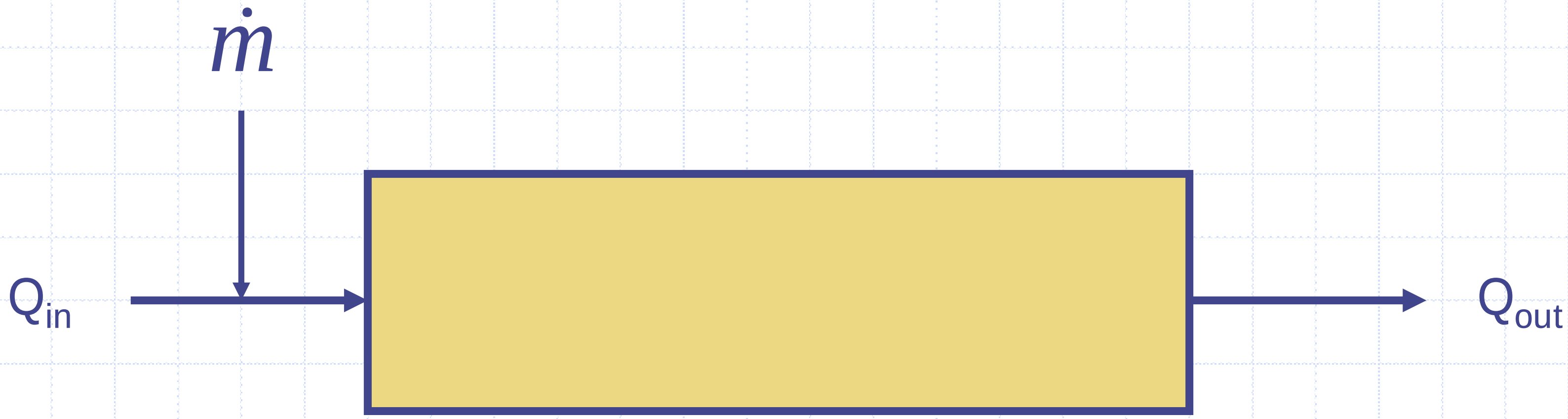
# 5 Reactor Vessels

- Motivation
- Fully-mixed reactors
- Single & multiple tanks with pulse, step and continuous inputs
- Dispersed flow reactors with pulse and continuous inputs
- Examples

# Introduction




A tank, reservoir, pond or reactor with **controlled** in/out flow

If $Q_{in} = Q_{out} = Q$ then $t_{res} = \tau = t^* = V/Q$

Used interchangeably

Generally more interest in what comes out than what's inside reactor

# Applications

- Natural ponds and reservoirs
- Engineered systems (settling basins, constructed wetlands, combustion facilities, chemical reactors, thermo-cyclers...)
- Laboratory set-ups: simple configurations with known mixing so you can predict/control the fate processes

# Wastewater Treatment Plants

Primary settling

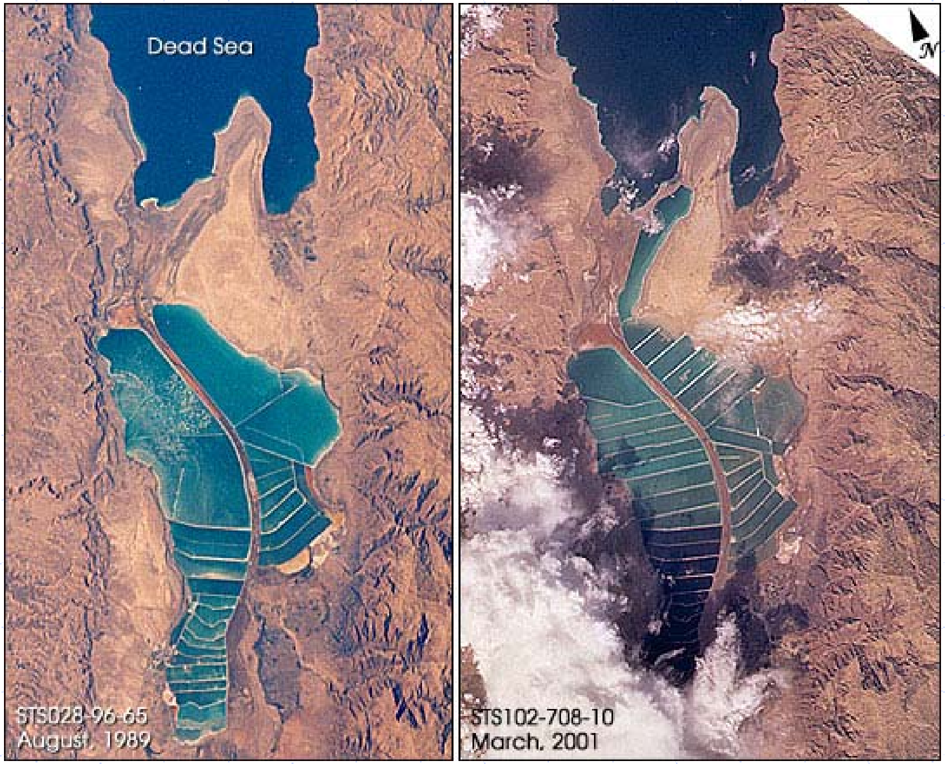
Secondary settling

Waste stabilization

# Constructed Wetlands

# Potash Evaporation Ponds

Southern shoreline Dead Sea

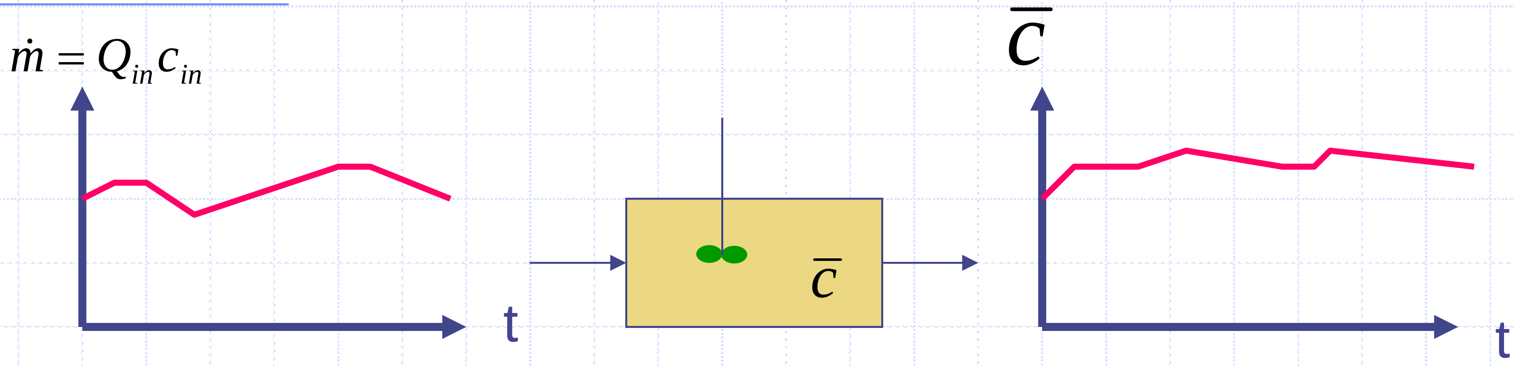


# Classification

- Flow: continuous flow or batch
- Spatial structure: well-mixed or 1-, 2-, 3-D
- Loading: continuous, intermittent (step) or instantaneous (pulse)
- Single reactor or reactors-in-series

Initially look at single continuously stirred tank reactor (CSTR)

# Well-mixed tank, arbitrary input



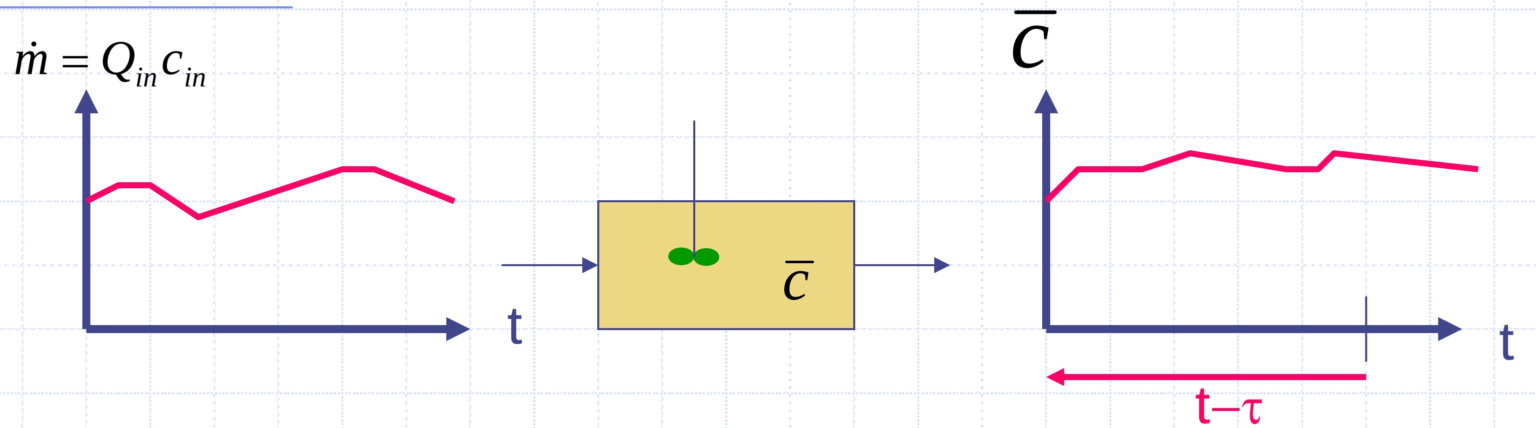

$$\frac{dV}{dt} = Q_{in}(t) - Q_{out}(t)$$

Conservation of volume

$$\frac{d(cV)}{dt} = c_{in}(t)Q_{in}(t) - c(t)Q_{out}(t) + r_i V$$

Conservation of mass

# Well-mixed tank




$$\frac{dc}{dt} = \frac{c_{in}(t) - c}{t^*} - kc$$

If $Q_{in} = Q_{out}$ = const, V = const; t* = V/Q; and $r_i$ = -kc

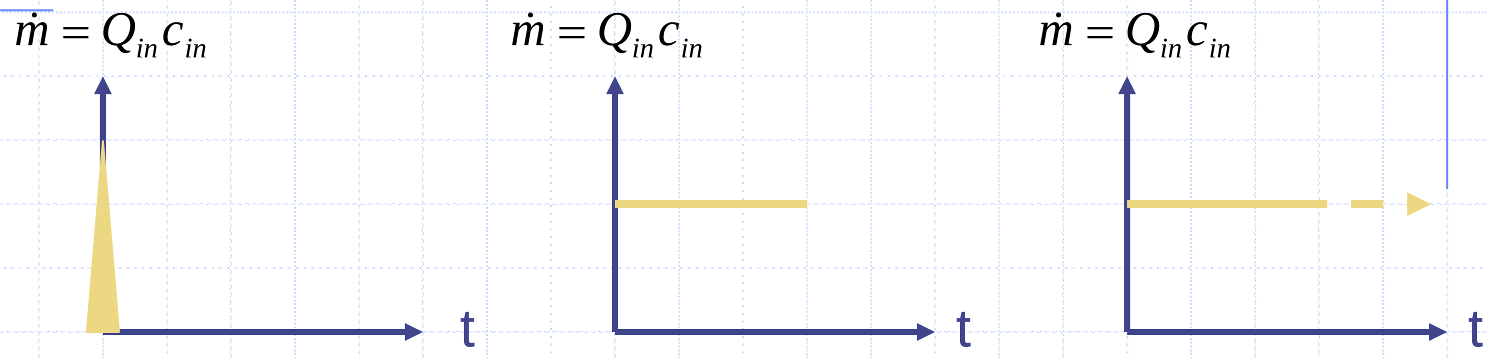
$$c(t) = c_o e^{-(t/t^* + kt)} + \int_0^{t/t^*} c_{in}(\tau) e^{-[(t-\tau)/t^* + k(t-\tau)]} d(\tau / t^*)$$

IC

Convolution integral (exponential filter that credits inputs w/ decreasing weight going backwards in time)

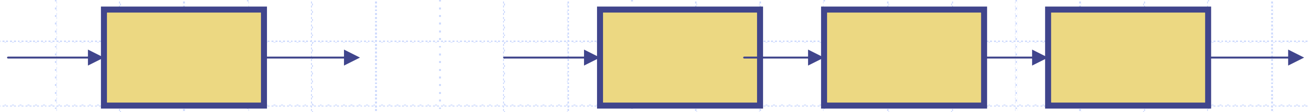
# Roadmap to solutions (3x2)

