Reactor Characteristics

Introduction

Chemical, biological and physical processes in nature and in engineered systems usually take place in what we call "reactors." Reactors are defined by a real or imaginary boundary that physically confines the processes. Lakes, segments of a river, and settling tanks in treatment plants are examples of reactors. Most, but not all, reactors experience continuous flow (in and out). Sequencing batch reactors have a sequence of states including fill, react, and empty. It is important to know the mixing level and residence time in reactors, since they both affect the degree of process reaction that occurs while the fluid (usually water) and its components (often pollutants) pass through the reactor.

Chlorine contactor tanks are designed to maximize the contact time between chlorine and pathogens before the water is delivered to consumers. Thus the design objective is to maximize the time that it takes for water to travel from the tank influent to the effluent. Tracer studies can be used to determine the hydraulic characteristics of a reactor such as the disinfection contact tanks at water treatment plants. The results from tracer studies are used to obtain accurate estimates of the effective contact time. In this laboratory students will experiment with different reactor designs with the goal of maximizing the contact time.

Reactor Classifications

Dispersion

Mixing levels give rise to three categories of reactors; completely mixed flow (CMFR), plug flow (PFR) and flow with dispersion (FDR). The plug flow reactor is an idealized extreme not attainable in practice. All real reactors fall under the category of FDR or CMFR.

Boundary Conditions

The reactor inlet and outlet boundary conditions significantly affect the reactor response to the addition of a pulse of tracer. If dispersion is possible across a boundary, then the boundary is open. An example of a reactor with open boundaries is a section of a river. If a tracer is added to a section of a river it is possible for some of the tracer to move upstream, illustrating that an arbitrary section of a river is an open reactor (Figure 5-1). This is equivalent to letting the reactor be

![Figure 5-1 Schematic of a reactor with open boundary conditions](image-url)
defined as a section of a long reactor. One of the characteristics of open boundaries is that some of the tracer introduced at the reactor inlet can be carried upstream and thus the residence time for a conservative tracer can be greater than the hydraulic residence time!

A "closed" reactor is one where the reactor has a diffusion or dispersion coefficient different than those of the entrance or exit (Figure Error! Reference source not found.). Typically exit and entrance diffusion/dispersion are much less than the diffusion/dispersion in the reactor. An example of a reactor with closed boundaries is a tank with small inlet and outlet pipes.

### Reactor Modeling

Reactors can be studied by measuring the effluent concentration after the addition of a spike or pulse of a tracer in the influent or after a step function change in input concentration. The resulting response curves can be non dimensionalized by plotting $\frac{C(t/\theta)}{C_r}$ as a function of $t/\theta$ where $\theta$ is the hydraulic residence time. The term $t/\theta$ will be defined as $t^*$.

The non dimensional response curves from pulse inputs and step inputs are know as E curves and F curves respectively. The E curve is the exit age or residence time distribution curve and the F curve represents the fraction of tracer molecules having an exit age younger than $t^*$. The E and F curves are related by

$$F_{(t^*)} = \int_{0}^{t^*} E_{(t^*)} dt^* \tag{5.3}$$

The $F_{(t^*)}$ curve can either be obtained by integrating $E_{(t^*)}$ or by applying a step function change in influent concentration to a reactor and monitoring the effluent concentration. In that case $F_{(t^*)}$ is defined as

$$F_{(t^*)} = \frac{C}{C_{in}} \tag{5.4}$$

The following sections will include typical E and F curves for different reactor types.

#### Completely Mixed Flow Reactor

Complete mix flow regimes can be approximated quite closely in practice. In the case of CMF reactors, there is not an analytical solution to the advective dispersion equation
so we revert to a simple mass balance. For a completely mixed reactor a mass balance on a conservative tracer yields the following differential equation:

\[
∀_r \frac{dC}{dt} = (C_{in} - C)Q \quad 5.5
\]

where \( Q \) is the volumetric flow rate and \( ∀_r \) is the volume of the reactor.

