BAE 820 Physical Principles of Environmental Systems

Type of reactors

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Ideal reactors

- A reactor is an apparatus in which chemical, biological, and physical processes (reactions) proceed intentionally, purposefully, and in a controlled manner.
- Ideal reactors are model systems for which the transport and mixing processes are exactly defined. They serve as abstract analogs of effective reactors. Their properties are chosen such that they can easily be described in mathematical terms.
- Whereas real reactors deviate in their behavior from the ideal reactors, they can frequently be described sufficiently accurately by ideal reactors.

Mass balance for a reactor

Input = Output +Reaction loss + Accumulation

$$N_{Af} = N_{Ae} + \int_V (-r_A)dV + \frac{dN_A}{dt}$$

In which

- N_{Af} is feed rate of solute A;
- N_{Ae} is effluent rate from the system;
- $\int_V (-r_A)dV$ is integral of reaction loss over the total volume of the system.

The equation is the basis for the development of reactor design. Specifically, we can determine either the time or the reactor volume required for a specific rate of conversion of the reactants to products.

Batch and continuous systems

- Batch reactor
  - A fixed volume (mass) of material is treated for a specified length of time. Periodically reactants can be added and products can be removed from the system.
  - Typical batch reactors are test tubes in the laboratory (frequently closed systems).
- Continuous flow reactor
  - Material is introduced and removed from the reactor at specific rates on continuous basis.

Batch reactor

- For a batch reactor, $N_{Af} = N_{Ae} = 0$, therefore,

$$-\frac{dN_A}{dt} = \int_V (-r_A)dV$$

- If the reactor is perfectly mixed, the rate of reaction is the same throughout,

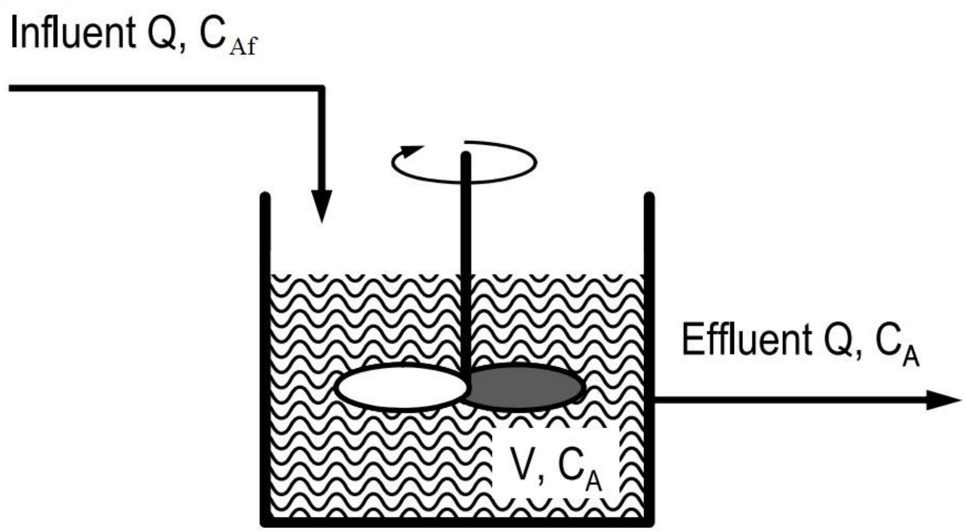
$$-r_A = -\frac{1}{V}\frac{dN_A}{dt} = -\frac{1}{V}\frac{d(C_A V)}{dt} = -\frac{dC_A}{dt} - C_A\frac{d\ln V}{dt}$$

- With constant volume,

$$-r_A = -\frac{dC_A}{dt}$$

The Continuous-Flow Stirred Tank Reactor (CSTR)

- Analogous to the batch reactor the CSTR consists of an ideally mixed volume.
  - No concentration gradients inside the reactor.
  - The feed is instantaneously mixed in the reactor.
  - The effluent concentrations is the same as the concentrations everywhere in the reactor at all times.