Inputs




Pulse | Step | Continuous

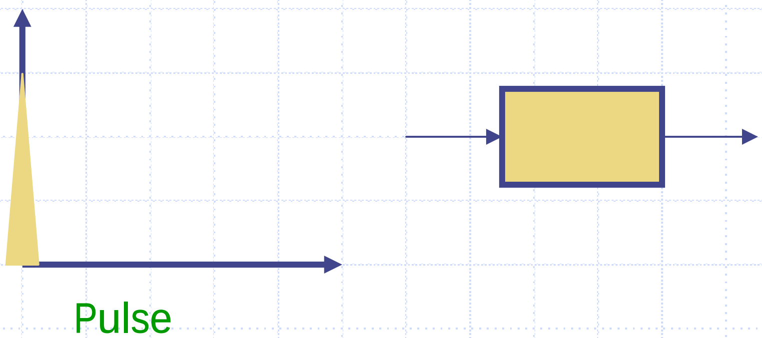
Reactors



Single | Multiple

# Pulse input to single tank

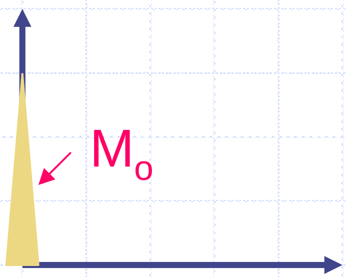
$$\dot{m} = Q_{in} c_{in}$$




- May have practical significance—e.g. instantaneous spill
- More commonly used as a diagnostic; Produces stronger gradients than other types of inputs

# Pulse input, single tank, cont'd

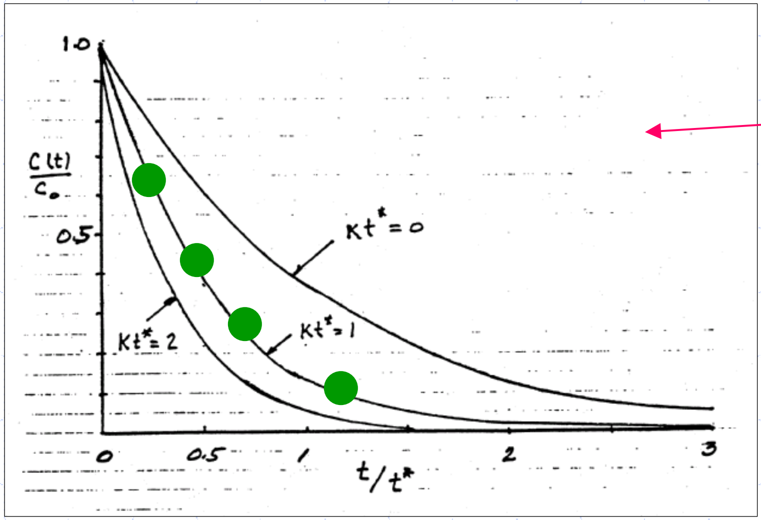
$$\dot{m} = Q_{in} c_{in}$$




Pulse

$$c(t) = \frac{M_o}{V} e^{-(t/t^* + kt)}$$

$c_o = M_o/V$ (not initial conc.)




$$\frac{c(t)}{c_o} = e^{-(t/t^* + kt)}$$

Know t* and $c_o$;

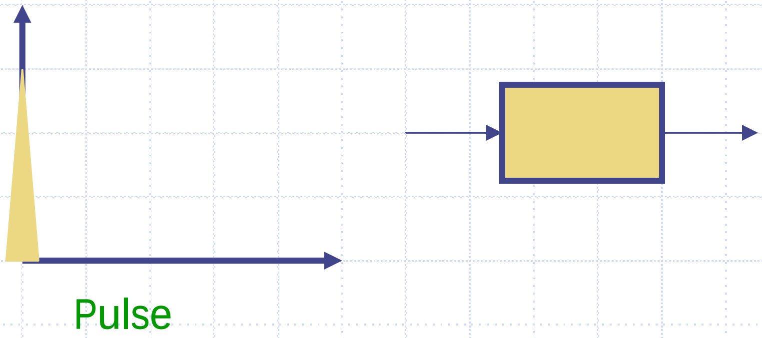
Plot $c/c_o$ vs t/t*

Determine kt* = > k

WE 5-2

# Pulse input, single tank, cont'd

$$\dot{m} = Q_{in} c_{in}$$




General case:

$$\frac{c(t)}{c_o} = e^{-(t/t^* + kt)}$$

Special cases:

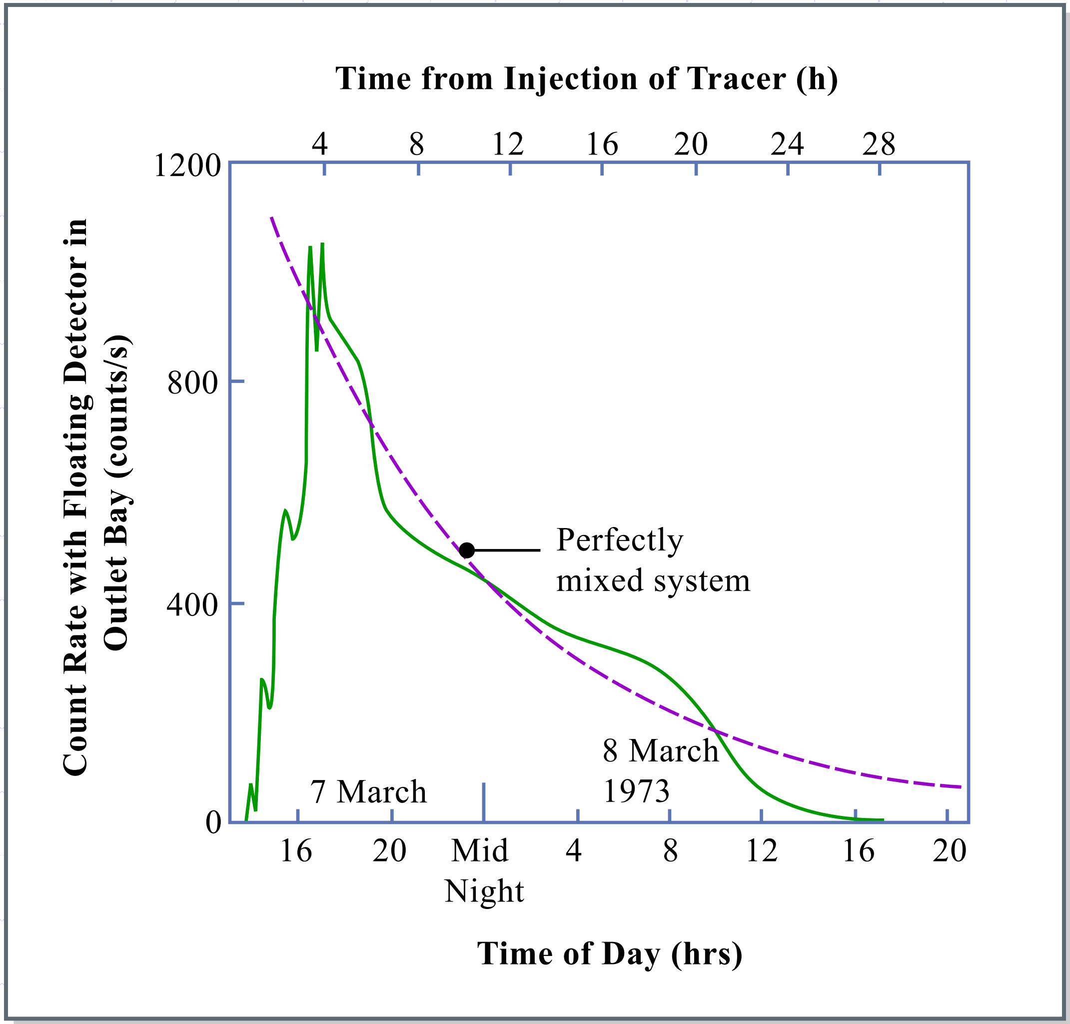
$$\frac{c(t)}{c_o} = e^{-kt}$$

No flow; batch reactor

$$\frac{c(t)}{c_o} = e^{-t/t^*} = e^{-tQ/V}$$

No loss; just flushing

# In practice never exactly well-mixed




White, (1974)

Figure by MIT OCW.

- Data versus theory tells how close to well mixed
- Ways to mix
  - Directed discharge and intake
  - Baffles
  - Stirrers
- May need to avoid over-mixing (benthic flux chambers)

# Benthic Flux Chambers

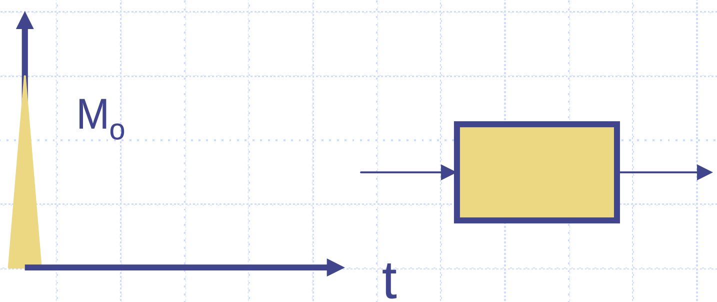
# Slight diversion: Residence time properties of reactor vessels

