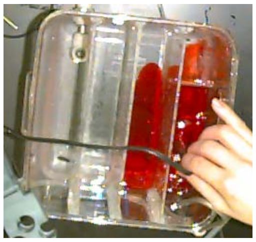
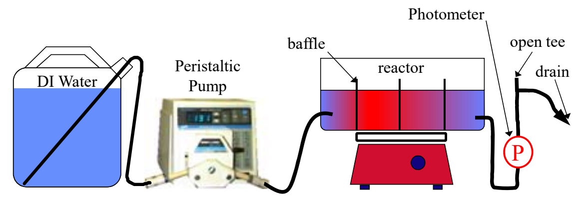
Reactors



The Case of the Chlorine Contact Tank

Reactor Characteristics: Designing a Chlorine Contact Tank



Outline

- Objectives of chlorine contact tanks
- Reactors in environmental engineering
- Advection, dispersion, and reaction
- Tracer studies and reactor characterization
- Data analysis and curve fitting
- Experimental design and ideas to probe

Chlorine Contact Tanks

- Widely employed in water and wastewater plants as the last step in the treatment process
- Takes place in a "clearwell" or "contact tank"
- Key design parameter: **contact time**

Disinfection CT Credits

To get credit for 99.9% inactivation of *Giardia*:

Contact time (min)

chlorine	pH 6.5		pH 7.5	
(mg/L)	2°C	10°C	2°C	10°C
0.5	300	178	430	254
1	159	94	228	134

Inactivation is a function of _______, ____________ ______, and ___________.

Contact Time Definition

- The contact time for purposes of chlorine disinfection is defined by the EPA as
  - The time that it takes for 10% of the mass of a tracer pulse to arrive at the effluent of the tank
  - Or equivalently, the time it takes for the effluent concentration to reach 10% of the influent concentration after a tracer is added continuously to the influent

EPA Contact Time Credit

Contact time = (baffle factor)(hydraulic residence time)

Baffling Condition	Baffle Factor (BF) t^* at $F = 0.1$	Extent of Baffles	Typical Unit Processes
Unbaffled (CMFR)	0.1	No baffles, agitated basin with low length to width ratio, high inlet and outlet flow velocities	Clearwell, storage tank, no perforated inlet or outlet, inlet or outlet submerged.
Poorly baffled	0.3	Single or multiple unbaffled inlets and outlets, no intrabasin baffles	Many conventional sedimentation basins. Storage tanks with two or three baffles.
Average	0.5	Baffled inlet or outlet with some intrabasin baffles	Some (few) sedimentation basins. Highly baffled storage tanks.
Superior	0.7	Perforated inlet baffles, serpentine or perforated intrabasin baffles, outlet weir or perforated launders	Filters. Contact tanks with serpentine baffling
Perfect (PFR)	1.0	Very high length to width ratio (pipeline flow), perforated inlet, outlet and intrabasin baffles	Sections of pipe ten times longer than their diameter.

The Meaning of Life… for Contact Tanks

- Minimally – To meet EPA regulations
- Better – To obtain as high a contact time as possible with a given tank
- Or – To build as small a tank as possible that meets the EPA regulations

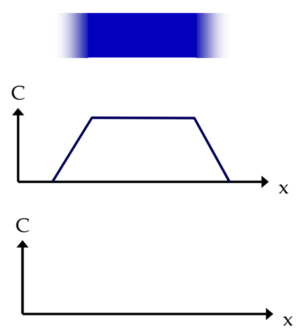
Reactors

- Reactor: a "container" where a reaction occurs
- Examples:
  - Clear well at water treatment plant (chlorine contact)
  - Activated sludge tank at wastewater treatment plant
  - Treated wastewater discharge into a stream: stream = reactor
  - Treated wastewater discharge into Cayuga lake: lake = reactor
  - Gas tank leaking into soil: soil = reactor

Advection: mean flow

$$\frac{\partial C}{\partial t}_{\text{advection}} = -\mathrm{u}\frac{\partial C}{\partial x}$$

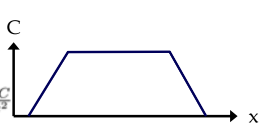
What does it look like a short time later?