Mass balance for CSTR

Assuming steady state and the rate of the reaction is uniform throughout the reactor.

$$\mathrm{N_{Af}} = \mathrm{N_{Ae}} + \int_V (-\mathrm{r_A})dV + \frac{dN_A}{dt} = \mathrm{N_{Ae}} + \mathrm{r_A}V$$

Thus, the volume of CSTR

$$\mathrm{V} = \frac{\mathrm{N_{Af}} - \mathrm{N_{Ae}}}{-\mathrm{r_A}} = \frac{\mathrm{Q_f C_{Af}} - \mathrm{Q_e C_A}}{-\mathrm{r_A}}$$

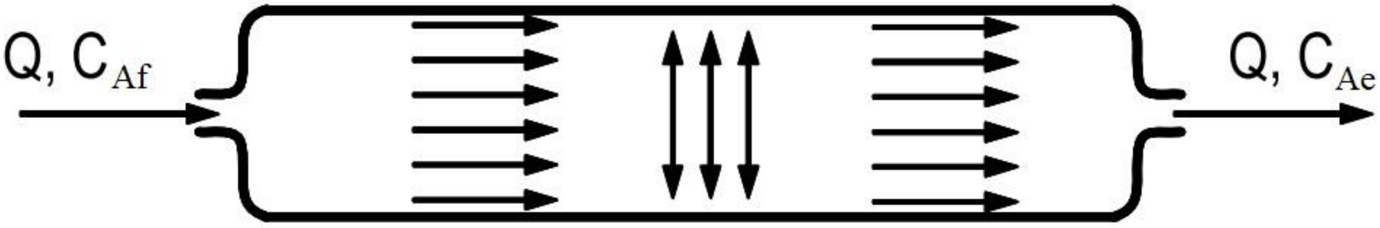
For first order reactions (with $r_A = -kC_A$), when $Q_f = Q_e = Q$

$$\frac{C_A}{C_{Af}} = \frac{1}{1+k(\frac{V}{Q})} \qquad \mathrm{V} = \frac{\mathrm{Q_f C_{Af}} - \mathrm{Q_e C_A}}{-\mathrm{kC_A}} = \frac{Q}{k}\frac{x}{(1-x)}$$

Where V/Q has unit of time , and is called the mean detention time or residence time of the reactor t_d. $x = 1 - C_A/C_{Af}$ is the conversion.

The Plug-Flow Reactor (PFR)

- In PFR, the reactants are continuously consumed as they flow along the length of the reactor and an axial concentration gradient develops.
  - Complete mixing only transverse to the direction of flow.
  - The reaction rate is a function of the axial direction.
  - Amount of influent and effluent are equal.



Mass balance for PFR

Assuming steady state, and the rate r_A is constant within a small volume element ΔV.

$$N_A\,(z+\Delta z) - N_A\,(z) = -r_A \Delta V$$

$$dN_A = -r_A\, dV = -r_A\, A_c dz$$

In which A_c is the cross-sectional area.
For first order reactions (with $r_A = -kC_A$)

$$Q\frac{dC_A}{dV} = -kC_A$$

$$\frac{C_A}{C_{Af}} = \exp(-kV/Q), \qquad V = \frac{Q}{k}\ln\frac{C_{Af}}{C_A} = \frac{Q}{k}\ln\frac{1}{1-x}$$

If 50% 0f C_{Af} has to be converted into products, the v=0.693Q/k is the reactor volume required.

