial facility is planned just upstream of the 1st segment and it is necessary to estimate effect of ww discharge. A series of dye experiments have been run and each of the segments was found to behave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

$$Q_{river} = 5 m^3/sec$$

$$k = 0{,}2 day^{-1}$$

$$C_0 = 30 g/m^3$$

PLUG FLOW REACTOR-(PFR)



→ No mixing in the axial direction.

→ 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.

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

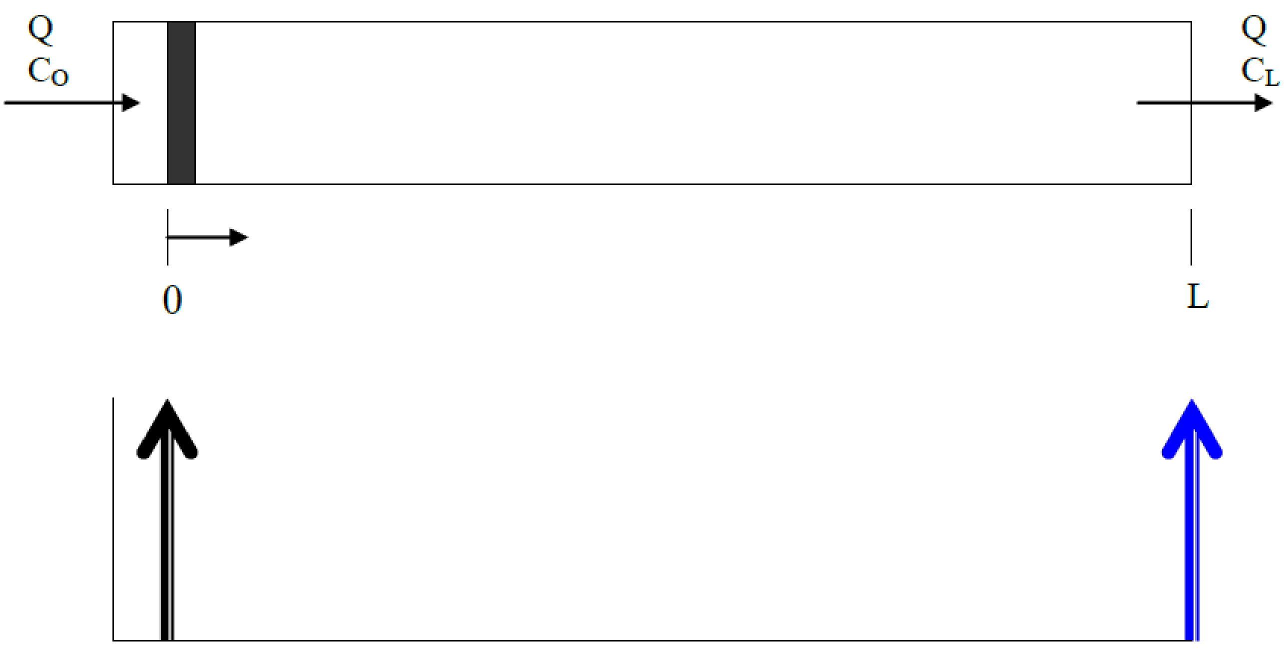
***Application*:**

→ Used to study river systems

IDEAL PLUG FLOW REACTOR

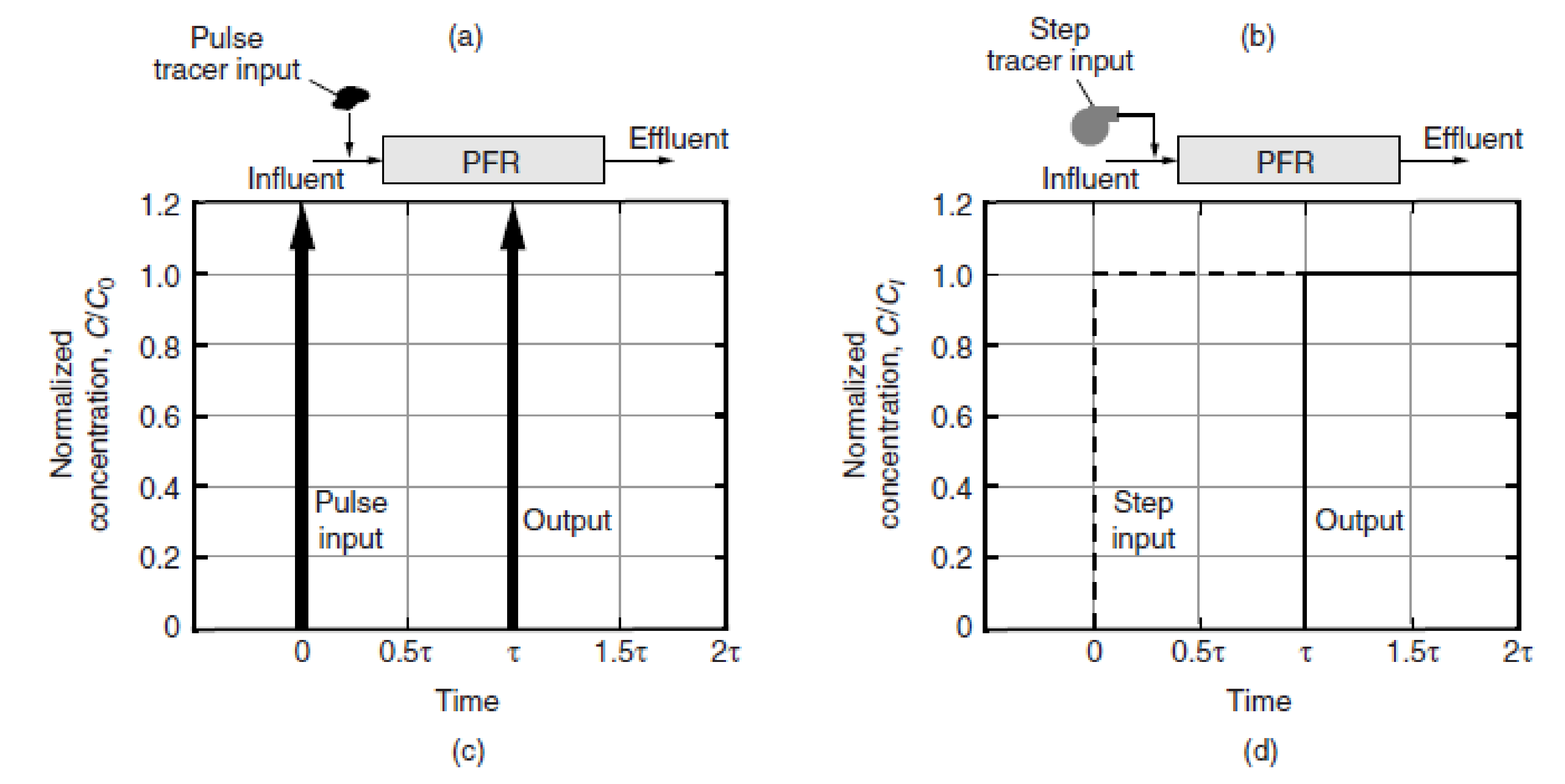
Characteristics of ideal plug flow

- PERFECT MIXING IN THE RADIAL DIMENSION (UNIFORM CROSS SECTION CONCENTRATION)
- NO MIXING IN THE AXIAL DIRECTION, OR NO AXIAL DISPERSION (SEGREGATED FLOW)