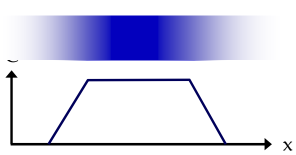
Dispersion: velocity fluctuations

Fick's first law $\mathrm{J} = -\mathrm{D}_d \frac{\partial C}{\partial x}$

Fick's second law $\frac{\partial C}{\partial t}_{\text{dispersion}} = \mathrm{D}_d \frac{\partial^2 C}{\partial x^2}$

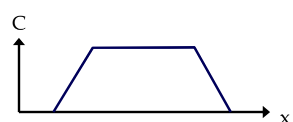


What does it look like a short time later?

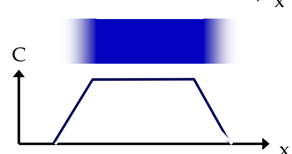


Reaction

$$\frac{\partial C}{\partial t}_{\text{reaction}} = \mathrm{r} = -\mathrm{kC}$$



What does it look like a short time later?



Advection/Dispersion/Reaction

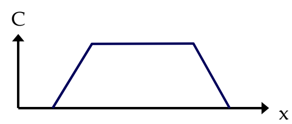
$$\frac{\partial C}{\partial t}_{\text{total}} = D_d \frac{\partial^2 C}{\partial x^2} - u\frac{\partial C}{\partial x} + r$$

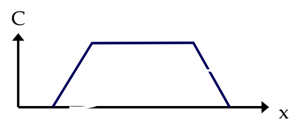
In three dimensions

$$\frac{\partial C}{\partial t} = D_d \nabla^2 C - u\nabla C + r$$

where

$$\nabla = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$$

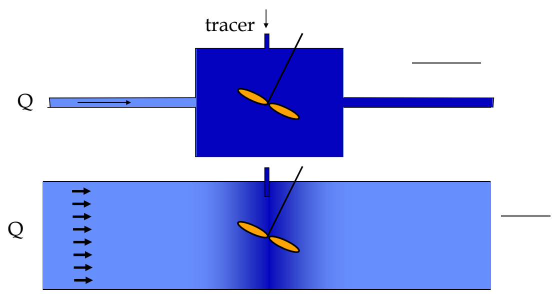




Reactors: Closed vs. Open

- Closed: have little dispersion across the inlet and outlet boundaries
  - Well defined reactor volume
  - Examples
    - ______________________________
    - _____
- Open: have significant dispersion across the inlet and outlet boundaries
  - Backmixing
  - Example
    - ______

Reactors: Defining the Control Volume



Reactor Characterization

- Time scales
  - hydraulic residence time
  - average time for tracer to get from inlet to outlet
- Closed systems
  - "dead volume" $\bar{t}$ ___ θ
- Open systems
  - dispersion upstream $\bar{t}$ ___ θ ?
  - "dead volume" $\bar{t}$ ___ θ

$$\theta = \frac{V_r}{Q} = \underline{\qquad\qquad}$$

$$\bar{t} = \frac{\int_0^\infty t \cdot C(t)\,dt}{\int_0^\infty C(t)\,dt}$$

Peclet Number

- Ratio of advection to dispersion
  - how far does advection carry the fluid/width of tracer plume
- High Peclet means primarily advection (_______________)
- Low Peclet means lots of mixing

$$Pe = \frac{U}{D_d/L}$$

Characterize a Tank: Tracer Studies

- Tracers
  - Desirable properties
  - Candidates
  - Measuring techniques
- Choosing a tracer concentration
  - Measurement range
  - Interferences ________________________
- Density matching
- Pulse vs. Step ___________________

Ideal Tracer

- same properties as fluid
  - viscosity
  - temperature
  - density
  - non reactive
- additional properties
  - low background concentrations
  - easily measured
  - cheap
  - non toxic

Real Tracers

Tracer type	distinguishing property	analytical instrument	examples
salt	conductivity	Conductivity meter	NaCl
Dyes	color	Spectrophoto-meter	methylene blue
fluorescent dye	fluorescence	Fluorometer	rhodamine WT
acid	protons	pH probe	HCl
Dissolved gas	Gas	Gas chromatograph	Sulfur hexafluoride