Comparison of reactor volume for a CSTR and a PFR

$$\mathrm{V_{CSTR}} = \frac{Q}{k}\frac{x}{(1-x)}$$

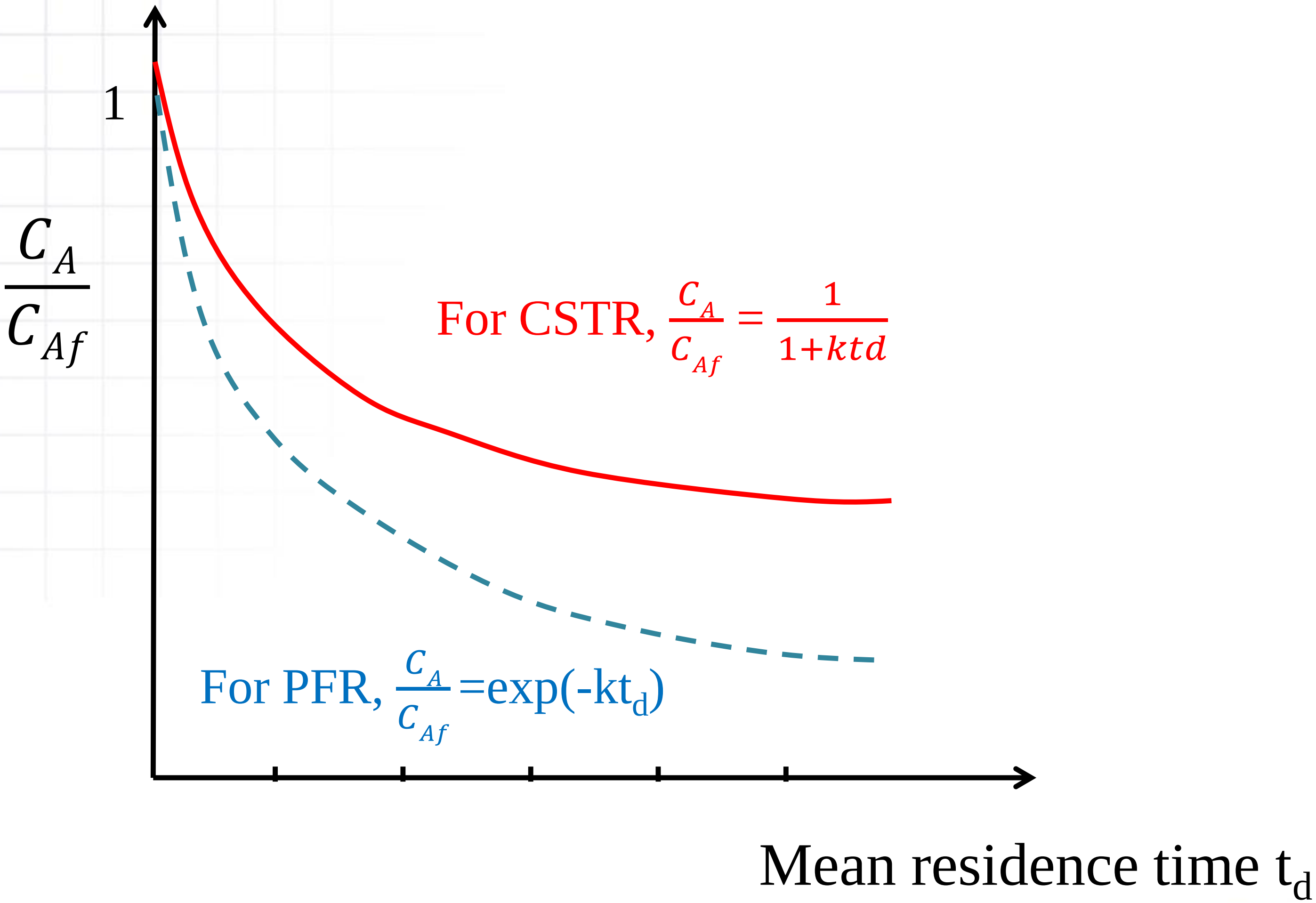
$$\mathrm{V_{PFR}} = \frac{Q}{k}\ln\frac{1}{1-x}$$

$$\frac{\mathrm{V_{CSTR}}}{\mathrm{V_{PFR}}} = \frac{x}{(1-x)\ln\frac{1}{1-x}}$$

If the desired conversion is x_A=0.6, then the ratio of volume is 1.63. Thus a 63% larger volume of CSTR than that of a PFR is required to achieve a 60% conversion.