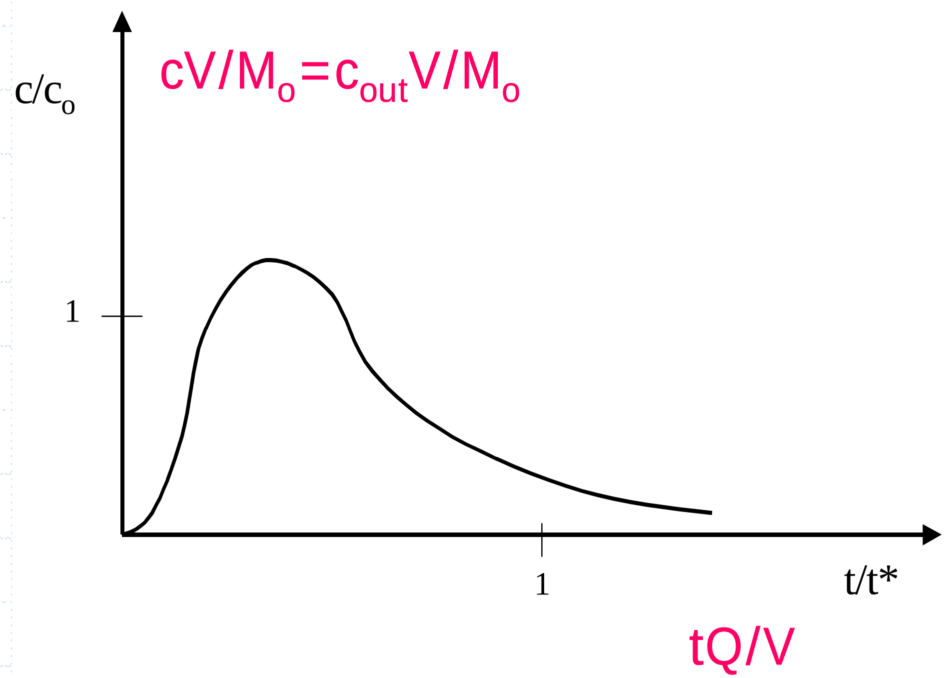
Not necessarily well-mixed

But known residence time

$C_o = M_o/V$ $t^* = V/Q$

$$\dot{m} = Q_{in} c_{in}$$

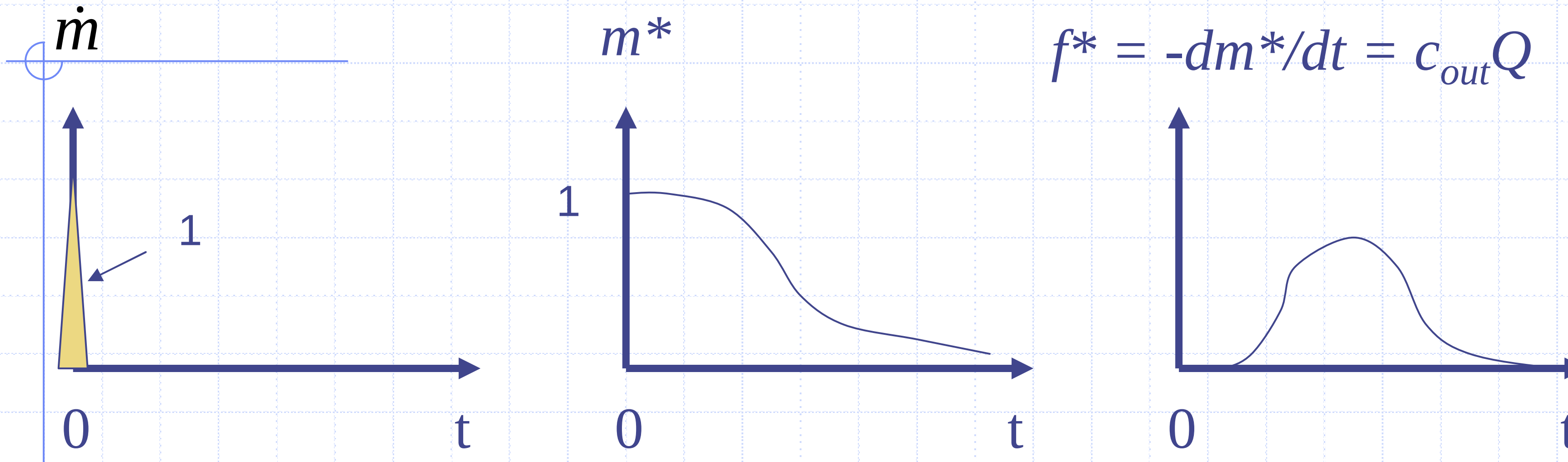



Residence time distribution

Unit impulse response

# Recall from Chapter 4




Rate of injection — Mass remaining in system — Mass leaving rate

$$t^* = V/Q$$

$$c_o = \frac{M_o}{V} = \frac{1}{V}$$

$$f^* = c_{out}Q = \frac{c_{out}}{c_o}\frac{Q}{V} = \frac{c_{out}}{c_o t^*}$$

$$\int_0^\infty f^* dt = 1 \Rightarrow \boxed{\int_0^\infty \frac{c_{out}}{c_o} d\left(\frac{t}{t^*}\right) = 1}$$

0th Moment

$$\int_0^\infty f^* t dt = t^* \quad or \quad \frac{1}{t^*}\int_0^\infty f^* t dt = 1$$

$$\Rightarrow \boxed{\int_0^\infty \frac{c_{out}}{c_o}\left(\frac{t}{t^*}\right) d\left(\frac{t}{t^*}\right) = 1}$$

1st Moment

# RTD, cont'd

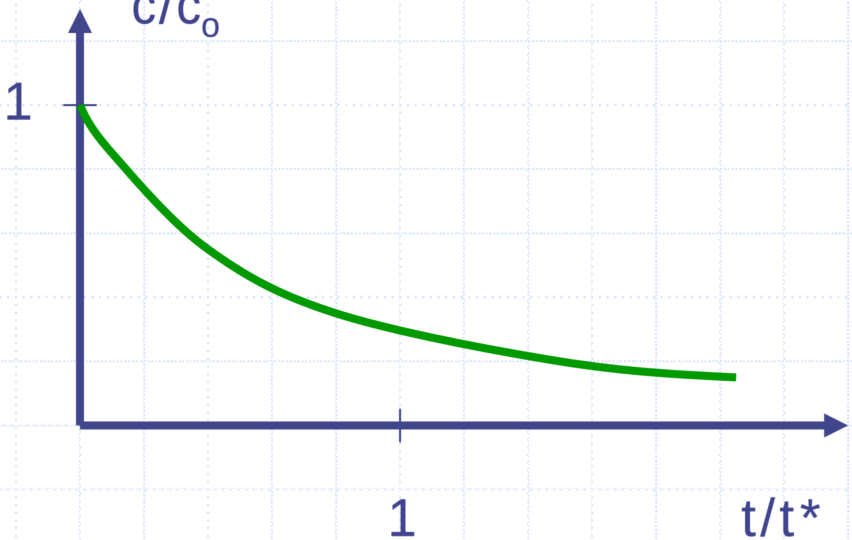
0th and 1st moments of normalized distribution ($c_{out}/c_o$ vs $t/t^*$) are both unity

For well mixed tank, k=0 (CSTR)

$$\frac{c_{out}}{c_o} = \frac{c}{c_o} = e^{-t/t^*}$$

$$\int_o^\infty e^{-t/t^*} d(t/t^*) = 1$$

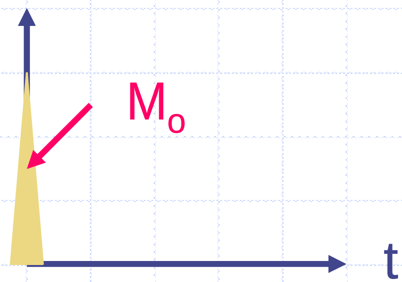
$$\int_o^\infty e^{-t/t^*} (t/t^*) d(t/t^*) = 1$$




Area under curve and center of mass are both one

# Pulse input to tanks-in-series

$$\dot{m} = Q_{in} c_{in}$$





$$\frac{dc_i}{dt} = \frac{c_{i-1} - c_i}{t^*} - kc_i$$

$$\frac{c}{c_o} = \frac{n^n}{(n-1)!}\left[\frac{t}{nt^*}\right]^{n-1} e^{-(t/t^* + kt)}$$

$C_o = M_o/nV$; $t^* = V/Q$ = res. time of each tank; total res time = $nt^*$

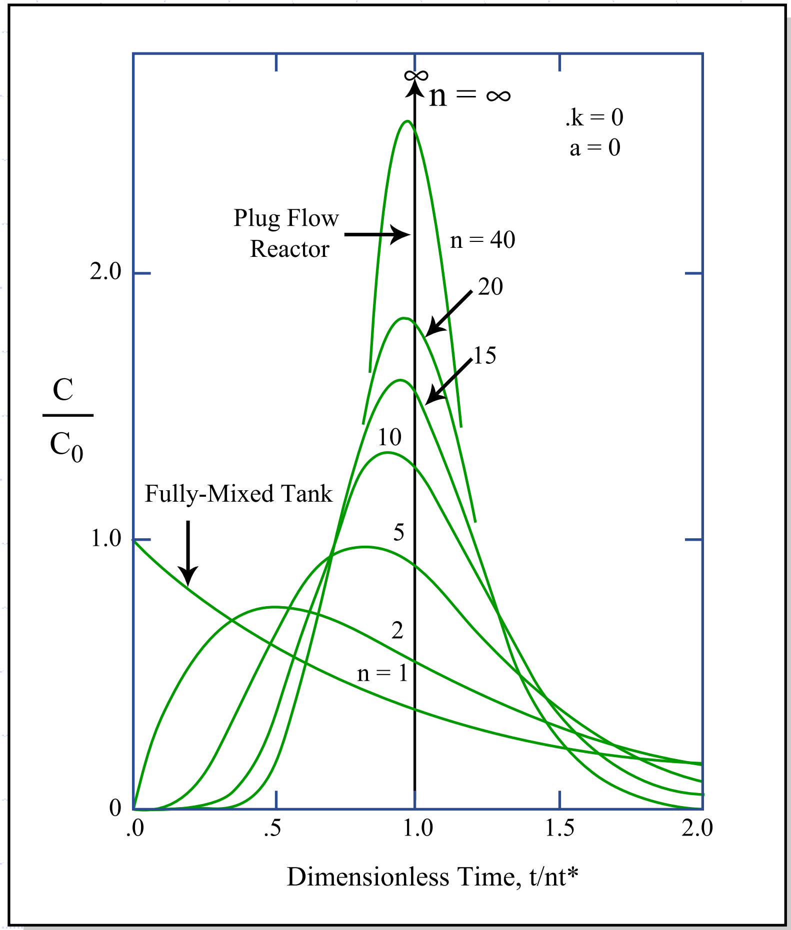



Figure by MIT OCW.

# Pulse input to tanks-in-series

Area under curve and center of mass are both one

$$\int_0^\infty \frac{c(t/nt^*)}{c_o} d\left(\frac{t}{nt^*}\right) = 1$$

$$\int_0^\infty \frac{c(t/nt^*)}{c_o} \left(\frac{t}{nt^*}\right) d\left(\frac{t}{nt^*}\right) = 1$$

Limits of plug flow and fully well-mixed

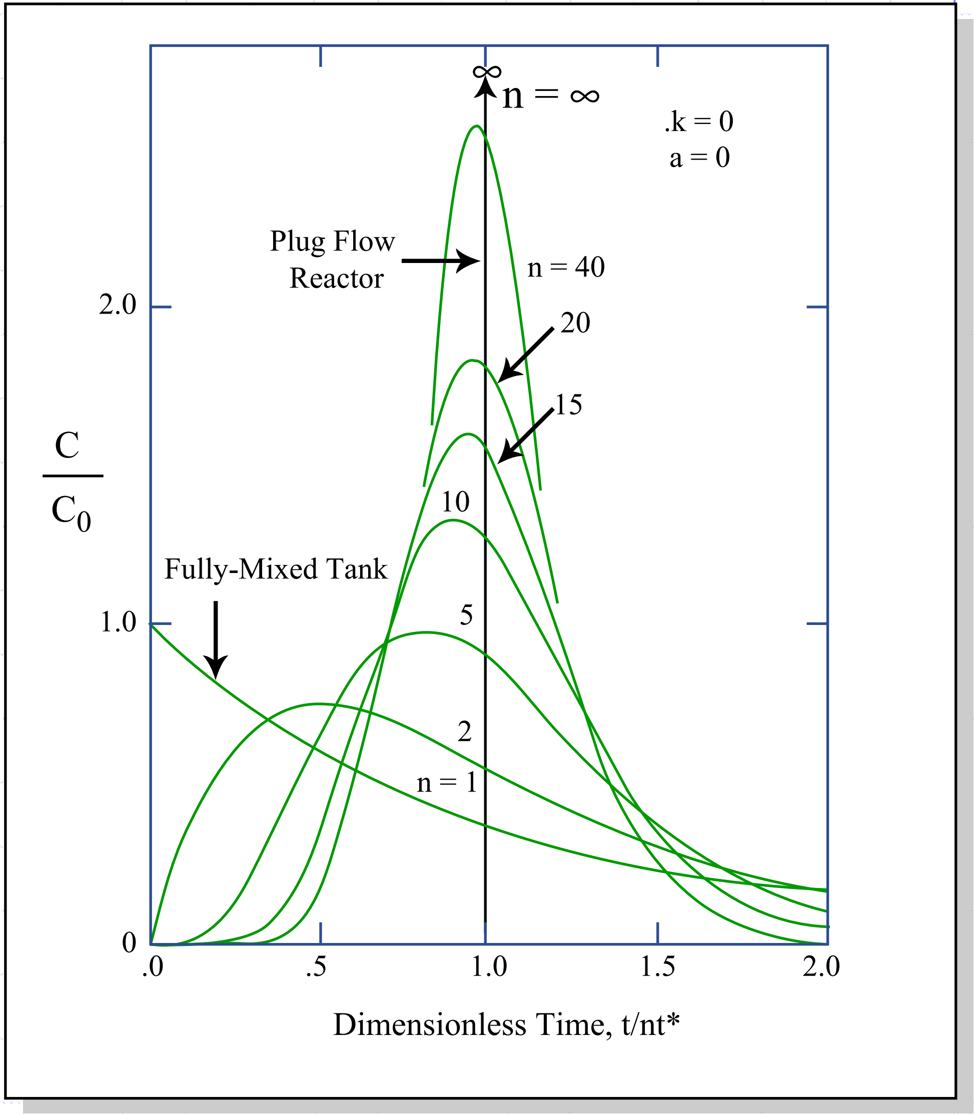



Figure by MIT OCW.

