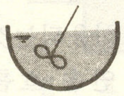
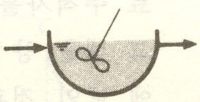
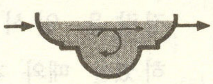
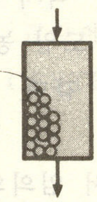
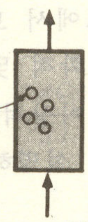
1. Reactors

- Reactors : Batch reactors vs. Continuous-flow reactors
- Completely stirred tank reactor (CSTR or CMF, Completely mixed flow reactor, CFSTR, Continuous flow stirred tank reactor) and Plug-flow reactor

반응기의 종류	그림	설명 또는 응용
회분 반응기 Batch		반응기의 도입 및 배출 흐름이 없다. 액상 내용물은 완전 혼합된다. 가령, 제 3 장에서 설명한 BOD 시험은 병으로 만든 회분 반응기에서 행한다.
플럭 흐름 반응기 (관형 흐름 반응기) Plug-flow		유체 입자는 도입 될 때와 마찬가지 순서로 탱크를 거쳐 흘러서 배출된다. 유체 입자는 이론적 체류 시간과 같은 시간 동안 탱크 안에 체류한다. 이러한 형태의 흐름은 길이 대 폭의 비가 큰 긴 탱크에서 볼 수 있는 것으로, 길이 방향에서의 분산은 최소이거나 없다.
연속 흐름 교반 탱크 반응기 (완전 혼합 반응기) CSTR		입자가 탱크 안에 도입되면 즉시 반응기 전체에서 분산되어 완전 혼합이 일어난다. 입자는 그 통계적 모집단에 비례하여 반응기에서 배출된다. 원형 또는 장방형 탱크에서 내용물을 균일하게 연속적으로 재분산시키면 완전 혼합을 이룰 수 있다.
임의 흐름 반응기 Arbitrary-flow		플럭 흐름과 완전 혼합 사이의 임의의 부분 혼합이 이루어지는 흐름을 임의 흐름이라 한다.
충전층 반응기 Packed-bed		충전층 반응기는 자갈, 슬랙, 도자기, 플라스틱과 같은 충전 매체를 채운 것이다. 흐름이 완전히 차게 하기도 하고(혐기성 여상), 간헐적으로 공급하기도 한다(살수 여상).
유동층 반응기 Fluidized-bed		유동층 반응기는 충전층 반응기와 여러 면에서 비슷하나, 이때는 충전 매체가 유체(공기 또는 물)의 상향 흐름에 의하여 층 전체에 팽창되게 한다. 충전 공극율은 유량을 조절하여 변화시킬 수 있다.

1.1 Introduction on Reactor Models

Batch reactor

- no flow in or out (no transport across the boundary of the reactor)
- Contents are mixed.
- may contain a single or multiple fluids (e.g., air and water)
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Completely stirred tank reactor

- Generally constant flow in and out
- Contents are thoroughly mixed (Perfect mixing assumption).
- Concentration of a species in the effluent is equal to its concentration throughout the reactor.
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Plug-flow reactor

- A tube through which fluid flows
- Assumptions: (1) The tube has constant cross-section at all axial positions, (2) the fluid velocity is uniform over the cross-section of the tube, and (3) no mixing in the axial direction of the tube (mass transport occurs only by advection).
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(1) and (2) are the most important key concepts for the reactor modeling.

1.2 Reactor Material Balances

Material balance equation follows this general form

Accumulation rate = Inflow rate – Outflow rate ± Net transformation rate

Net transformation rate : gain "+" and loss "-"

Inflow rate =

Outflow rate =

Accumulation rate =

where Q_{in} = flow rates of fluid in [L^3/T];

Q_{out} = flow rate of fluid out [L^3/T];

C_{in} = concentration of species in the inflow [M/L^3] or [moles/L^3];

C_{out} = concentration of the species in the outflow [M/L^3] or [moles/L^3];

C = concentration of the species [M/L^3] or [moles/L^3];

V = fluid volume [L^3]; and

t = elapsed time [T].