Equation 5.5 can be used to predict a variety of effluent responses to tracer inputs such as the pulse input used in this experiment. If a volume of tracer is discharged directly into a reactor so that the initial concentration of tracer in the reactor is \( C_0 = \frac{C_{tr} ∀_r}{∀_r} \) and the input concentration is zero \( (C_{in} = 0) \) the solution to the differential equation is:

\[
E_{(t/θ)} = \frac{C_{(t/θ)} ∀_r}{C_{tr} ∀_r} e^{\left(-\frac{t}{θ}\right)} \quad 5.6
\]

or in the dimensionless form

\[
E_{(t')} = \frac{C_{(t')} ∀_r}{C_{tr} ∀_r} e^{\left(-t'\right)} \quad 5.7
\]

where \( E_{(t')} \) is the exit age or residence time distribution curve, \( ∀_r \) is the reactor volume, \( ∀_{tr} \) is the tracer volume, and \( C_{tr} \) is the tracer concentration. If a reactor has a complete mix flow regime its response, \( E_{(t')} \), to a pulse input should plot as a straight line on a semi-logarithmic plot. Response curves for a CMFR are shown in Figure 5-3.

The time for 10% of the pulse to arrive at the effluent of a CMFR is approximately \( 0.1_t^* \).

**Plug Flow Reactor**

Plug flow regimes are impossible to attain because mass transport must be by advection alone. There can be no differential displacement of tracer relative to the average advective velocity. In practice some mixing will occur due to molecular diffusion, turbulent dispersion, and/or fluid shear. For the case of the plug flow reactor the advective dispersion equation 5.11 reduces to:
\[
\frac{\partial C}{\partial t} = -U \frac{\partial C}{\partial x}
\]

5.9

The velocity, \( U \), serves to transform the directional concentration gradient into a temporal concentration gradient. In other words, a conservative substance moves with the advective flow of the fluid. The solutions to this differential equation for a pulse input and for a step input are shown graphically in Figure 5-4. The time for 10% of the pulse to arrive at the effluent of a PFR is \( t^* \) since all of the pulse arrives at the same time.

![Figure 5-4 Pulse and step input in a plug flow reactor.](image)

**Flow with Dispersion**

Real flow reactors that aren’t completely mixed exhibit behavior that is between plug flow and completely mixed. The reactor flow behavior is a function of the relative strength of the mixing process (or dispersion) compared to the advective flow. Analytical solutions that describe these real reactors are more difficult and in most cases a parameter describing the dispersion is fit to the data rather than predicted a priori. Two models for arbitrary mixing levels are described below.

**Open Boundary conditions: One Dimensional Advective Dispersive Equation**

The governing differential equation for a conservative (i.e., non-reactive) substance in a reactor that has advective transport (i.e., flow) and some mixing (dispersion) in the direction of flow (x-plane) is given in equation 5.11.

\[
\frac{\partial C}{\partial t} = -U \frac{\partial C}{\partial x} + D_a \frac{\partial^2 C}{\partial x^2}
\]

5.11

\( C \) = concentration of a conservative substance
\( U \) = average fluid velocity in the x direction
\( D_a \) = longitudinal dispersion coefficient
\( t \) = time

The dispersion is described by a single parameter that is the same in the reactor as it is at the inlet and outlet for open boundary conditions. The solution to equation 5.11 for the case of complete mixing in y-z plane and advective and dispersive transport only in the x direction for any x and t (after t=0) gives:

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

5.12

where \( M \) = mass of conservative material in the spike, \( D_d \) = axial dispersion coefficient [L^2/T], \( x' = x - Ut \), \( U \) = longitudinal advective velocity in the reactor, and \( A \) is the cross-sectional area of the reactor. A measure of dispersion can be obtained directly from
equation 5.12. From this equation we expect a maximum value of $C$ at $t = x/U$. At this time $C(x,t) = \frac{M}{A\sqrt{4\pi D_d t}}$. If the mass of the tracer input ($M$) and reactor cross-sectional area ($A$) are known, then $D_d$ can be estimated. Equation 5.12 can be made dimensionless to more clearly reveal the important parameters. The dispersion coefficient can be made dimensionless by dividing by a velocity and a length.

$$Pe = \frac{UL}{D_d} \quad 5.13$$

where $L$ is the length of the reactor and $U$ is the mean advective velocity. The dimensionless parameter $Pe$ (Peclet number) is used to characterize the level of dispersion in a reactor. The Peclet number is the ratio of advective to dispersive transport. In the limiting cases when $Pe = 0$ (very high dispersion) we have a complete mix regime (CMFR) and when $Pe = \infty$ ($D_d = 0$, no dispersion) we have a plug flow reactor (PF).