# Advantages of Plug Flow?

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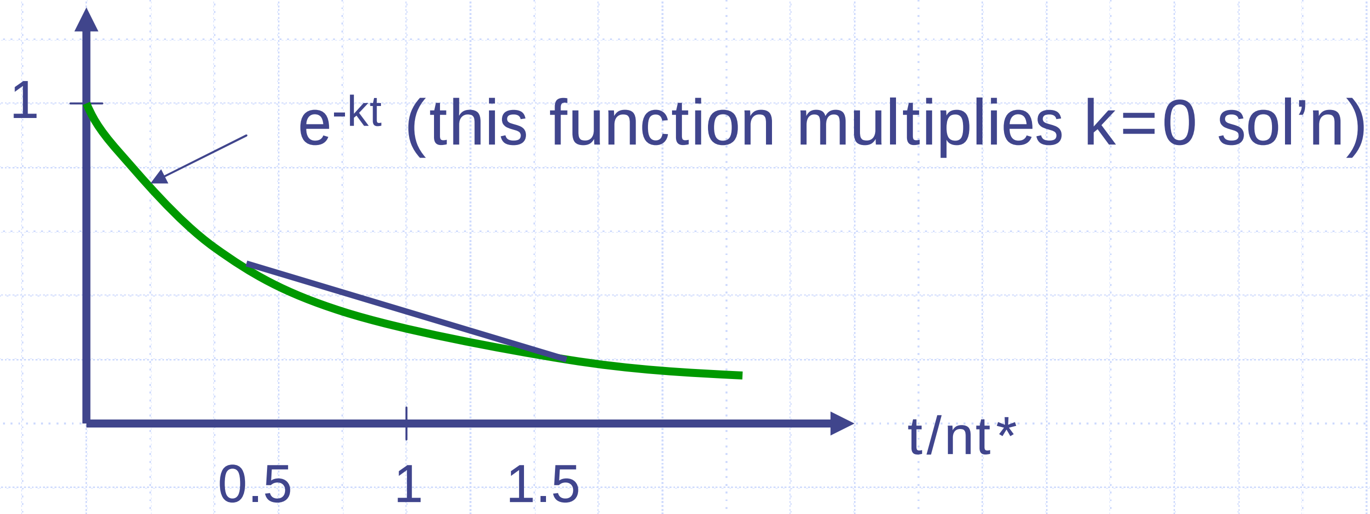
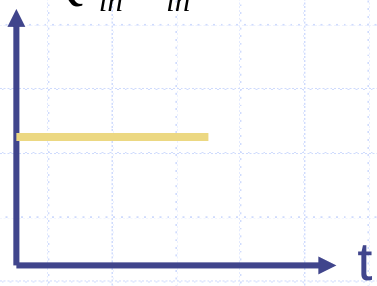



Everything "cooks" the same time. The mean residence time of a water parcel is always nt* (by definition) but under plug flow all parcels reside for nt*

This advantage obviously applies for continuous and step injections as well

# Step input, single and multiple

$$\dot{m} = Q_{in} c_{in}$$




Step

$$c(t) = c_o e^{-(t/t^*+kt)} + \frac{\bar{c}_{in}}{1+kt^*}\left[1-e^{-(t/t^*+kt)}\right]$$

$$\frac{c(t)}{c_{in}} = \frac{1}{(t^*\kappa)^n}\left[1-e^{-\kappa t}\left(1+\kappa t+\frac{(\kappa t)^2}{2}+\ldots+\frac{(\kappa t)^{n-1}}{(n-1)!}\right)\right]$$

$$\kappa = k + 1/t^*$$

# Multiple reactors, k = 0

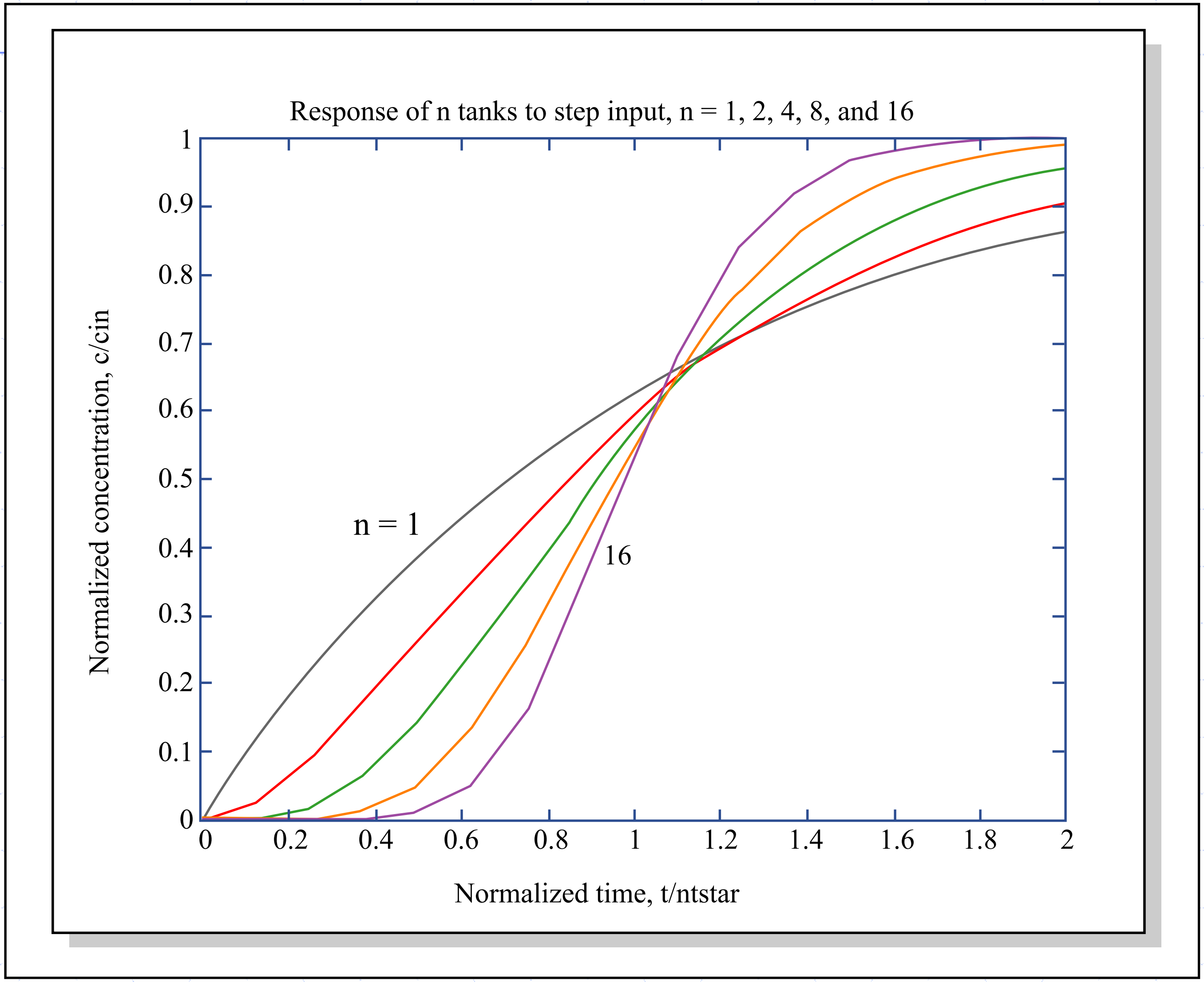
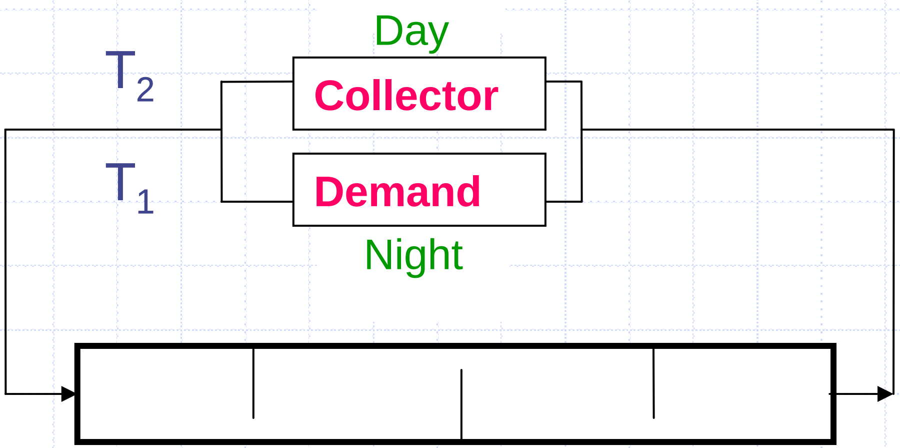



Figure by MIT OCW.

# WE 5-3 Thermal storage tank




t = start of the "day") (when tank has cold water at T = $T_1$ and you want to keep T = $T_1$

$$\frac{T(t)-T_1}{T_2-T_1}=\frac{1}{(t*\kappa)^n}\left[1-e^{-\kappa t}\left(1+\kappa t+\frac{(\kappa t)^2}{2}+\ldots+\frac{(\kappa t)^{n-1}}{(n-1)!}\right)\right]$$

$$R(t)=\frac{100\%}{nt*}\int_0^t\frac{T_2-T(t)}{\Delta T_0}dt$$

Percent of theoretical cooling (or heating) potential, a measure of hydraulic efficiency of storage system

# Thermal storage tank, cont'd

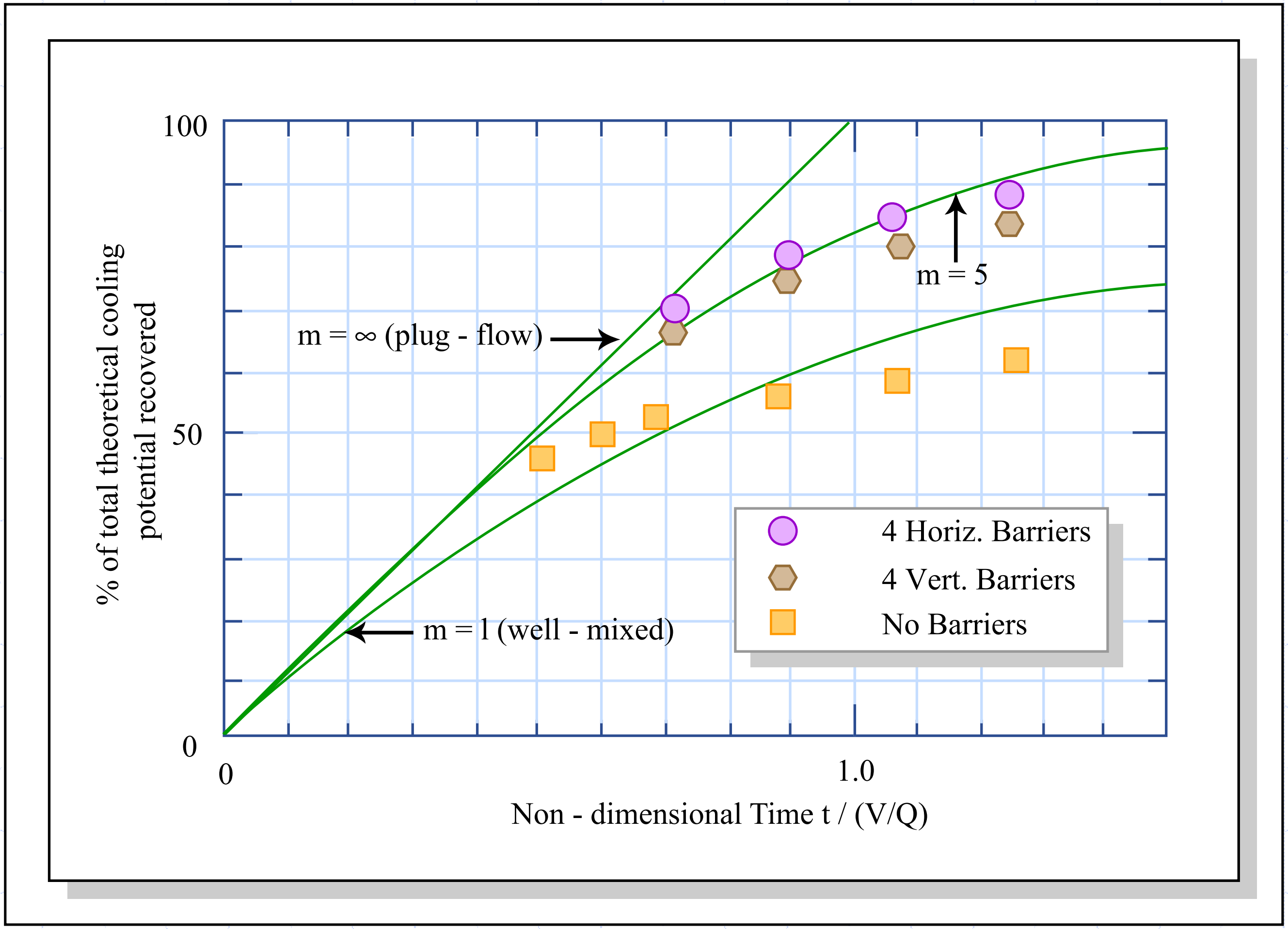
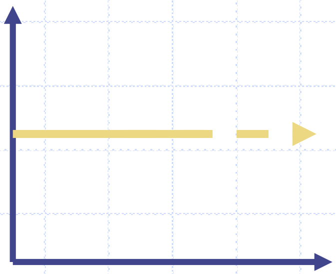



Figure by MIT OCW.