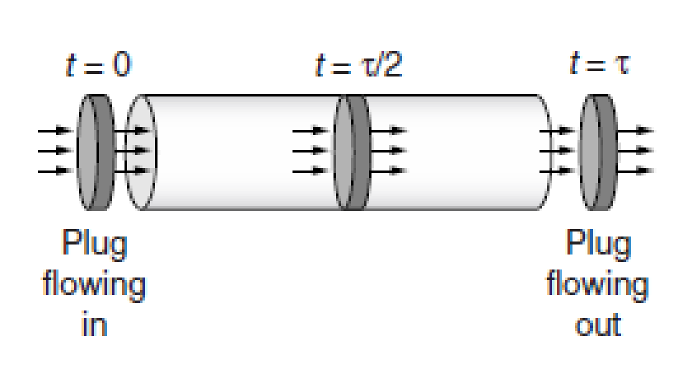
http://ceae.colorado.edu/~silverst/cven5534/IDEAL%20PLUG%20FLOW%20REACTOR.pdf

PLUG FLOW REACTOR-(PFR)



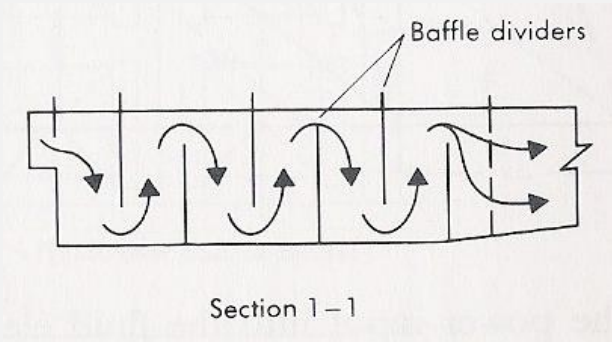
An effluent tracer (conservative) signal is exactly the same as the input , except that is transposed in time by t_R.

PLUG FLOW REACTORS (PFR)



- 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

→ PF conditions are achieved by designing long and narrow reactors or 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 $\Delta\forall$)

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

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

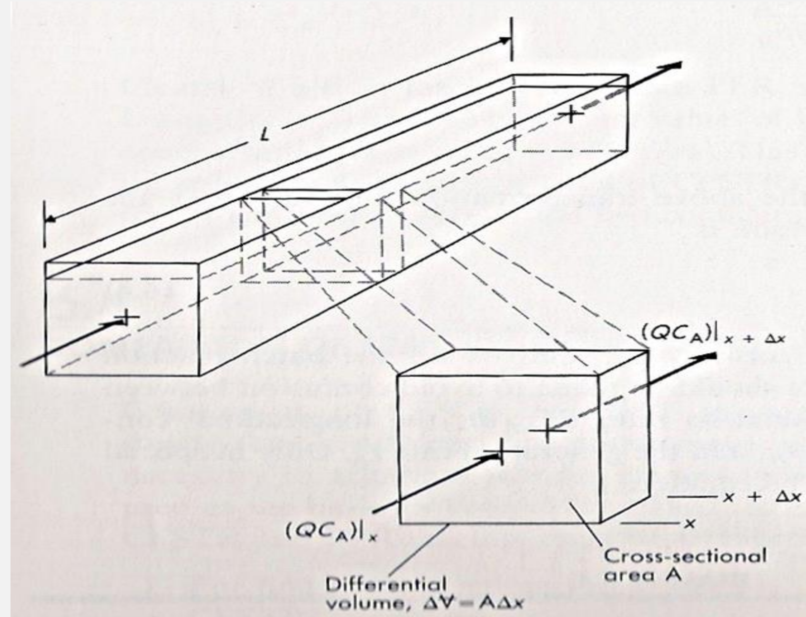
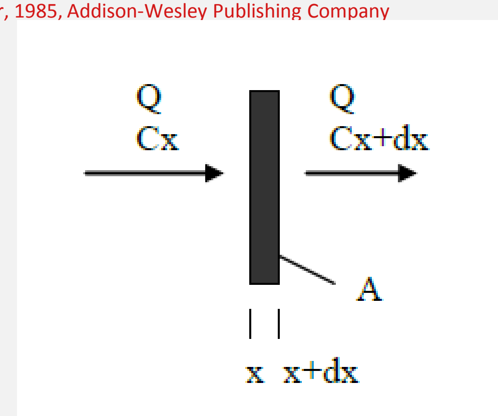


FIGURE 6.8
Definition sketch for the analysis of a PFR.