The time can be normalized by dividing by the hydraulic residence time.

$$t^* = \frac{tU}{L} \quad 5.14$$

Combining Equations 5.13 and 5.14 we obtain $D_d t = t^* Pe L^2$ for substitution into Equation 5.12. The concentration can be normalized by the mass of the tracer and the volume, $\forall$, of the reactor.

$$\forall = AL \quad 5.15$$

$$E(x^*) = \frac{C(x,t)\forall}{M} \quad 5.16$$

The position in the reactor where the concentration measurements are made can be changed to the reactor effluent by substituting $L$ for $x$. Substituting Equation 5.14 into the definition of $x^*$ we obtain:

$$x^* = (L - Ut)^2 = (1 - t^*)^2 L^2 \quad 5.17$$

The resulting dimensionless form of Equation 5.12 is given in Equation 5.18.

$$E(x^*) = \frac{Pe}{\sqrt{4\pi t^*}} \exp \left[ \frac{-(1-t^*)^2 Pe}{4t^*} \right] \quad 5.18$$
Response curves for the advective dispersion equation are shown in Figures 5-5 and 5-6. The exit age curve is highly skewed for low $Pe$ because tracer that is in the reactor longer has more time for dispersion. As the Peclet number increases the dispersion decreases and the response becomes closer to plug flow.

Flow through porous media (such as groundwater through soil) is a type of flow with dispersion. The above equations can be applied by recognizing that the relevant water velocity is the pore water velocity. The pore water velocity is $U = \frac{Q}{A\varepsilon}$ where $A$ is the cross-sectional area of the porous media and $\varepsilon$ (volume of voids/total volume) is the porosity of the porous media.

The form of equation 5.21 is exactly like the normal distribution curve:

$$\frac{CA}{M} = \frac{1}{\sigma_x \sqrt{2\pi}} \exp\left[-\frac{x^2}{4\sigma_x^2}\right]$$

where

$$\sigma_x^2 = 2D_d t$$

Or in dimensionless form:

$$\frac{\sigma_x^2}{L^2} = 2t^* Pe$$

The variance in concentration over space ($\sigma_x^2$) is the variance in concentrations taken from many different positions in the reactor at some single moment in time, $t$. The variance in $x$ ($\sigma_x^2$) has dimensions of length squared.

**Closed Boundary Conditions: Completely Mixed Flow Reactor in Series**

Completely mixed flow reactors are sometimes connected in series to create a reactor system with flow characteristics in between CMFR and PFR. CMFRs in series increase
overall process efficiency because the reactants are at higher concentrations in the first reactors than they would be in a single large CMFR. Thus the total reactor volume can be smaller with a series of CMFRs. Similarly the reaction process can be made more efficient given the same reactor volume if is divided into series CMFRs.

Non ideal reactors with mixing levels between that of CMFRs and PFRs and reactors containing baffles can also be modeled as a series of CMFRs. In this case the mixing level for the system is represented by the number of CMFRs that are used to represent the non-ideal reactor. The equation describing the concentration of a conservative tracer in the Nth reactor is given in equation 5.24.

$$\frac{C_N(t)}{M} = \frac{N^N}{(N-1)!} \left( \frac{t}{\theta} \right)^{N-1} e^{-\frac{N}{\theta}}$$  \hspace{1cm} 5.24

The non-dimensional form of equation 5.24 is given in equation 5.25

$$E_N(t') = \frac{N^N}{(N-1)!} \left( \frac{t'}{\theta} \right)^{N-1} e^{-\frac{N}{\theta}}$$  \hspace{1cm} 5.25

It can be shown that equations 5.18 and 5.25 converge for large N when

$$Pe = 2N$$  \hspace{1cm} 5.26

Equation 5.24 is limited to integral values of N. The model could be extended to include non integral values of N if the factorial function were replaced with the \(\Gamma\) function. Note that the \(\Gamma\) function is not defined as an extension of the factorial function in Excel. Instead use the functions EXP(GAMMALN(N)) to calculate the \(\Gamma\) function.