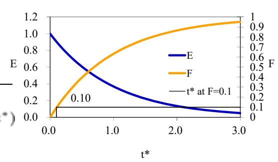
Reactor Theory: CMFR

$$\forall_r \frac{dC}{dt} = (C_{in} - C)\,Q$$

r = reactor
tr = tracer
t = time

$$t^* = \frac{t}{\theta} = \frac{tQ}{\forall_r}$$

$$\frac{C_{(t)}\forall_r}{C_{tr}\forall_{tr}} = e^{\left(\frac{-t}{\theta}\right)}$$



$$E_{(t^*)} = \frac{C_{(t^*)}\forall_r}{C_{tr}\forall_{tr}} = e^{(-t^*)}$$

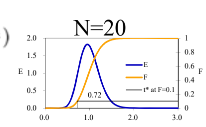
$$F_{(t^*)} = \int_0^{t^*} E_{(t^*)}\,dt^*$$

E and F curves

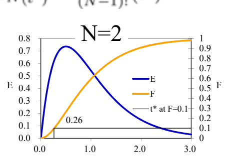
- The E curve is a dimensionless measure of the output tracer concentration from a spike input.
- The F curve is a dimensionless measure of the cumulative output from a spike input
- The F curve is also a dimensionless measure of the output tracer concentration from a step input

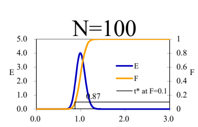
Reactor Theory: Series CMFR

$$\frac{C_{N(t/\theta)}\forall_r}{C_{tr}\forall_{tr}} = \frac{N^N}{(N-1)!}\left(\frac{t}{\theta}\right)^{N-1} e^{\left(\frac{-Nt}{\theta}\right)}$$



$$E_{N(t^*)} = \frac{N^N}{(N-1)!}(t^*)^{N-1} e^{(-Nt^*)}$$





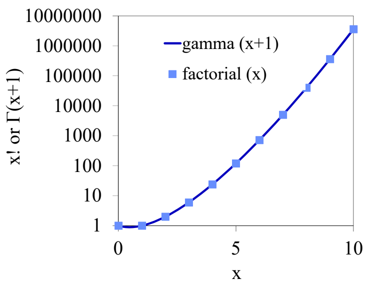
Gamma Function to Replace Factorial?

- We will be using solver to find N. It would be better if we had a continuous function rather than one that only works for whole numbers $E_{N(t^*)} = \frac{N^N}{(N-1)!}(t^*)^{N-1} e^{(-Nt^*)}$
- The (complete) gamma function is defined to be an extension of the factorial to complex and real number arguments. It is related to the factorial by

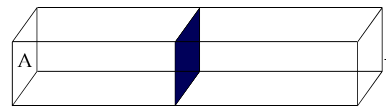
$$\Gamma(n) = (n-1)!$$

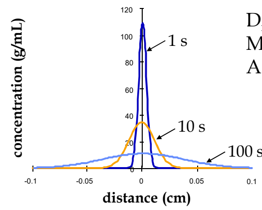
$$E_{N(t^*)} = \frac{N^N}{\Gamma(N)}(t^*)^{N-1} e^{(-Nt^*)}$$

Γ(x+1)



1-D Dispersion





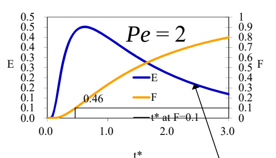
$D_m = 0.673 \times 10^{-5}$ cm²/s
M = 1 g
A = 1 cm²

$$C_{(x,t)} = \frac{M}{A\sqrt{4\pi D_m t}}\exp\left(\frac{-x^2}{4D_m t}\right)$$

1-D Advective Dispersion Equation

$$\mathrm{C(x,t)} = \frac{M}{A\sqrt{4\pi D_d t}}\exp\left[\frac{-x'^2}{4D_d t}\right]$$

$$E_{(t^*)} = \sqrt{\frac{Pe}{4\pi t^*}}\exp\left[\frac{-(1-t^*)^2 Pe}{4t^*}\right]$$



$$Pe = \frac{UL}{D_d} =$$

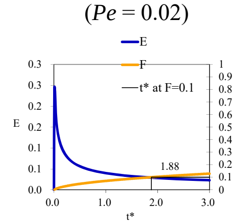
$$t^* = \frac{tU}{L}$$

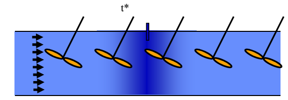
$$x' = x - Ut$$

Note: This reactor has more dispersion than a series CMFR with N = 2, but it has a longer contact time!