An ideal PFR can achieve the same conversion as that of a CSTR but using a much smaller volume of the reactor.

Comparison of concentrations in a CSTR and a PFR



General design equations fro CSTR and PFR

For CSTR,

$$V = \frac{N_{Af} - N_{Ae}}{-r_A} = \frac{N_{Af} x}{-r_A}$$

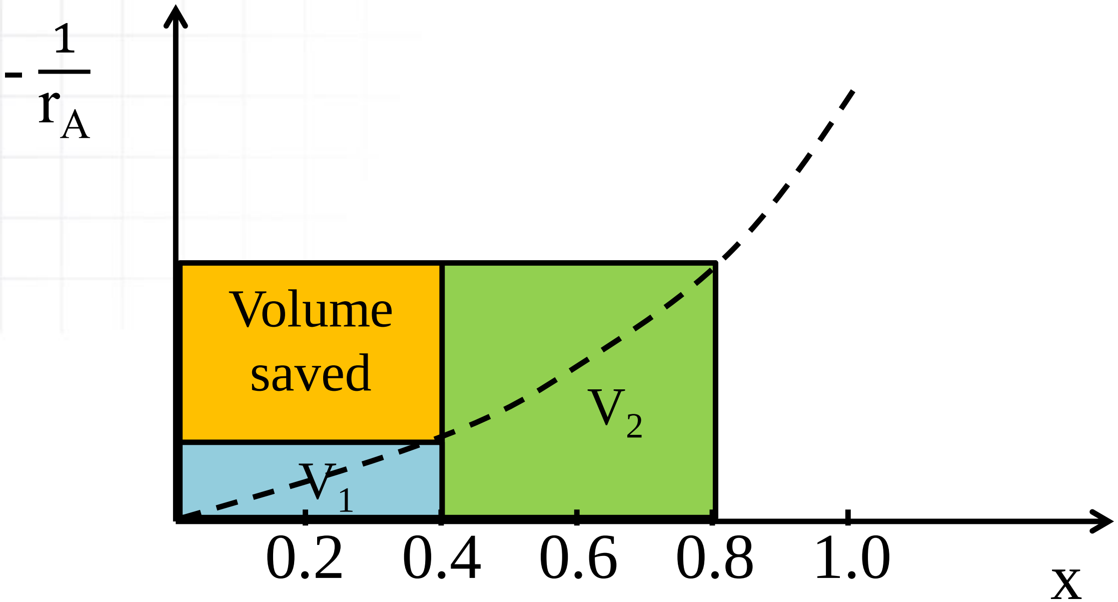
For PFR,

$$dV = -\frac{1}{r_A} dN_A, \qquad V = N_{Af} \int \left(-\frac{1}{r_A}\right) dx$$

The rate of disappearance of A, $-r_A$, is a function of concentrations of the reactants, and thus can be expressed as a function of the conversion x.