Response curves for the advective dispersion equation are shown in Figure 5-7. Notice that the effluent concentration begins to rise much more quickly in series CMFRs than in the advective dispersion model. This distinction between the two models lessens as the number of reactors increases and the \(Pe\) increases.

**Reactor Studies**

**Measuring Reactor Characteristics**

One of the easiest methods to determine the mixing (dispersion) characteristics of a reactor is to add a spike input of a conservative material and then monitor the
concentration of the material in the reactor effluent. The variance of tracer concentration versus time ($\sigma_i^2$, with dimensions of time squared) can be measured by sampling at a single point in the reactor at many different times and can be computed using the following equations.

$$\sigma_i^2 = \frac{\int_{0}^{\infty} C(t)(t - \bar{t})^2 dt}{\int_{0}^{\infty} C(t) dt} = \frac{0}{\int_{0}^{\infty} C(t) dt} - \bar{t}^2$$

where

$$\bar{t} = \frac{\int_{0}^{\infty} t \cdot C(t) dt}{\int_{0}^{\infty} C(t) dt}$$

For discrete data points:

$$\sigma_i^2 = \frac{\sum_{i=0}^{n} t_i^2 \cdot C_i \Delta t}{\sum_{i=0}^{n} C_i \Delta t} - \bar{t}^2$$

and

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

Inlet and outlet boundary conditions affect the response obtained from a reactor. Closed reactors have little dispersion across their inlet and outlet boundaries whereas "open" reactors can have significant dispersion across their inlet and outlet boundaries. Typically open systems have no physical boundaries in the direction of flow. An example of an open system would be a river segment. Closed systems have small inlets and outlets that minimize dispersion across the inlet and outlet regions. An example of a closed system is a tank (or a lake) with a small inlet and outlet. The reactor used in the lab is closed. The $\bar{t}$ in equation 5.31 is the measured average residence time for the tracer in the reactor. For ideal closed reactors the measured residence time, $\bar{t}$, is equal to the theoretical hydraulic residence time ($\theta = \text{reactor volume}/\text{flow rate}$). For open reactors $\bar{t}$ can exceed the hydraulic residence time. If $\bar{t}$ is less than the hydraulic residence time it may indicate that the reactor contains "dead volume" or "short circuiting" such that some volume of the reactor is effectively unused.
The above equations suggest that from the reactor response to a spike input we can compute the dispersion coefficient for the reactor. We have two options for measuring reactor response:

1) synoptic measurements: at a fixed time sampling many points along the axis of the reactor will yield a Gaussian curve of concentration vs. distance. In practice synoptic measurements are difficult because it requires sampling devices that are time-coordinated. By combining equations 5.22, 5.30, and 5.31 it is possible to estimate the dispersion coefficient from synoptic measurements.

2) single point sampling: measure the concentration at a fixed position along the x axis of the reactor for many times. If the reactor length is fixed at L and measurements are made at the effluent of the reactor (observe the concentration of a tracer at x = L as a function of time) then x is no longer a variable and C(x,t) becomes C(t) only. The response curve obtained through single point sampling is skewed. The curve “spread” changes during the sampling period and the response curve is skewed.

**Peclet Number Estimation**

For single point sampling of the effluent response curve, skew increases as the dispersion level in the reactor increases. The degree of skew depends on the dispersion coefficient, the velocity in the x-direction, and the length of the reactor. Peclet values in the range 100<Pe<∞ result in a symmetric response curve.

Response curve skew makes the assumption of a symmetrical normal distribution curve inappropriate and a new relationship between the variance and the dispersion coefficient (or Pe) has to be determined. Boundary conditions affect the determination of the dispersion coefficient. The relationship between the Peclet number and variance for open systems is given by:

\[ \sigma_i^2 = \left( \frac{2}{Pe} + \frac{8}{Pe^2} \right) \cdot \theta^2 \quad 5.33 \]

For closed systems the relationship is:

\[ \sigma_i^2 = \left[ \frac{2}{Pe} - \frac{2}{Pe^2} \left( 1 - e^{-Pe} \right) \right] \cdot \theta^2 \quad 5.34 \]

The term \( \frac{2}{Pe} \) in equations 5.33 and 5.34 is dominant for Peclet numbers much greater than 10 as is shown in Figure 5-8. The additional terms in equations 5.33 and 5.34 are corrections for skewedness in the response curve. These skewedness corrections are not very significant for Peclet numbers greater than 10. Thus for Peclet numbers greater than 10 the Peclet number can be determined using equation 5.35 for both open and closed systems.