1-D Advective Dispersion Extremes: High Dispersion

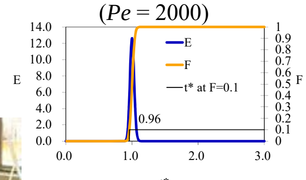
- How can it take 1.9 residence times for 10% of the tracer to come out?
- Why is the contact time so good?
- Why is F so small at 3 residence times?
- Hey! That's not fair!





1-D Advective Dispersion Extremes: Low Dispersion

- Approaches plug flow!



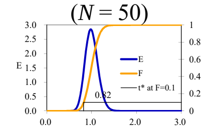
CMFR in series ≡ Advective Dispersion

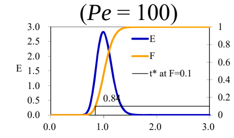
They both approach plug flow!

$$E_{N(t^*)} = \frac{N^N}{(N-1)!}(t^*)^{N-1}e^{(-Nt^*)}$$

$$E_{(t^*)} = \sqrt{\frac{Pe}{4\pi t^*}}\exp\left[\frac{-(1-t^*)^2 Pe}{4t^*}\right]$$

$$Pe \cong 2N$$





Goals of plug flow without dead volume

- Many CMFR in series ____________
- High Peclet number ____________
  - Laminar pipe flow
  - Turbulent pipe flow
  - Porous media flow
- Eliminating “Dead volume”
  - Requires more mixing!
  - Turbulent pipe flow: Serpentine channels
  - Turbulent jets: Perforated baffles

Serpentine Chlorine Contact Tanks

Model as_________________. Baffle Factor of________.

Distribution Tank (Honduras)

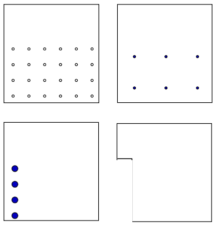
- How would you model this tank?
- _________
- _________________
  ____
  ____
  ____

Baffle Factor of________.

Experiment Design Options

- Baffles
  - With holes
    - (pattern, diameter, number)
    - **Head loss**
    - Jet Reynolds number
  - Partial baffles
- Reactor flow rate
- Reactor depth
- Porous media
  - Packing material

➢Mean circulation patterns
➢Serpentine vs. series CMFR
  ➢Risk of dead volumes



Plotting F

- Where do these terms come from?

$$E_{(t^*)} = \frac{C_{(t^*)}\forall_r}{C_{tr}\forall_{tr}} \qquad t^* = \frac{t}{\theta} \qquad \theta = \frac{\forall_r}{Q}$$

$$\left.\begin{aligned} F_{(t^*)} &= \int_0^{t^*} E_{(t^*)} dt^* & F_{(t^*)} &= f\left(\forall_r, Q, t, C_{(t)}, C_{tr}, \forall_{tr}\right) \\ F_{(t^*)} &= \sum_{i=0}^{n(t^*)} E_{(i)} \Delta t_i^* & F_{(t^*)} &= f\left(C_{(t)}, t, \theta, M_{tr}\right) \end{aligned}\right\}$$

$$F_{(t^*)} = f\left(t^*, Pe \text{ or } N\right)$$

Mass Conservation

- What is the purpose of checking mass conservation? ______________________
- Four ways to check

At infinity… At all times

$$\forall_{tr} C_{tr} \stackrel{?}{=} \sum_{i=0}^{\infty} Q C_i \Delta t_i \qquad \forall_{tr} C_{tr} \stackrel{?}{=} \sum_{i=0}^{n} Q C_i \Delta t_i + \forall_r C_{r\ mixed_n}$$

dimensionless $1 \stackrel{?}{=} F_{(\infty)}$ $\qquad 1 \stackrel{?}{=} \sum_{i=0}^{n} E_i \Delta t_i^* + \frac{C_{r\ mixed(t^*)}\forall_r}{C_{tr}\forall_{tr}}$