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



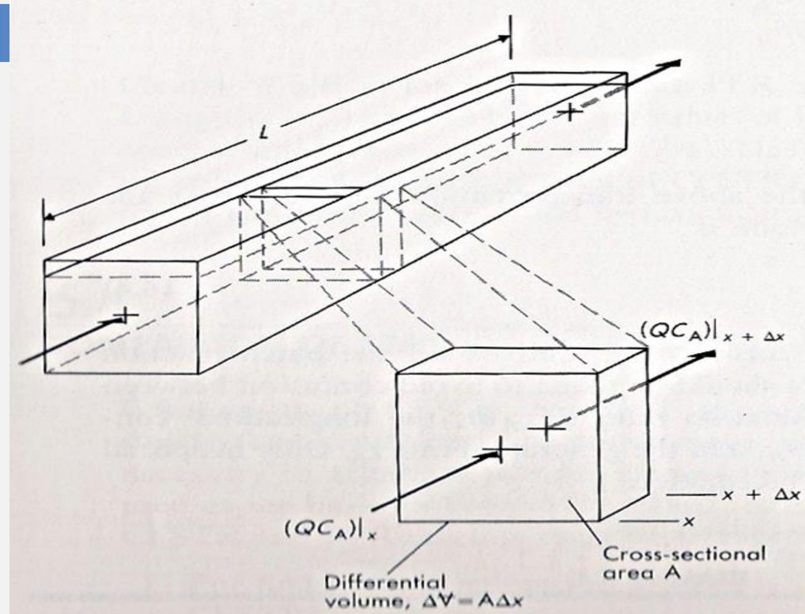
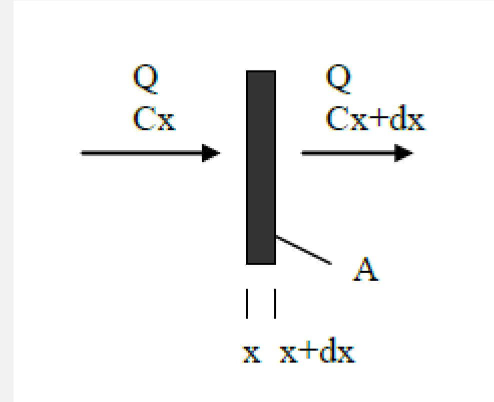


FIGURE 6.8
Definition sketch for the analysis of a PFR.



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

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

PFR
Unsteady-state conditions

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

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

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

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 $r_a=-kC_A$

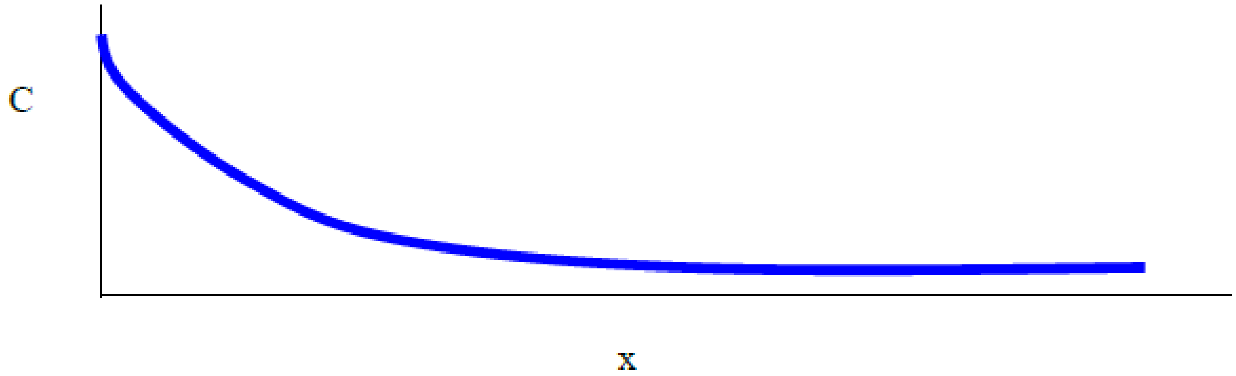
Determine the steady-state effluent concentration as a function of t_R .