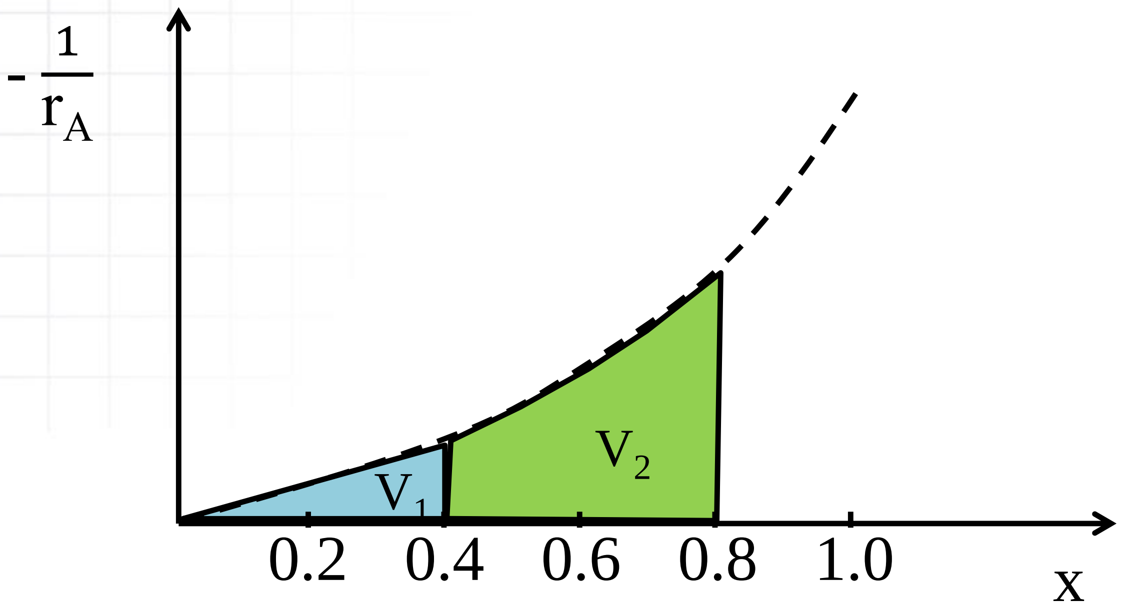
Two CSTR in series

Consider two CSTR in series, if 40% conversion is achieved in the first reactor, and the second reactor accomplished 80% overall conversion of reactant A entering reactor 1. What are the total reactor volume saved comparing with using only one CSTR?