Geyer and Golay (1983), Adams (1986)

# Continuous input single & multiple

$$\dot{m} = Q_{in} c_{in}$$



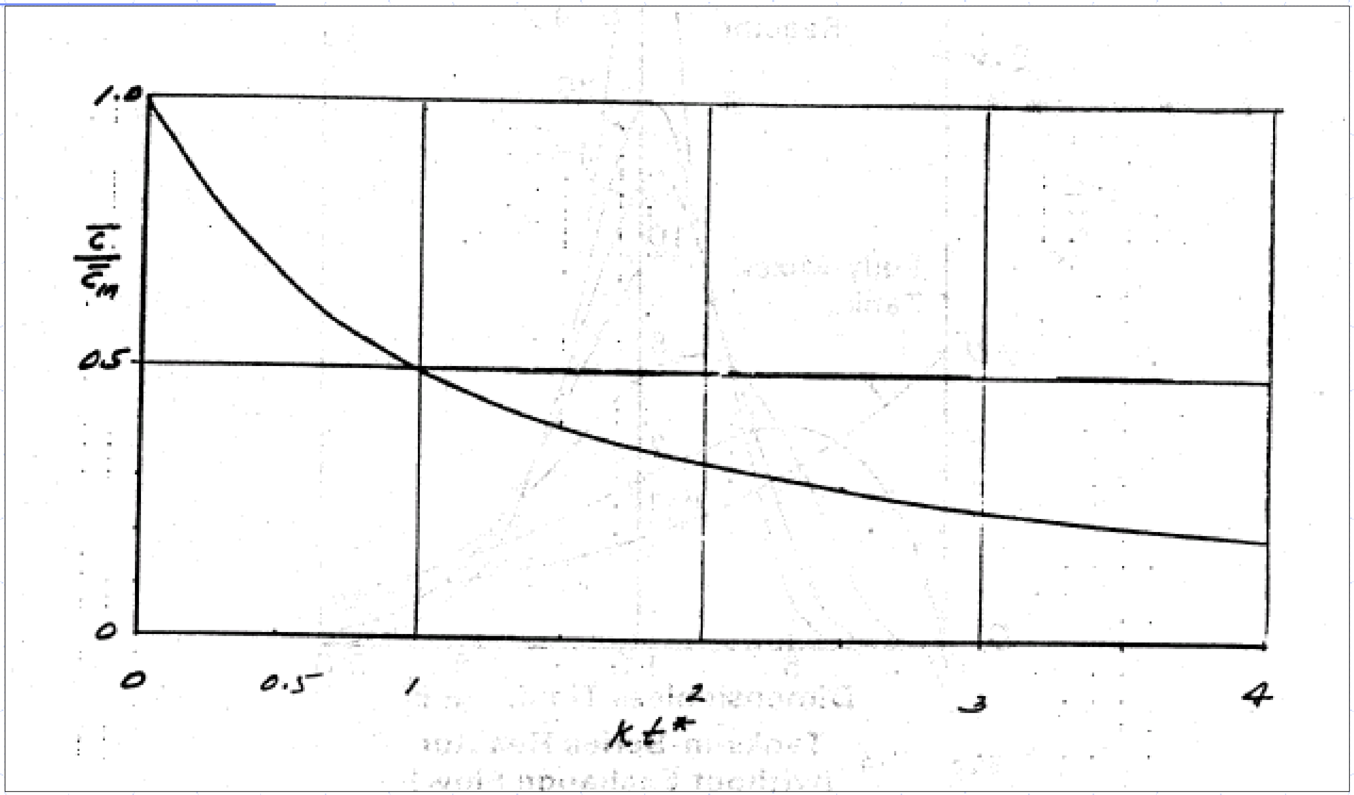
Continuous

From step input solutions for large t

$$\frac{\bar{c}}{\bar{c}_{in}} = \frac{1}{1 + kt^*}$$

$$\frac{\bar{c}_{out}}{\bar{c}_{in}} = \frac{1}{(1 + kt^*)^n}$$

# Continuous input, single tank



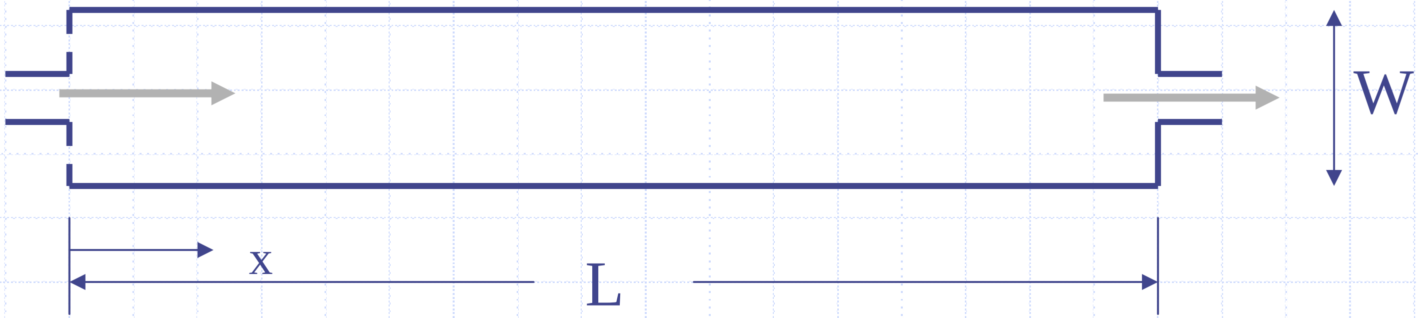
# Continuous input single & multiple

$$\frac{\bar{c}_{out}}{\bar{c}_{in}} = \frac{1}{(1 + kt^*)^n}$$

(knt* = 1; constant total volume)

| n | kt* | $c_{out}/c_{in}$ |
|---|---|---|
| 1 | 1 | 0.5 |
| 2 | 0.5 | 0.44 |
| 5 | 0.2 | 0.40 |
| 10 | 0.1 | 0.386 |
| 100 | 0.01 | 0.37 |
| infinity | 0 | $e^{-1}$ |

# Dispersed flow reactor




Engineer delayed response (--> plug flow) by making the reactor long & narrow. Density stratification should also be minimal (see Sect 5.4.1)

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}=\frac{1}{A}\frac{\partial}{\partial x}\left(E_L A\frac{\partial c}{\partial x}\right)-kc$$

(Small) entrance and exit sections may be treated differently

# Pulse input

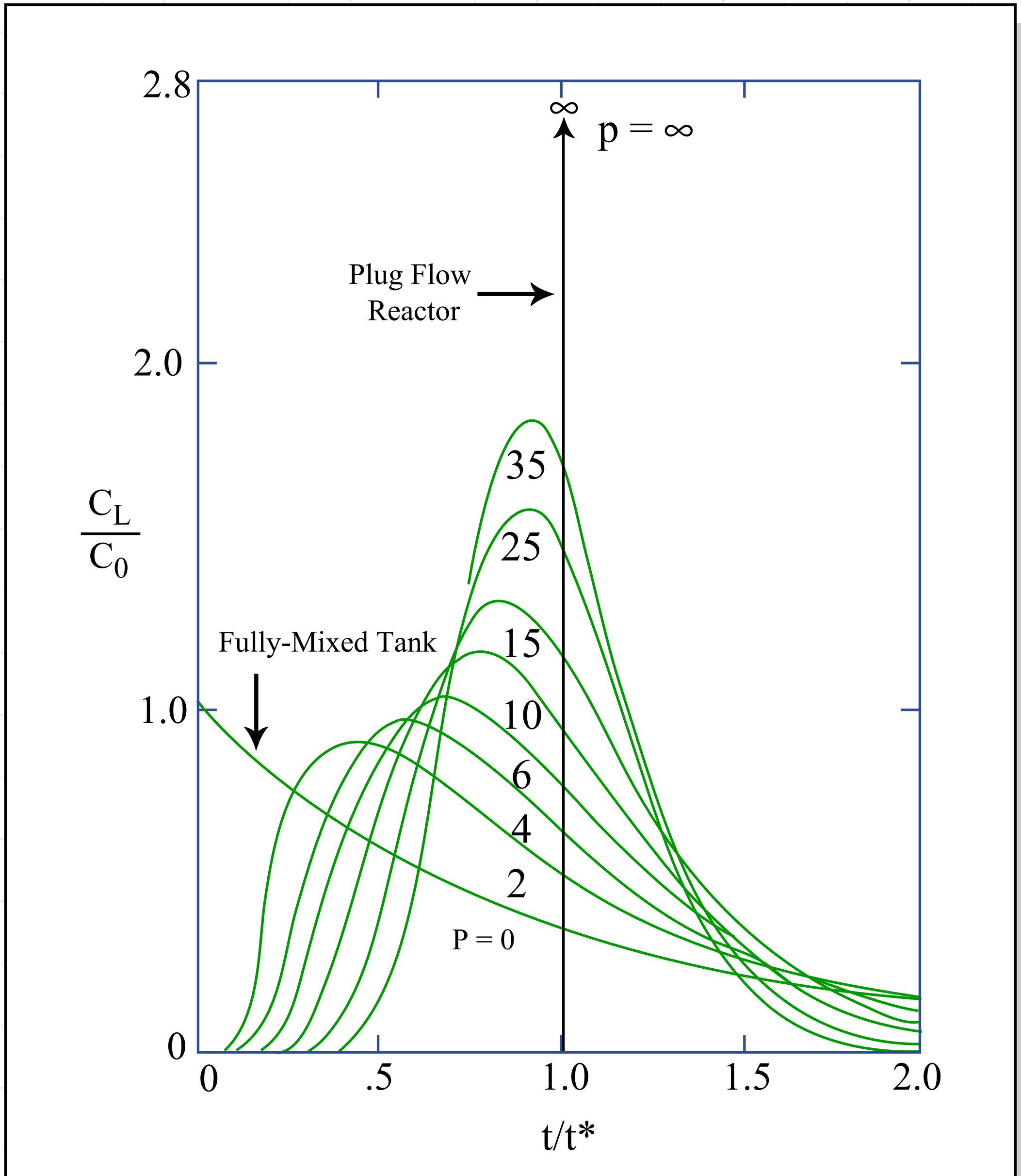
$Q_{in} = Q_{out}$ = const; A = const; k = 0 and pulse input at x =0

$$\frac{c_L}{c_o} = 2\sum_{i=1}^{\infty} \frac{\mu_i\left(\frac{Pe}{2}\sin\mu_i + \mu_i\cos\mu_i\right)}{\left(\frac{Pe^2}{4} + Pe + \mu_i{}^2\right)} \exp\left[\frac{Pe}{2} - \frac{\left(\frac{Pe^2}{4} + \mu_i{}^2\right)}{Pe}\left(\frac{t}{t*}\right)\right]$$

$c_o = M_o/V$; $Pe = UL/E_L$

$$\mu_i = \cot^{-1}\left(\frac{\mu_i}{P} - \frac{Pe}{4\mu_i}\right)$$

# Dispersed flow, pulse input




- A lot like tanks-in-series
- Greater n or Pe (lower $E_L$) => plug flow
- Pe ~ 2n-1 ( WE 5-5)
- Elongation sometimes done with baffles

Figure by MIT OCW.