For general chemical reactions,

Net transformation rate =

where r = net rate of degradation of species concentration due to the reaction [M/T,L^3] or [moles/T,L^3].

For examples,

For flux across fluid interface,

Net transformation rate =

where J_{gl} = the species flux across the interface area [M/L^2] or [moles/L^2]; and

A = interface area [L^2].

Residence time, θ

Mean residence time of fluid molecule (hydraulic retention time in the water-based system)

Sometimes, more than one material balance equation is needed to describe a system.

1.3 Reactor Models

Batch Reactor

$$\frac{d(C \cdot V)}{dt} = \text{net transformation rate} = r \cdot V$$

$$\frac{dC}{dt} = r \quad \text{or} \quad \frac{d(C \cdot V)}{dt} = J \cdot A$$

EXAMPLE 5.A.2 ***Species Decay in a Batch Reactor as a Function of Reaction Order***

A species is placed in a batch reactor, where it decays by either a zeroth-, first-, or second-order reaction. Derive equations to describe the change in species concentration and characteristic times in each case. Plot the results.

<u>CSTR</u>

$$\frac{d(C \cdot V)}{dt} = Q \cdot C_{in} - Q \cdot C + r \cdot V$$

Since V = constant

$$\frac{dC}{dt} = \frac{1}{\theta} \cdot (C_{in} - C) + r$$

where θ = V/Q

If there is no reaction occurred in the reactor (just

Under steady state conditions (dC/ct = 0), a time dependent solution, C(t) is not required. For example, a zero order reaction