Solution for Example 2 (Derivation of Effluent Cocnentration Equation)

$$\frac{dCx}{d\tau} = r_C$$

Comments

1. At steady-state, the concentration of a reactant at any single point along the PFR is constant at Cx. Overall a stable concentration profile is obtained at steady state, with the concentration varying in space as the reaction occurs along the flow path.



http://ceae.colorado.edu/~silverst/cven5534/IDEAL%20PLUG%20FLOW%20REACTOR.pdf

For a 1st order reaction, $r = -kC$, in a PFR at steady state

$$\frac{dC}{d\tau} = -kC$$

$$\int_{C_o}^{C_L} \frac{dC}{C} = \int_0^{\tau} -k\,d\tau$$

$$C_L = C_0 \exp(-k\tau)$$

http://ceae.colorado.edu/~silverst/cven5534/IDEAL%20PLUG%20FLOW%20REACTOR.pdf

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:

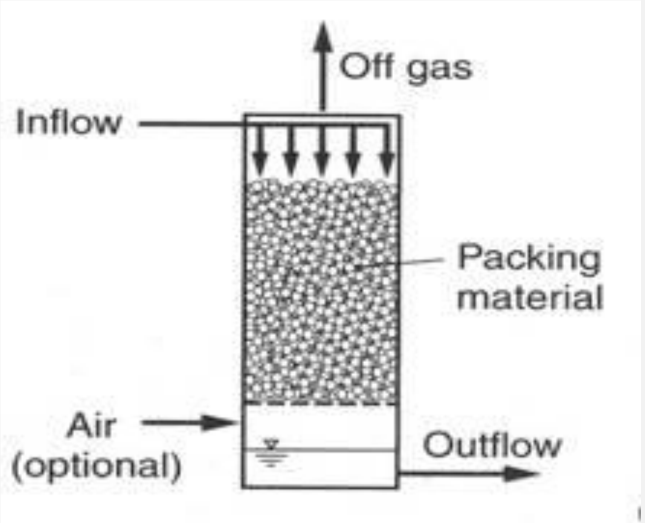
Determine the volume of a PFR to provide the same degree of treatment for the conditions given Example 1.

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)**

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)

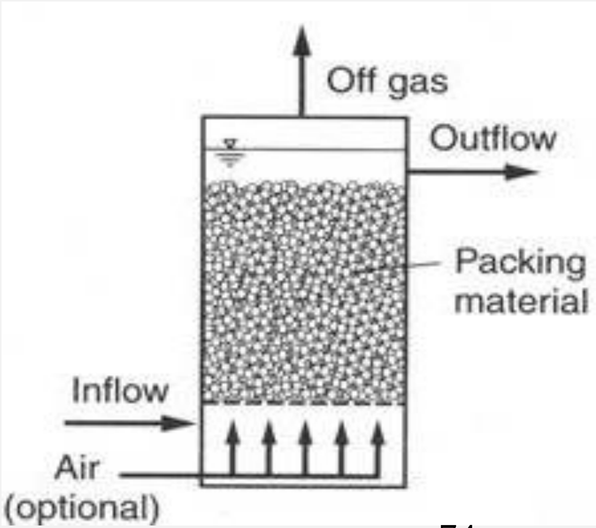
Application:

→ 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