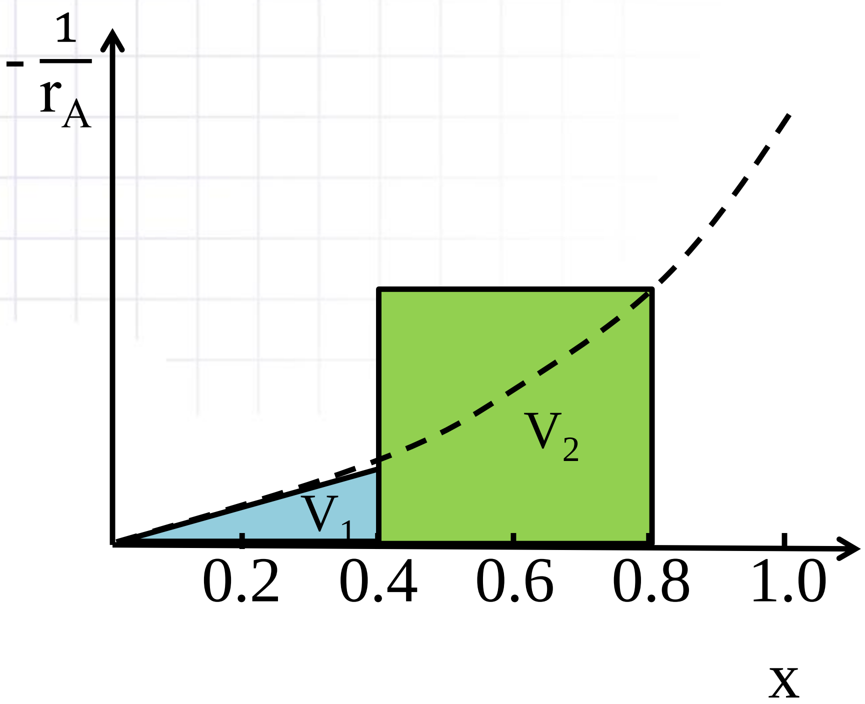
Two PFR in series

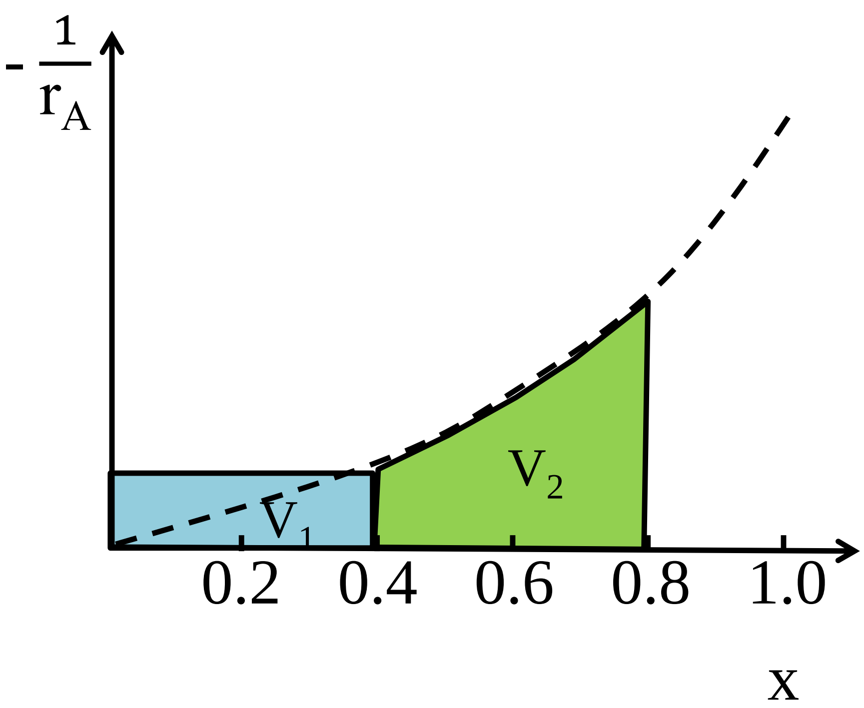
Can we save any volume by using two PFR in series?



One CSTR and one PFR in series

How to arrange to minimize total reactor volume? It depends on shape of the curve and the intermediate concentration.





Example: CSTR model for a surface impoundment

Surface impoundment is often used for treatment of wastewater, and it can be considered as a CSTR with complete mixing within the aqueous phase. The average biodegradation rate is 0.05 h^{-1}; the rate constant for settling of biomass is estimated to be 2.2×10^{-6} h^{-1}; the rate constant for volatilization is 2×10^{-5} h^{-1}. Estimate the reduction efficiency when the mean detention time is 1 days.

Solution:

The overall rate constant k=0.05 h^{-1}.

Assuming it is a CSTR, $\frac{C_A}{C_{Af}} = \frac{1}{1+kt_d} = \frac{1}{1+0.05\times24} = 0.45$.

The reduction efficiency is around 55%.

Example: FPR model for a combustion incinerator

Consider a waste containing benzene being incinerated using an airstream at a velocity of 5 m/s. A typical length of the incinerator chamber is 10 m. Typical inlet temperature is 900ºC and outlet temperature is 800ºC. The average rate constant is estimated to be around 4 s^{-1}. Estimate the reduction efficiency

Solution:

The detention time t_d=10/5=2 s.

Assuming it is a PFR, $\frac{C_A}{C_{Af}}$ =exp(-kt_d) =exp(-4×2)=0.0003

The reduction efficiency is around 99.97%.

CSTR or PFR?

- For many degradation reactions PFR result in better performance than the CSTR (back mixed). However, for many processes, mixing is a central element of the process, e.g., with aeration (gas exchange), generation of turbulence for the acceleration of flocculation and precipitation. Mixing contradicts the characteristics of the PFR.
- Therefore, intermediate solutions with defined mixed ranges (e.g., a cascade of CSTR, or PFR with turbulence) are used. These solutions combine the advantages of mixing with the extra performance offered by PFR.
- Also recirculation (i.e., return of sludge and internal recirculation in the activated sludge process) leads to back mixing and brings the behavior and performance of a PFR closer to those of a mixed system.
- Back mixed systems are a necessity for autocatalytic processes. Back mixing brings the catalyst from where it is produced back to the influent of the reactor, where it is most required. Many microbial processes are autocatalytic, thus completely mixed or back mixed reactors or systems with recirculation flow are typical for biological treatment systems.