![Figure 5-8. Relationship between equations 5.33 through 5.34.](image-url)
Reactor Characteristics

Mass Conservation

When a pulse of conservative tracer is added to a continuous flow reactor, all of the tracer is expected to leave the reactor eventually. The mass of a substance that has left the reactor is given in equation 5.36.

\[ M_{out} = \sum_{i=0}^{n} Q C_i \Delta t_i \]  

where \( Q \) is the flow rate and \( M \) is the mass of any substance whose concentration is given by \( C \). If \( Q \) and \( \Delta t \) are constant, then equation 5.36 can be rewritten as

\[ M_{out} = Q \Delta t \sum_{i=0}^{n} C_i \]  

Equation 5.37 can be used to determine if all of the tracer was measured in the reactor effluent. Alternately, mass conservation can be checked by plotting the \( F \) curve and checking if the plot approaches 1. If some of the tracer is in the reactor at the end of the experiment then the following equation can be used to test for mass closure.

\[ M_{in} = M_{out} + \Delta M_{stored} \]  

Tracers

A conservative tracer will be used to characterize each of the reactors. Typical tracers include salt and various dyes. For the experiment we will use hydrogen ions as the conservative tracer. Normally hydrogen ions would not be a good choice because they are reactive. In the laboratory we can circumvent that problem by using distilled water to eliminate potential reactants. The hydrogen ion concentration will be measured using a pH probe. The hydrogen ions will be added as hydrochloric acid.

A reasonable number of hydrogen ions to add can be calculated based on the following constraints. An excessively high concentration of hydrogen ions will cause low pH values that may not be measured accurately. Low concentrations of hydrogen ions will not be conservative because some reactions will occur with carbonates that have dissolved in the distilled water from the atmosphere. The concentration of total carbonates can be obtained by setting the ANC to zero and solving for pH, then solving for \( Ct \). The concentration of bicarbonate, the only reactive species at low pH can be calculated based on the \( Ct \) and the pH. The concentration of bicarbonate is approximately 2.2 \( \mu \)M in distilled water. To reduce the error caused by reaction with bicarbonate the target hydrogen ion concentration should be at least 100x the bicarbonate concentration. Given these constraints a first guess for a reasonable number of hydrogen ions is that the hydrogen ion concentration of a completely mixed reactor containing the requisite tracer addition should be equivalent to pH 3.66 (or 220 \( \mu \)Moles H\(^+\) per liter of reactor).

Addition constraints for the tracer are that if a highly concentrated tracer is used, then there will be a significant density difference between the tracer and the water in the
reactor. If density matching is used to increase the density of the fluid in the reactor, then
the high ionic strength of the reactor fluid will change the activity coefficient of \( H^+ \). If a
very dilute tracer is used then a large volume of tracer will need to be added and the
volume of tracer could become a large fraction of the reactor volume and thus the pulse
could no longer be modeled as having negligible volume.

**Density Matching**

A common problem when using tracers is that the tracer may have a different density
than the fluid that is in the reactors. This is normally not a problem for reactors with low
Peclet numbers or high levels of turbulence. However, density effects should not be
overlooked since some of the tracer could easily sink to the bottom of the reactor and
remain there. To compensate for the tracer density, the density of the water being pumped
into the reactors will be increased by adding sodium chloride.

The solution density due to the addition of hydrochloric acid is approximately:

\[
\rho_{\text{solution}} = \rho_{H_2O} + 17.9 N_{HCl}
\]

where \( N_{HCl} \) has units of \( \text{eq/L} \) and density is in \( \text{kg/m}^3 \).