# Dispersed flow vs tanks-in-series

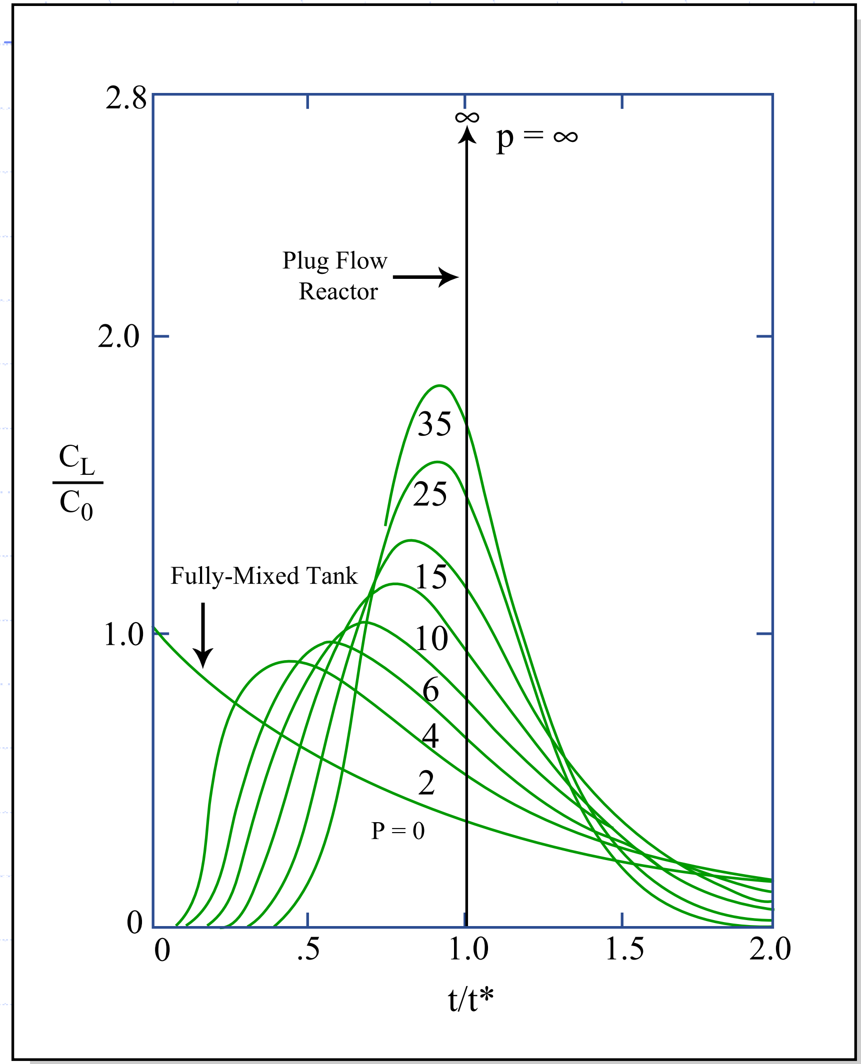



Figure by MIT OCW.

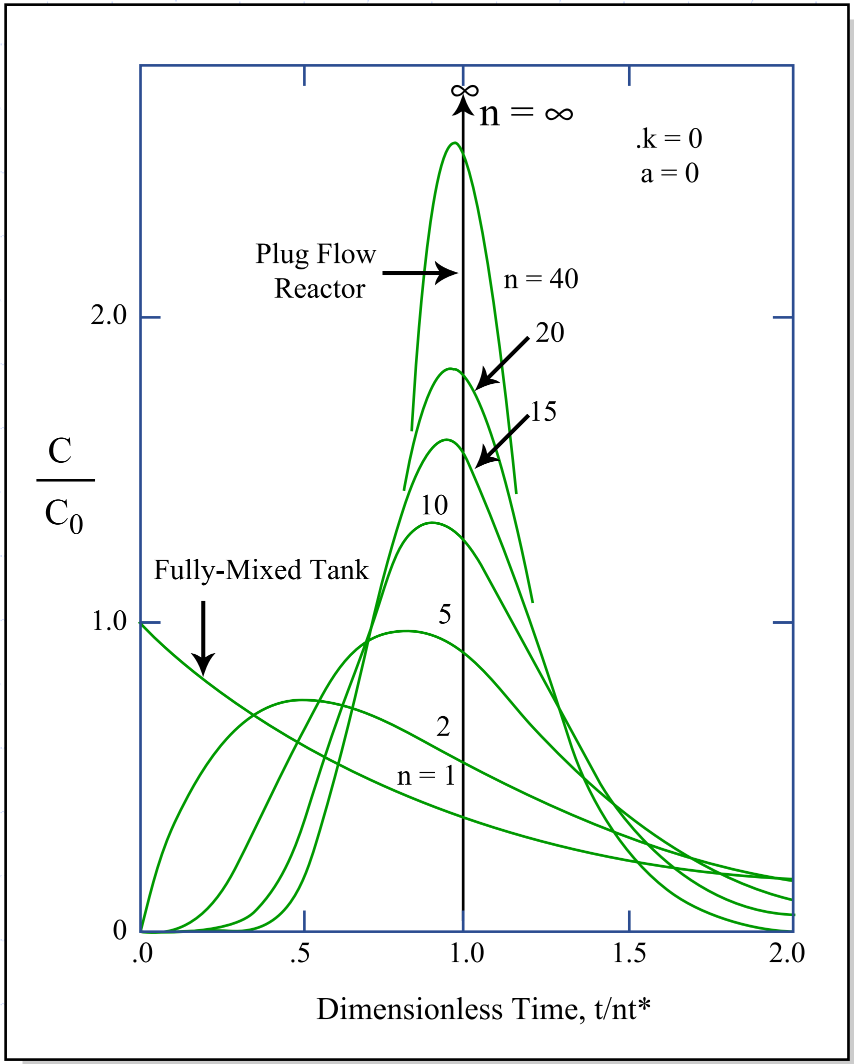
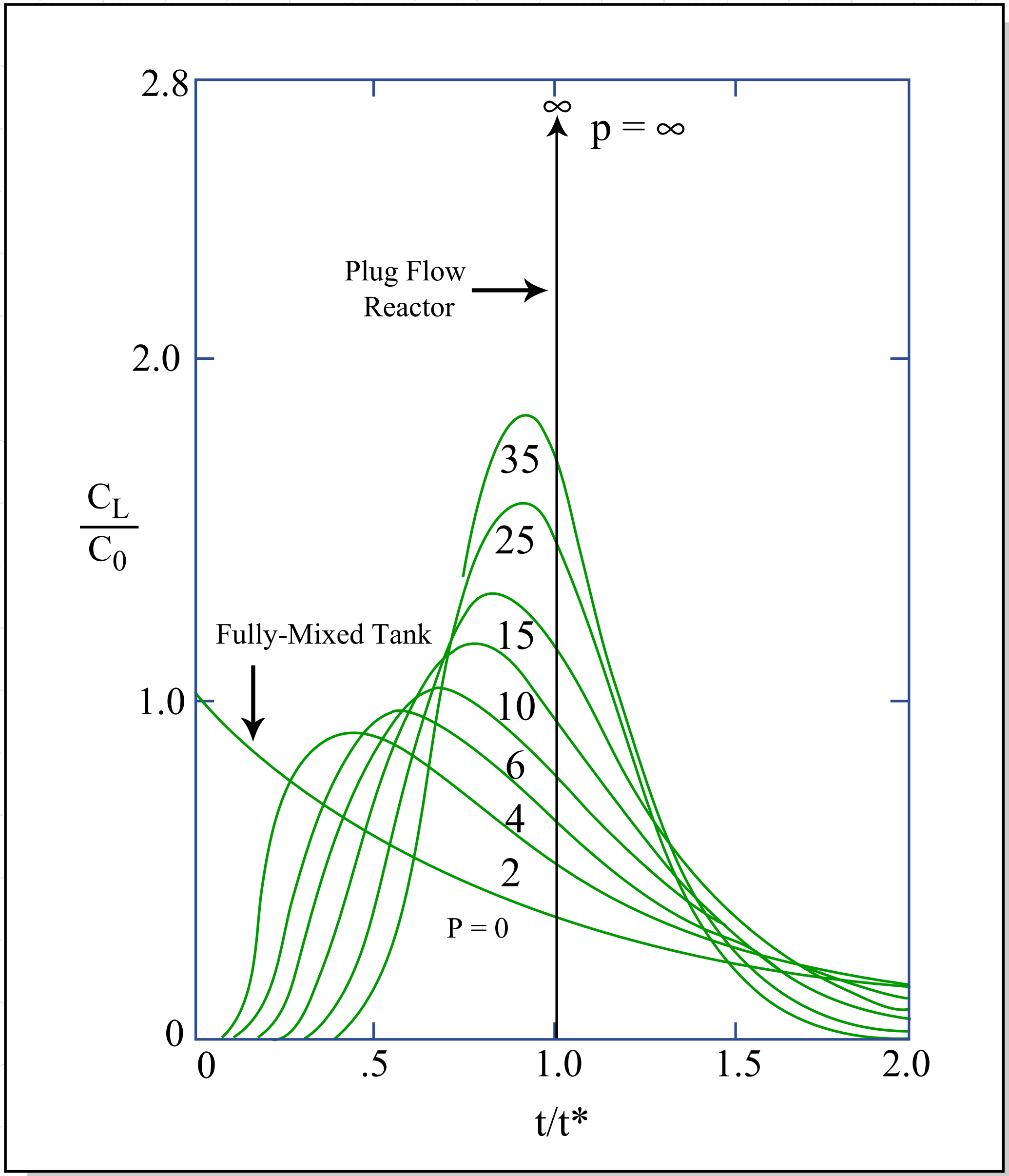



Figure by MIT OCW.

# Dispersed flow reactor




Area under curve and center of mass again are both one

$$\int_0^\infty \frac{c(t/nt^*)}{c_o} d\left(\frac{t}{nt^*}\right) = 1$$

$$\int_0^\infty \frac{c(t/nt^*)}{c_o} \left(\frac{t}{nt^*}\right) d\left(\frac{t}{nt^*}\right) = 1$$

Limits of plug flow and fully well-mixed

Figure by MIT OCW.

# (Idealized) effect of central baffle

$$Pe = \frac{UL}{E_L} = \frac{Q}{HB}\frac{A}{B}\frac{1}{E_L} = \frac{QA}{HE_L B^2}$$

$$E_L \cong \frac{0.01U^2 B^2}{u_* H} \sim \frac{UB^2}{H}$$

$$Pe = \frac{UL}{E_L} \sim \frac{ULH}{UB^2} \sim \frac{LH}{B^2}$$

If $E_L$ = const, B decreases by 2x, so Pe increases by 4x; real increase could be even more

L increases by 2x and B decreases by 2x, so Pe increases by 8x.

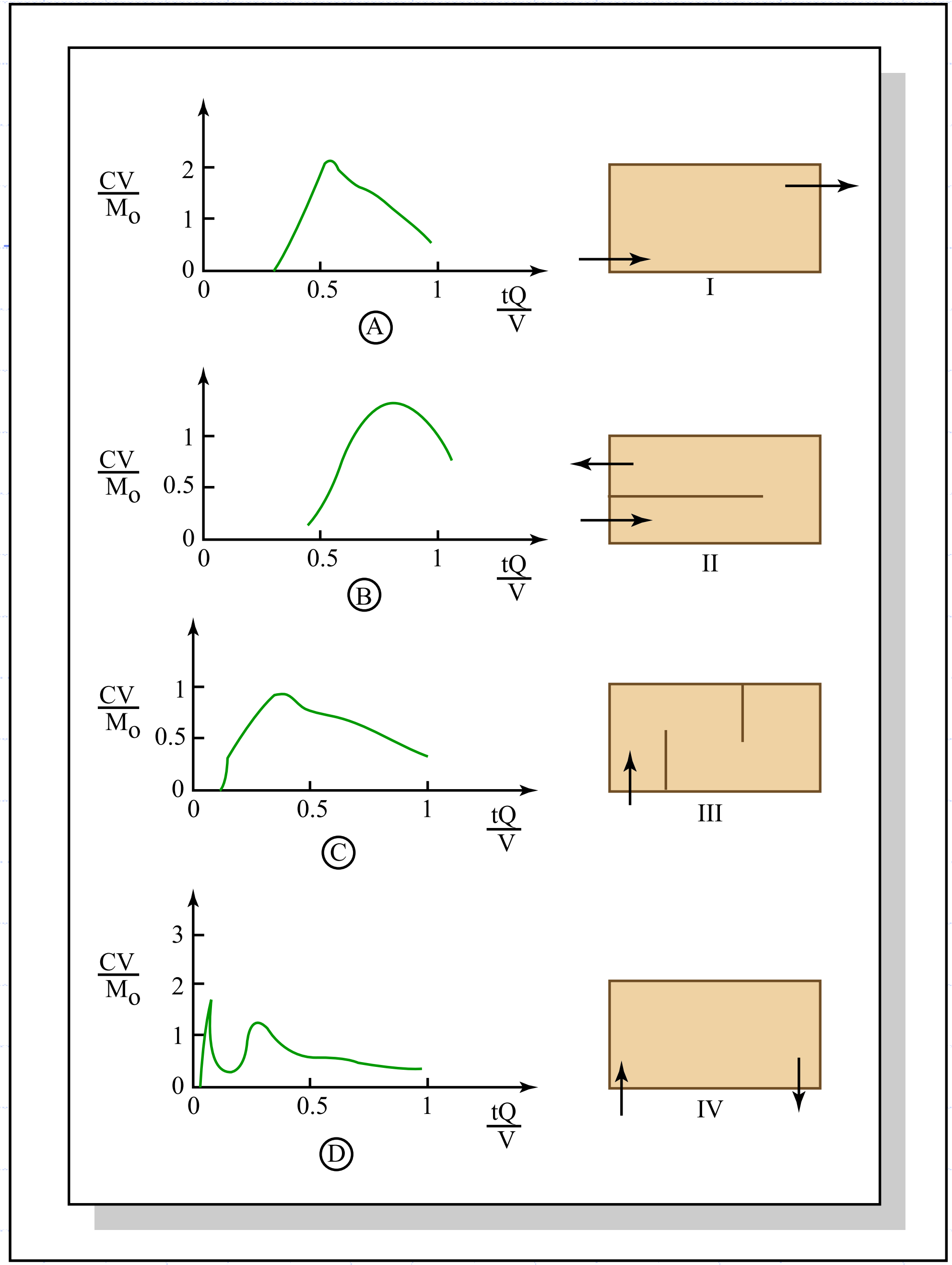



Figure by MIT OCW.