Characteristic times…

- What is the difference between θ and $\bar{t}$?

$$\theta = \frac{\forall_r}{Q} \qquad \bar{t} = \frac{\sum_{i=0}^{n} t_i \cdot C_i \Delta t}{\sum_{i=0}^{n} C_i \Delta t}$$

- $\bar{t}$ is only defined correctly if all of the tracer is accounted for!!!!!!
- What does it mean if θ is greater than $\bar{t}$?
- What does it mean if θ is less than $\bar{t}$?
- What other technique could you use to measure the tracer residence time?

$$\theta_{tracer} \neq \frac{\forall_r}{Q}$$

Comparison with Models

- Which model do you expect might describe perforated baffle reactors?
- Which model do you expect might describe serpentine reactors?

$$E_{N(t^*)} = \frac{N^N}{(N-1)!}(t^*)^{N-1} e^{(-Nt^*)}$$

$$E_{(t^*)} = \sqrt{\frac{Pe}{4\pi t^*}} \exp\left[\frac{-(1-t^*)^2 Pe}{4t^*}\right]$$

Estimating the Peclet number (or the number of CMFR in series)

$$Pe = \frac{2\theta^2}{\sigma_t^2} \qquad \sigma_t^2 = \frac{\sum_{i=0}^{n} t_i^2 \cdot C_i \Delta t}{\sum_{i=0}^{n} C_i \Delta t} - \bar{t}^2$$

Requires data from the entire tracer curve

model	data
$E_{(t^*)} = \sqrt{\frac{Pe}{4\pi t^*}} \exp\left[\frac{-(1-t^*)^2 Pe}{4t^*}\right]$	$E_{(t^*)} = \frac{C_{(t^*)} \forall_r}{C_{tr} \forall_{tr}}$

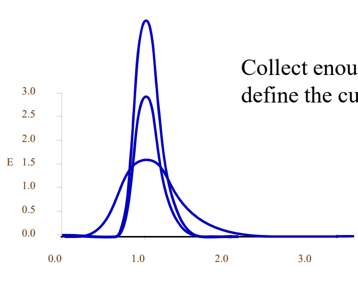
Use multiple variable regression analysis.
Minimize the SSE (sum of the squared errors) between the model and the data by changing (Q or volume) and (*Pe or N)* (use Solver)

Data Analysis Requirements: 2 goals

- Measure the baffle factor
  - Can be as simple as finding the time when 10% of the tracer gets to the effluent
- Compare the data with the two reactor models
  - At minimum requires fitting N or Pe
  - But there is no reason to expect the hydraulic residence time to be the same as the tracer residence time – so fit θ also (by fitting Q or volume)

Curve fitting

- Changing θ, M_{tr}, and N or Pe



Collect enough data to define the curve!

Organizing Experiments

- Protocol for sharing resources? (baffles)
- What is the question you are trying to answer?
- Make sure you conduct experiments that provide data to answer that question!
- Jet Reynolds number is not an important parameter, but head loss is!
- Only vary one parameter at a time!!!!
- Distilled water
- How do you choose and control reactor volume?
- USE YOUR EYES!!!!!

Experiment ideas

- Vary a parameter over at least 3 values
- Effect of depth given serpentine path
- Baffles in the long direction
- Parallel pipe flow between inlet and outlet baffles
- Effect of Reynolds number (can you get the transition between laminar and turbulent flow in open channel flow)?

More ideas

- Use a Step function instead of a pulse
- Inlet and outlet conditions matter!
- Use red dye to see what is happening
- Create a spreadsheet that makes it easy to analyze the data
- How do you get model curves based on data t* as the x values? (This will make nonlinear regression analysis easier.)

Reactor analysis

- Using Mass conservation as a given (and require solver to fit 2 parameters)

$$\forall_{tr} C_{tr} \stackrel{?}{=} \sum_{i=0}^{n} Q C_i \Delta t_i + \forall_r C_{r\ mixed_n}$$