PFR

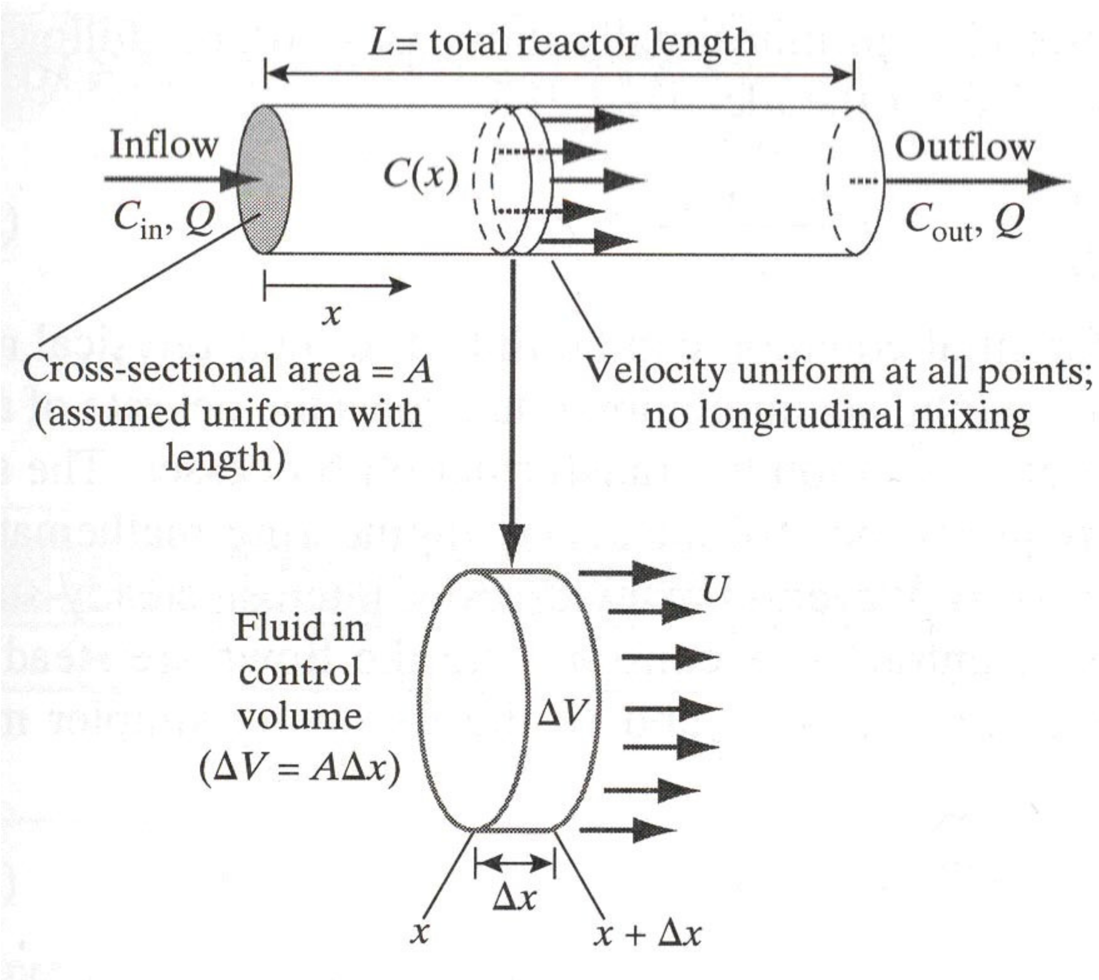

Figure 5.A.12 Schematic of an idealized plug-flow reactor and the control volume used for writing a material balance

Comparison between CSTR and PFR

EXAMPLE 5.A.1 ***Contrasting CMFR and PFR Model Behavior (continued)***

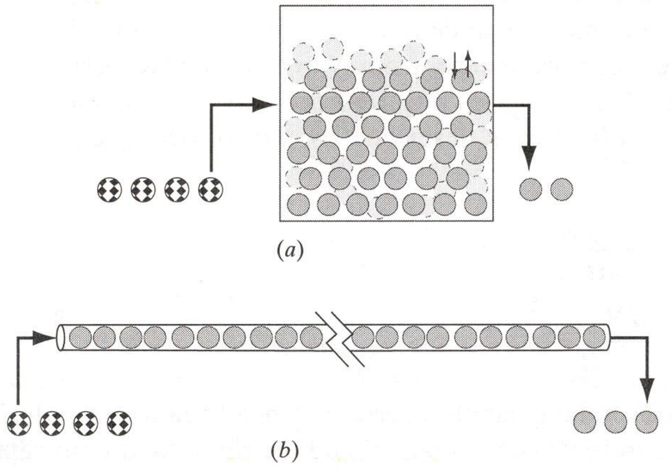

Figure 5.A.2 System illustrating the fluid flow characteristics of two reactor models: (*a*) a CMFR and (*b*) a PFR.

How will the total number of gray and spotted marbles in the two reactors change over time?

EXAMPLE 5.A.10 ***Comparing CMFR and PFR Performance***

Reactor performance is often characterized by calculating the ratio of the outlet concentration to the inlet concentration under steady-state conditions. Given fixed mean residence times, Θ, compare reactor performance for a CMFR and a PFR for contaminants that undergo zeroth-order, first-order, and second-order decay reactions.

SOLUTION Each of the required results has been calculated in Examples 5.A.5 and 5.A.9. The results are summarized in Table 5.A.1 and Figure 5.A.16.

For the case of a zeroth-order reaction, the reactor configuration does not affect performance: The CMFR and the PFR yield the same results. For all positive reaction orders, though, greater conversion is obtained in a PFR than in a CMFR. The difference in performance is negligible if the overall conversion is small ($C_{out}/C_{in} \sim 1$), but the difference becomes progressively greater as conversion increases ($C_{out}/C_{in} \rightarrow 0$).

Table 5.A.1 Comparison of the Steady-State Performance of CMFRs and PFRs

		C_{out}/C_{in}	
Reaction order	r	CMFR	PFR
Zeroth[a]	$-k_0$	$1 - \dfrac{k_0\Theta}{C_{in}}$	$1 - \dfrac{k_0\Theta}{C_{in}}$
First	$-k_1C$	$\dfrac{1}{1 + k_1\Theta}$	$\exp(-k_1\Theta)$
Second	$-2k_2C^2$	$\dfrac{(8k_2\Theta C_{in} + 1)^{1/2} - 1}{4k_2\Theta C_{in}}$	$\dfrac{1}{1 + 2k_2\Theta C_{in}}$

[a]Expressions are valid provided that $k_0\Theta \leq C_{in}$; otherwise, $C_{out} = 0$.