Residence time distribution

- The residence time distribution of a chemical reactor is a probability distribution function that describes the amount of time a fluid element could spend inside the reactor. Since each fluid element must at some time leave the reactor, the integral under the residence time distribution is unity.
- The residence time distribution is often used to characterize the mixing and the internal transport processes in a reactor. The comparison between the behavior of real reactors and their ideal models is useful for troubleshooting existing reactors, as well as in designing future reactors.

Residence time distribution of CSTR

- At time t_0 we add to the influent of the CSTR the quantity of N of a tracer material, which does not have a background concentration and which is immediately distributed over the entire reactor. The probability that the tracer material left the reactor after the time t is:

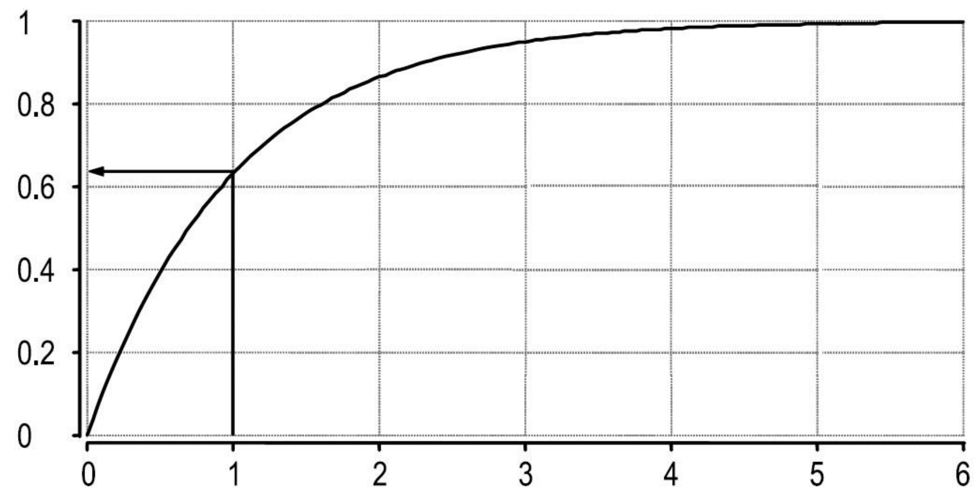
$F(t) = (N-C_tV)/N = 1-C_t/C_0$

$VdC_t/dt = -QC_t,$

$C_t = C_0\exp(-\frac{Q}{V}t)$

$F(t) = 1-\exp(-\frac{Q}{V}t) = 1-\exp(-\frac{t}{t_d})$

Cumulative frequency of residence time



$t=t_d$

Residence time in the unit of t_d

Example

- A CSTR in the steady state has an influent of 100 m^3 /h. What size is required such that 90% of the water remain in the reactor for more than 1 hour?
- Solution:

$$F(t) = 1-\exp(-\frac{t}{t_d}) = 0.1$$

$$\frac{t}{t_d} = -\ln(1-0.1) = 0.105$$

$$t_d = t/0.105 = 1/0.105 = 9.5 \text{ h}$$

$$V = Q\, t_d = 100 \times 9.5 = 950 \text{ m}^3$$

Nonideal reactors

- The reactors we have discussed thus far assumed ideal flow patterns,
  - As one extreme, no back mixing in PFR;
  - As the other extreme, complete mixing in CSTR.
- Natural environmental reactors fall somewhere between the two ideal reactors. The deviations are caused by fluid channeling, recycling, or stagnation points in the reactor.
- Two models have been used to explain nonideal flows in reactors.
  - Dispersion model: introduce a axial dispersion coefficient D_{ax}. When D_{ax}=0, we have PFR; and as $D_{ax} \rightarrow \infty$, we have CSTR.
  - Tanks-in-series model: model dispersion by using a series of CSTR.