Can you place the UIR (A-D) with the schematic cooling pond (I-IV)?

Cerco, 1977

# WE5-5 Dispersed flow vs tanks-in-series

River: L = 10 km; B = 20 m; H = 1 m; Q = 10m$^3$/s; S = 10$^{-4}$

What are equivalent values of Pe and n?

$$u_* \cong \sqrt{gHS} = \sqrt{10 \cdot 1 \cdot 10^{-4}} = 0.032 m/s$$

*u = Q/BH =0.5 m/s*

$$E_L = 0.01 U^2 B^2 / H u_* \cong 0.01 \cdot 0.5^2 \cdot 20^2 /(1 \cdot 0.032) \cong 30 m^2 / s$$

$$Pe = UL / E_L = 0.5 \cdot 10^4 / 30 = 167$$

$$n \cong P / 2 = 83.$$

A finite difference model using upwind differencing would want to use a spatial grid size of order 10$^4$/83 or 120 m

# Dispersed flow, continuous input


GE assuming steady state

$$u\frac{dc}{dx} = E_L \frac{d^2c}{dx^2} - kc$$

Boundary conditions

$$Qc_{in}\Big|_{x=0^-} = \left(Qc - AE_L\frac{dc}{dx}\right)\Big|_{x=0^+}$$ at x = 0 (Type III)

$$Qc\Big|_{x=L^-} = Qc\Big|_{x=L^+}$$ at x = L (Type II)

# Dispersed flow, continuous input

Solution (0 < x < L)

$$\frac{c(x)}{c_{in}} = g_o \exp\left(\frac{Pe\xi}{2}\right)\left\{(1+\alpha)\exp\left[\frac{\alpha Pe}{2}(1-\xi)\right] - (1-\alpha)\exp\left[\frac{\alpha Pe}{2}(\xi-1)\right]\right\}$$

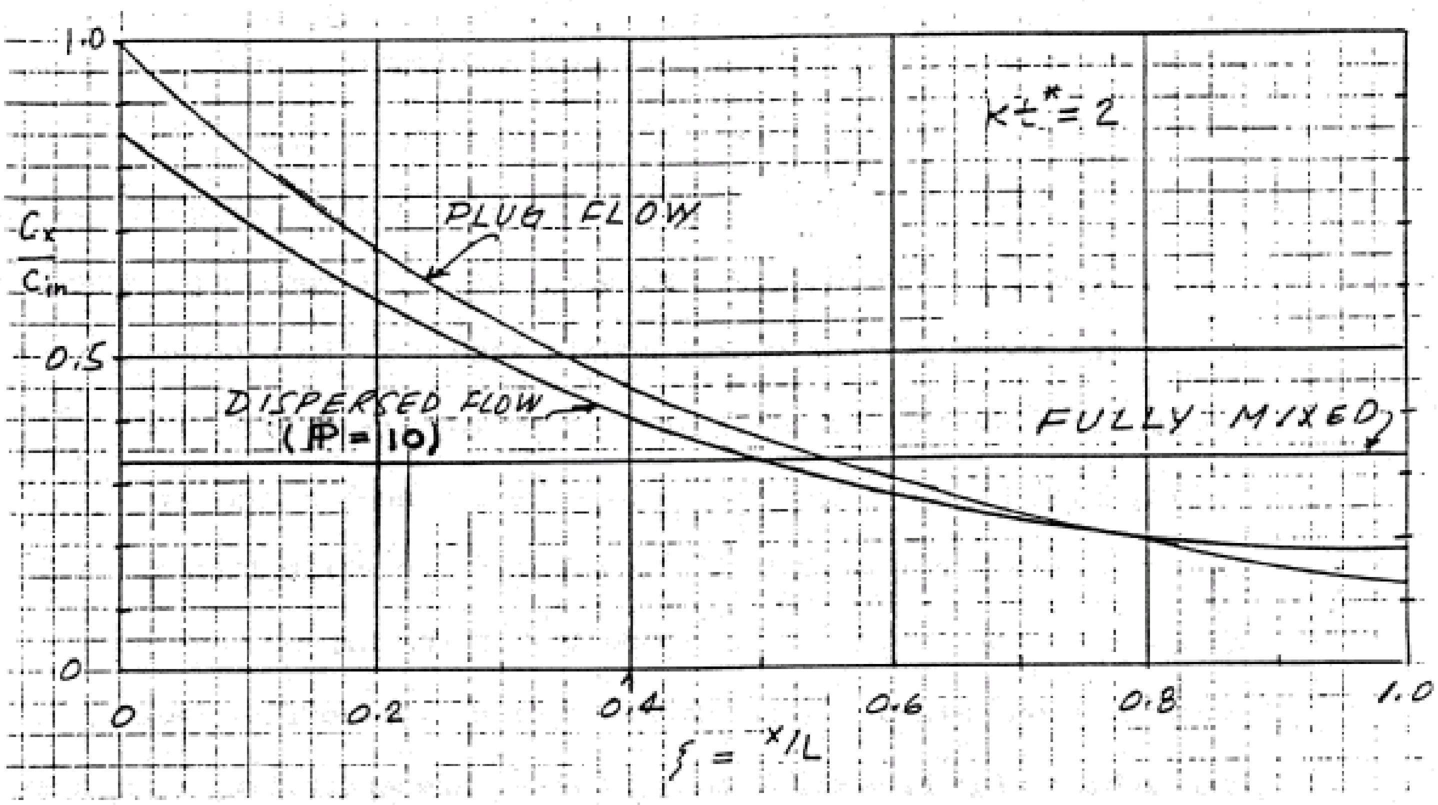
$$\xi = x / L$$

$$g_o = \frac{2}{(1+\alpha)^2 \exp\left(\frac{\alpha Pe}{2}\right) - (1-\alpha)^2 \exp\left(-\frac{\alpha Pe}{2}\right)}$$

$$a = \sqrt{\left[1 + \frac{4kL}{u}\left(\frac{1}{Pe}\right)\right]}$$

# Solution (0 < x < L)

Plug flow: greater loss at small x → lower concentration at large x




Note:

$c(x=0) < c_{in}$

# At outlet

Solution (x=L)

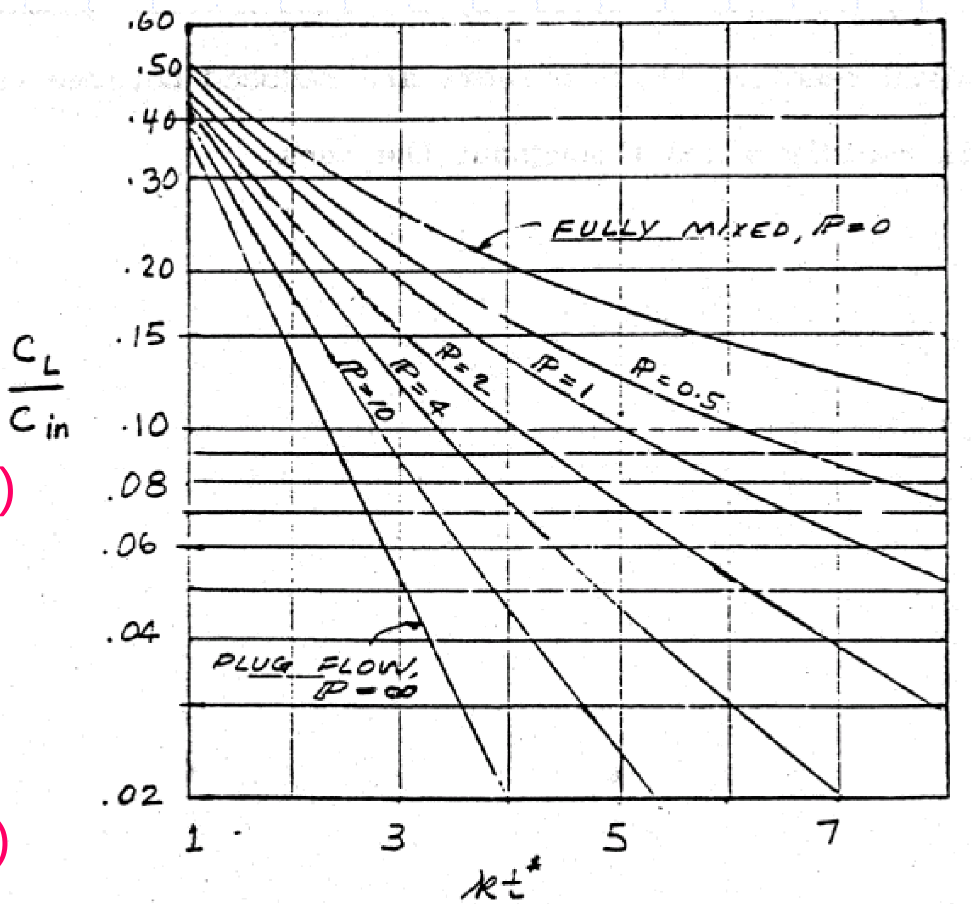
$$\frac{c_L}{c_{in}} = 2ag_o \exp(Pe/2)$$

For Pe --> 0 (well mixed)

$$\frac{c_L}{c_{in}} = \frac{1}{1+kt^*}$$

For Pe --> oo (plug flow)

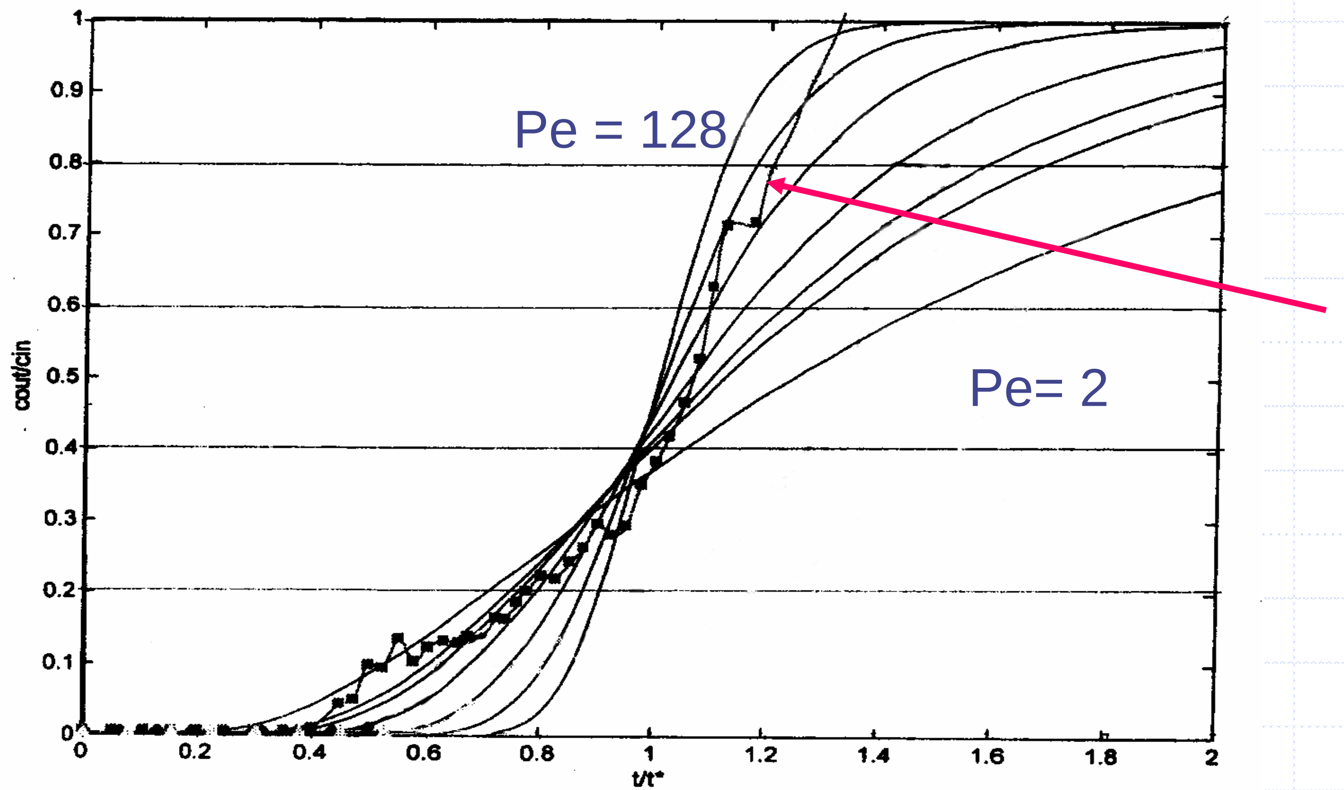
$$\frac{c_L}{c_{in}} = e^{-kL/u} = e^{-kt^*}$$