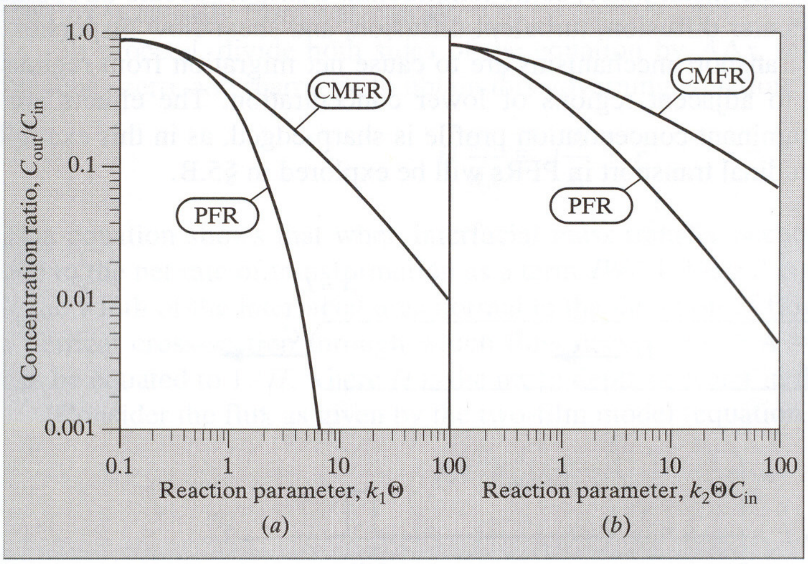

Figure 5.A.16 Steady-state reactor performance, comparing the outlet to inlet concentration ratio for a CMFR and a PFR for a species decaying by a homogeneous reaction of (*a*) first order or (*b*) second order.