The increase in density due to the addition of sodium chloride is approximately:

\[
\rho_{\text{solution}} = \rho_{H_2O} + 0.6985 C_{NaCl}
\]

where \( C_{NaCl} \) has units of \( \text{g/L} \). Equations 5.39 and 5.40 can be used to solve for the
necessary concentration of NaCl given the tracer concentration of HCl.

\[
C_{NaCl} = 25.6 N_{HCl}
\]

**Activity Corrections**

When we measure pH we are actually measure the activity of the hydrogen ion, \( \{H^+\} \).
The true concentration, \( [H^+] \), is equal to the activity divided by an activity coefficient.

\[
[C] = \frac{\{C\}}{\gamma}
\]

The activity coefficients for ions in an electrolyte are related to the concentration of ions.
The ionic strength, \( \mu \), is defined as

\[
\mu = \frac{1}{2} \sum_i C_i Z_i^2
\]

where \( C_i \) is the molar concentration [moles/L] of the \( i \)th ion, \( Z_i \) is its charge, and the
summation extends over all of the ions in the solution. The activity coefficient, \( \gamma_i \), is a
nonlinear function of the ionic strength. Several relationships have been proposed. The
Davies relationship for activity is valid for ionic strengths up to 0.5 M (see Figure 5-9).
Reactor Characteristics

The activity coefficient correction is generally unnecessary for dilute solutions. However, in this laboratory we will use sodium chloride for density matching and the concentration of sodium chloride will be high enough that the activity of the hydrogen ions will be significantly decreased.

**Acid Tracer Design**

The reactors are 30 cm long and 15 cm wide. If the depth is limited to 5 cm, then the total volume is 2.25 L and with the maximum pumping rate (380 mL/min) for our peristaltic pumps the residence time is 6 minutes. Acid tracer can be added as 0.05 M HCl. If the reactor volume is 2.25 L with 220 µeq/L of H⁺ then 500 µeq of H⁺ (or 10 mL 0.05 M HCl) are required.

The tracer can be poured directly into the first chamber of your reactor or it can be injected into the influent line. Red dye or methylene blue can also be added to the tracer or used separately to qualitatively observe the turbulence levels of the jets.

**Mass balance**

Collect data that makes it possible to perform a mass balance on hydrogen ions. Note that if it is expedient to shorten an experimental run such that there is a significant quantity of the tracer residual in the reactor, that the residual (stored) tracer can be measured by pouring the reactor contents into a container and measuring the pH of the resultant mixture.

**Reactor Design**

**Baffle Design**

Baffles can be added to tanks to decrease the ability of the solution to travel quickly from the tank inlet to the tank outlet. The goal of the baffle design depends on whether the tank is designed for a reaction or for separation. The baffles in reactors should generally be designed to achieve mixing in each of the baffled zones. The baffles in tanks designed for separation (clarifiers) should be designed to achieve uniform flow (a much more difficult goal to achieve). Mixing within each baffled zone could be achieved with a propeller mixer or by appropriately sized ports in the baffles. If port mixing is desired the energy for mixing is provided by the kinetic energy of the fluid flowing through the ports.
The flow characteristics of a baffled tank are complex and would require computational fluid dynamics to model. In lieu of developing a CFD model we will turn to dimensional analysis to help us characterize the mixing efficiency of a baffled reactor segment. The independent parameter that we will measure to characterize the reactor is its Peclet number.

The design goal is to determine the diameter and spacing of the ports required to achieve adequate mixing. The fluid flow out of the ports is jet flow. The jets entrain and mix with the surrounding fluid. To develop effective mixing the jet should be turbulent. The transition between turbulent and laminar behavior for jets occurs at a jet Reynolds number of a few hundred$^2$.

\[
\text{Re}_{\text{jet}} = \frac{V_{\text{jet}} d_{\text{jet}}}{\nu} \quad \text{or} \quad \text{Re}_{\text{jet}} = \frac{4Q_{\text{jet}}}{\pi d_{\text{jet}} V} \quad \text{or} \quad \text{Re}_{\text{jet}} = \frac{4Q_{\text{reactor}}}{n_{\text{ports}} \pi d_{\text{jet}} V}
\]

The optimal port spacing for maximum mixing could be based on the spread of the jet in the distance to the next baffle. Jets expand in the radial direction at a rate of approximately 10% of the distance the jet travels axially. Thus the port spacing could be in a rectangular grid with the distance between ports equal to 10% of the distance between baffles. This spacing may be smaller than practical since it will require a large number of ports.