# WE 5-6 Continuous solar disinfection

- SODIS: simple household treatment technology for destroying pathogens using UV and temperature
- Pioneered by EAWAG, SANDEC and others; studied by former MEng students in Nepal
- Continuous (or semi-continuous) operation more convenient than discrete bottles

# Dispersed flow reactor response to step input (eq 2.104), k = 0



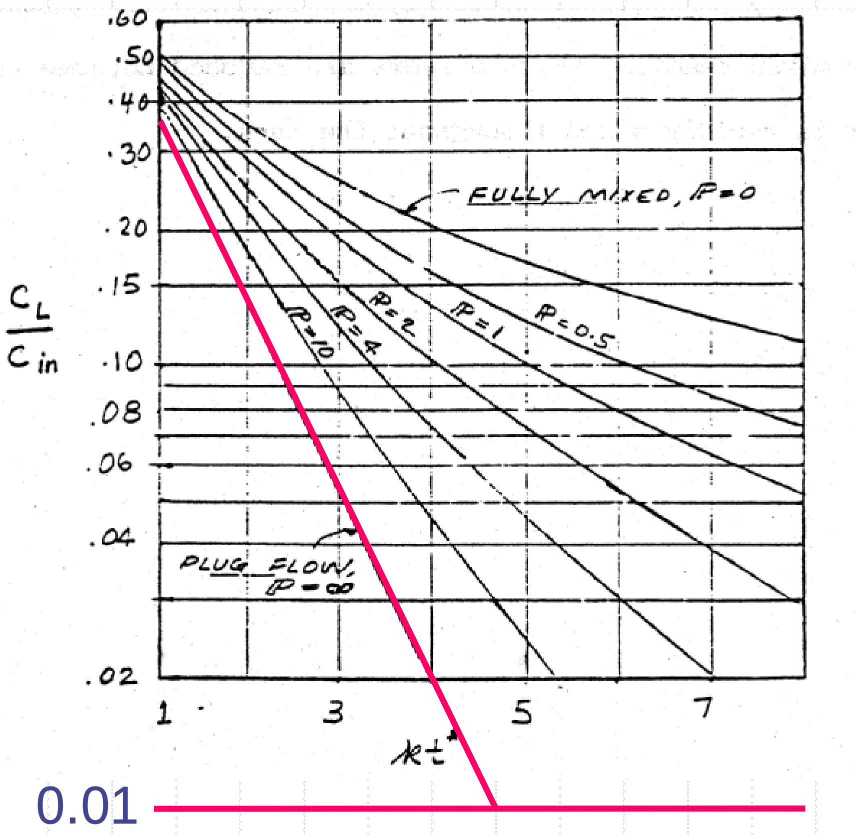

Infer 16 < Pe < 128

**$C_{out}/C_{in}$ vs t/t* for various values of Pe (2, 4, 8, 16, 32, 64, 128) compared with measurements (connected dots)**

Flores (2003)

# Continuous SODIS, cont'd

Measurements show 99% of pathogens killed for t* = 2 days ($c_{out}/c_{in}$ = 0.01). Use Eq. 5.40 to estimate first order removal rate (k) for plausible values of Pe & compare with plug flow reactor




Example

Pe = oo, $c_L/c_{in}$ = $c_{out}/c_{in}$ = 0.01

kt* = 4.6, k = 2.3 $d^{-1}$

# Continuous SODIS, cont'd

| Pe | k ($d^{-1}$) | $C_{out}/c_{in}$ (Plug Flow) | $\frac{C_{out}\text{ (Dispersed)}}{C_{out}\text{ (Plug flow)}}$ |
|---|---|---|---|
| 16 | 2.92 | 0.0029 | 3.45 |
| 32 | 2.62 | 0.0053 | 1.89 |
| 64 | 2.47 | 0.0072 | 1.39 |
| 128 | 2.38 | 0.0086 | 1.16 |
| oo | 2.30 | 0.0100 | 1.00 |

# Skimmer walls

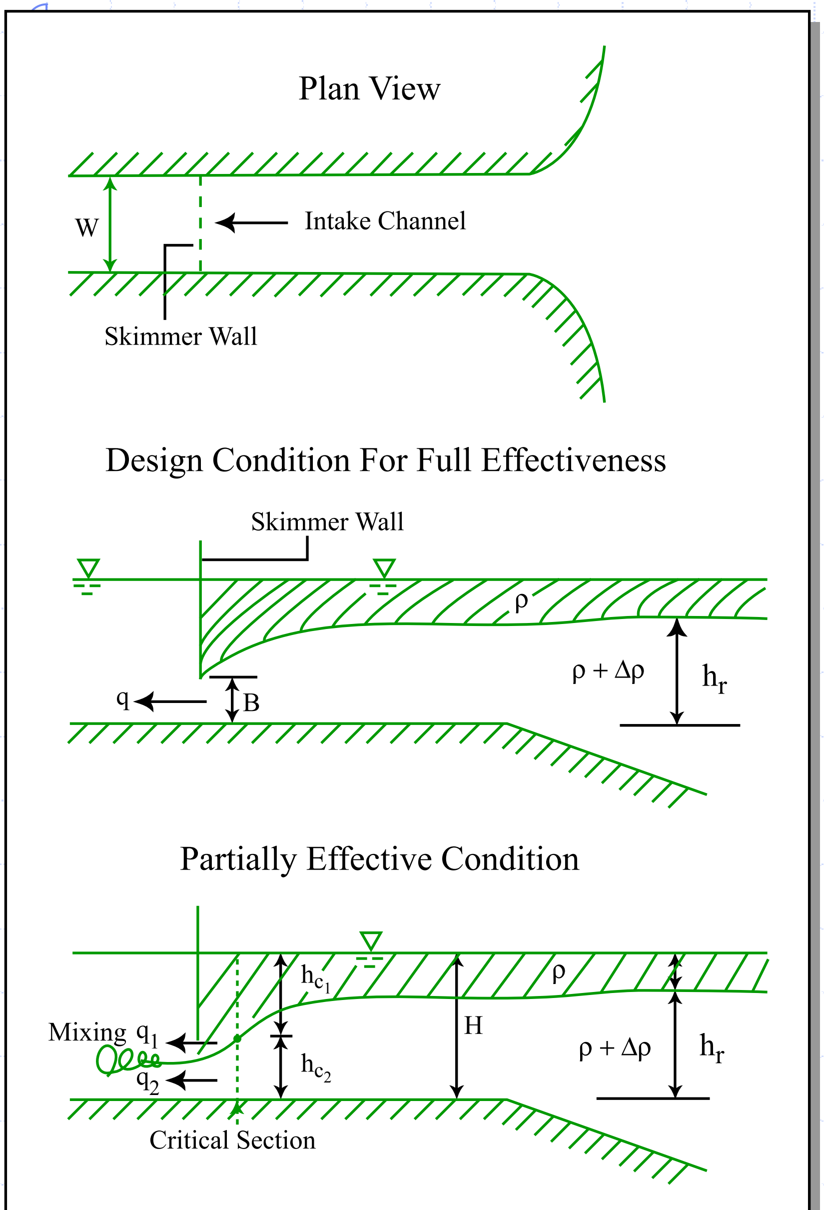



Figure by MIT OCW.

Selective withdrawal of water from density stratified tank or reservoir

Withdrawal of lower layer water tends to "suck down" upper layer. Bernoulli's equation used to compute max flow, draw down

Maximum flow per unit width

$$q_c = \left[ g' \left( \frac{2}{3} h_r \right)^3 \right]^{\frac{1}{2}}$$

$$F_r = \frac{q}{\sqrt{\left( g' h_r^3 \right)}} = \left( \frac{2}{3} \right)^{3/2}$$

For larger $F_r$, partially effective

# Partially-effective skimmer wall

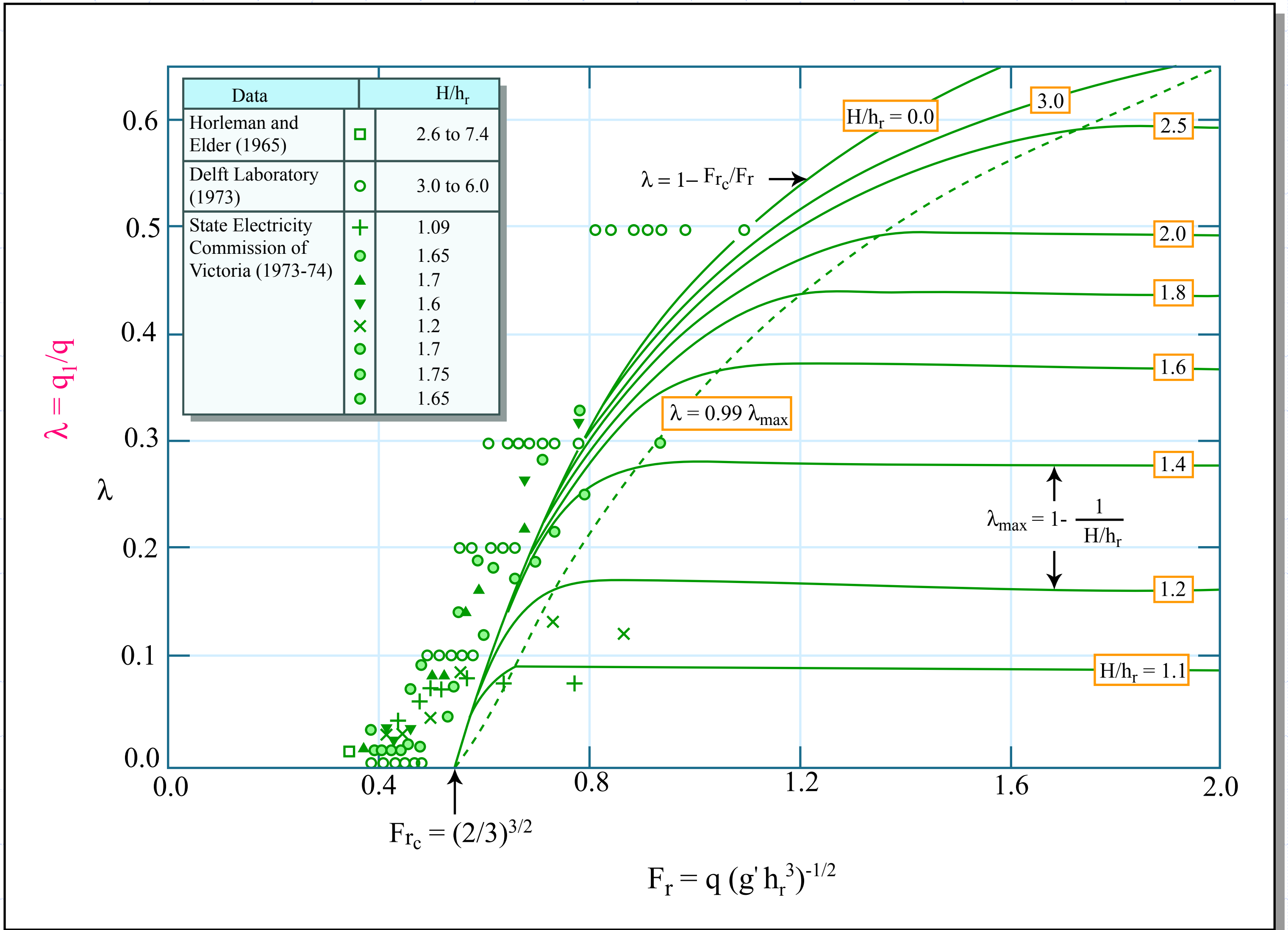



Figure by MIT OCW.

Jirka (1979)