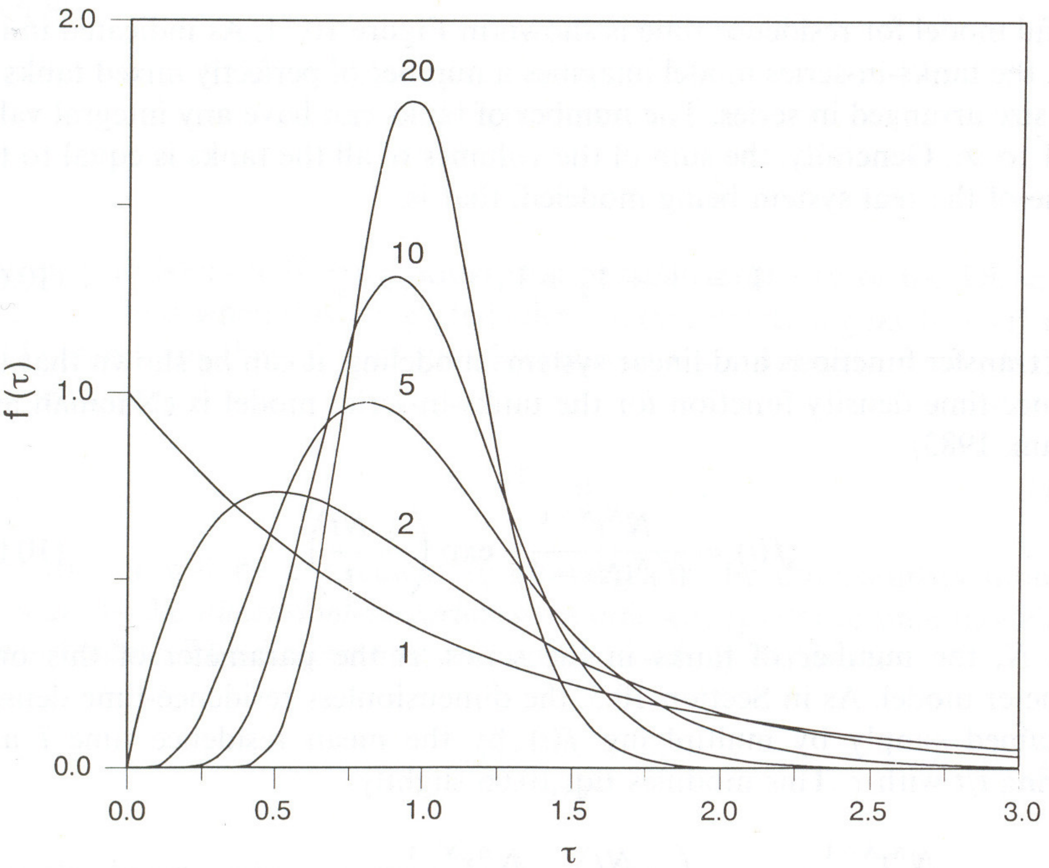

Figure 10.12. Dimensionless residence-time density for tanks-in-series model. The numbers next to the curves are the number of tanks in the series.

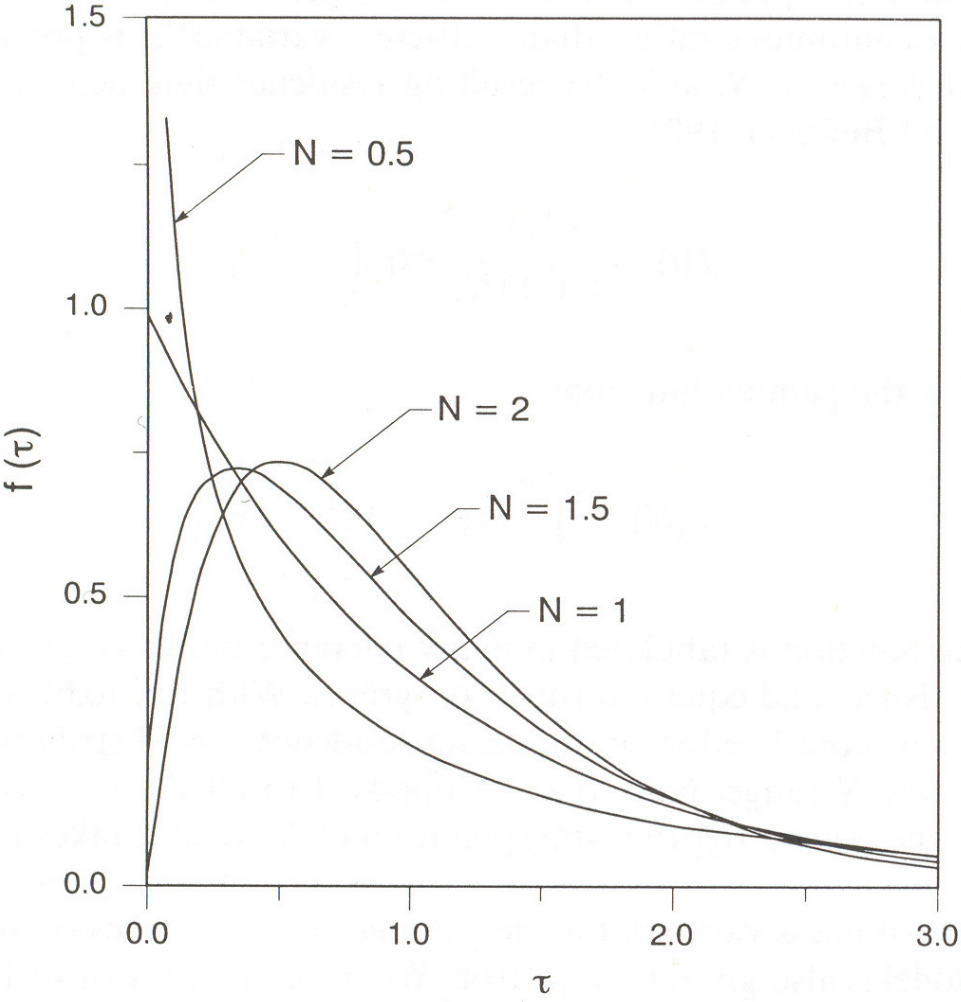

Figure 10.13. Gamma-function extension to the tanks-in-series model.