An additional constraint on port design is that the head loss through the ports not be excessive. The hydraulic grade line (and thus depth of each baffled reactor) will drop by a distance equal to the head loss through the ports. The head loss through the ports is given by the orifice equation

\[
Q_{\text{orifice}} = K_{\text{orifice}} A_{\text{orifice}} \sqrt{2g\Delta h}
\]

where the orifice coefficient, $K_{\text{orifice}}$, has a value of approximately 0.6, the area of the orifice is $A_{\text{orifice}}$, and the head loss through the orifice is $\Delta h$.

\[
Q_{\text{orifice}} = K_{\text{orifice}} \frac{\pi d_{\text{orifice}}^2}{4} \sqrt{2g\Delta h}
\]

\[
Q_{\text{reactor}} = n_{\text{orifice}} K_{\text{orifice}} \frac{\pi d_{\text{orifice}}^2}{4} \sqrt{2g\Delta h}
\]

where $n_{\text{orifice}}$ is the number of ports. Solving for the port diameter we obtain.

\[
d_{\text{orifice}} = \sqrt[4]{\frac{4Q_{\text{reactor}}}{\pi n_{\text{orifice}} K_{\text{orifice}} \sqrt{2g\Delta h}}}
\]

$^2$Personal communication with Dr. Cowen.
Chlorine Contact Tank Design

The design objective for chlorine contact tanks is to maximize the inactivation of pathogens by maximizing the contact time between the chlorine and the pathogens before the water is sent to the distribution system. This objective has been codified with the contact time for a tank defined as the time for the effluent of the tank to reach 10% of the influent value after a step change in the influent.

### Table 5-1. Comparison of $t^* \text{ at } F = 0.1$ for non-ideal reactors (Malcolm Pirnie, 1991)

<table>
<thead>
<tr>
<th>Baffling Condition</th>
<th>Guidance manual value of $t^* \text{ at } F = 0.1$</th>
<th>Extent of Baffles</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unbaffled (CMFR)</td>
<td>0.1</td>
<td>No baffles, agitated basin with low length to width ratio, high inlet and outlet flow velocities</td>
</tr>
<tr>
<td>Poorly baffled</td>
<td>0.3</td>
<td>Single or multiple unbaffled inlets and outlets, no intrabasin baffles</td>
</tr>
<tr>
<td>Average</td>
<td>0.5</td>
<td>Baffled inlet or outlet with some intrabasin baffles</td>
</tr>
<tr>
<td>Superior</td>
<td>0.7</td>
<td>Perforated inlet baffles, serpentine or perforated intrabasin baffles, outlet weir or perforated launders</td>
</tr>
<tr>
<td>Perfect (PFR)</td>
<td>1.0</td>
<td>Very high length to width ratio (pipeline flow), perforated inlet, outlet and intrabasin baffles</td>
</tr>
</tbody>
</table>

Procedures

The reactor you will be working with can be easily modified by installing various configurations of perforated baffles (Figure 5-10). Your objectives are

- to modify the reactor to obtain a maximum value of $t^* \text{ at } F = 0.1$
- to document your progress toward this goal by obtaining appropriate experimental data
- to compare your experimental data with appropriate models

Note that you are allowed to collaborate with other teams to obtain the results from additional tests. All data sharing must be documented in your report.

Baffle installation

The baffles can be installed by rolling a 3 mm diameter roll of putty and applying the putty to the bottom and one side of the baffle. Carefully install the baffle by rotating it.
into place (so the putty on the one side doesn’t have to slide) and then pressing it down (so the putty on the bottom doesn’t have to slide). Install the two bolts with wing nuts to hold the baffle in place. Add a roll of putty to the corner formed at the unsealed side of the baffle and press the putty into place.

**Testing protocol**

To establish the steady-state hydraulic profile of your reactor it will be necessary to operate at normal flow for a minute or more prior to injecting the tracer. The reactor volume can be adjusted by changing the reactor effluent weir height. Data collection can be by the pH meter software or by the Process Controller. The flow rate can also be varied. When choosing flow rates, consider that it will be necessary to run tests for several hydraulic residence times. As part of your experimental protocol ensure you have all of the necessary data for analysis including flow rates, tracer volumes, tracer concentration, reactor volumes, and tracer injection times.)

To ensure that everything is working properly I recommend that you begin by first testing a CMFR. Use the CMFR data to verify that you obtain mass balance and that you obtain the expected exit age response.

For each test make sure that you accurately measure the reactor volume, residual reactor pH, and the flow rate. The reactor volume should be measured by pouring the reactor contents into another container and then using the 5k electronic balance to determine the volume of water. Measure the residual concentration of hydrogen ions in the reactor by measuring the pH of the container contents. The flow rate can be accurately measured by massing an accurately timed sample from the pump (not from the reactor effluent).

The pH probes are extremely sensitive to voltage fluctuations. The peristaltic pumps produce small amounts of static electricity as the rollers squeeze over the pump tubing. The result is a small change in voltage level of the solution in the reactor. This voltage fluctuation will be picked up by the pH probe and cause poor quality data. To eliminate this problem a small grounding rod should be installed in the reactor and connected to an electrical ground. The stirrer housing is grounded and thus any metal that is directly connected to the stirrer housing is grounded. An alternate way to ground the reactor solution is to have the water flow through a short section of grounded metal tubing.

**Prelab Questions**

1) Calculate the concentration of bicarbonates in distilled water in equilibrium with the atmosphere. (This is similar to the Gran Plot prelab requiring the use of Solver.)

2) Calculate the change in hydraulic grade line between baffled sections of a reactor with a flow rate of 300 mL/min. The reactor baffles are perforated with 24 holes 1 mm in diameter.

3) Calculate the concentration of hydrogen ions in the reactor effluent given the following situation. You added enough NaCl to the distilled water flowing through the reactor to match the density of 0.05 N HCl. You measured the pH in the reactor effluent to be 4.0. (Hint: the activity of the hydrogen ions is less than 1.)
Data Analysis

Use a consistent set of units throughout your data analysis and include the units in your spreadsheet and report!

1) Convert the pH measurements into proton concentration including the correction for activity.

2) Create the data E curve from

\[ E_r = \frac{C_r}{M_r}. \]

3) Create model E curves for CMFR in series and for the one dimensional advective dispersion equation.

4) Use multivariable nonlinear regression to obtain the best fit between the model E curves and the data E curve by using Solver to minimize the sum of the squared errors. Allow Solver to vary the values of \( \theta, M_r \), and either N or Pe (depending on the model).

5) Compare \( M_r \) obtained using Solver with the actual \( M_r \) added and comment on any differences.

6) Compare \( \theta \) obtained using Solver with the measured value of \( \theta \) and comment on any differences.

7) Plot data and model E curves and if appropriate show both model E curves and explain which model fits best and compare with your expectations.

8) Evaluate whether there is any evidence of “dead volumes” or “short circuiting” in your reactor.

9) Make a recommendation for the design of a full scale chlorine contact tank. As part of your recommendation discuss the following:
   - Serpentine flow paths versus perforated baffled reactors.
   - Effects of scaling up to full size based on dimensional analysis.
   - Effects of Reynolds scale effects on modeling baffled and serpentine flow.
   - Cumulative head loss through the contact tank.

References


### Lab Prep Notes

#### Table 5-2. Equipment list

<table>
<thead>
<tr>
<th>Description</th>
<th>Supplier</th>
<th>Catalog number</th>
</tr>
</thead>
<tbody>
<tr>
<td>reactor with baffles</td>
<td>CEE shop</td>
<td></td>
</tr>
<tr>
<td>variable flow digital drive</td>
<td>Cole Parmer</td>
<td>H-07523-30</td>
</tr>
<tr>
<td>Easy-Load pump head</td>
<td>Cole Parmer</td>
<td>H-07518-00</td>
</tr>
<tr>
<td>PharMed tubing size 18</td>
<td>Cole Parmer</td>
<td>H-06485-18</td>
</tr>
<tr>
<td>20 liter HDPE Jerrican</td>
<td>Fisher Scientific</td>
<td>02-961-50C</td>
</tr>
</tbody>
</table>

#### Table 5-3. Reagent list

<table>
<thead>
<tr>
<th>Description</th>
<th>Supplier/Source</th>
<th>Catalog number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acid tracer 0.5 N HCl</td>
<td>MG Newell</td>
<td>07704-1</td>
</tr>
</tbody>
</table>

1) Use # 18 tubing for baffled tank.

2) Organize team research so they don’t use the same materials and so they answer different questions.