

2. Scaling Analysis and Basic Models for Aquatic Systems

In a previous chapter we derived the Conservation of Mass in both an integral and differential form. While these equations completely describe the fate of scalar species, they are difficult to solve directly for many real systems with complex boundaries and temporally varying inputs. In many cases, however, appropriate assumptions and approximations can be made to reduce the complexity of the governing equations and arrive at quick and simple solutions. This chapter begins with a basic discussion of scaling, an analysis technique that reveals terms that can be appropriately neglected in the governing equations. As specific examples, we derive two simple models, *Plug-Flow* and *Continuously-Stirred*, which are often used to represent aquatic systems.

Scale Analysis

The complexity of a system can be reduced by recognizing that the inherent spatial and temporal scales of any system constrain its behavior. Consider a small pond of volume, $V = 10 \text{ m}^3$, which is fed by a river with constant flow rate, $Q = 1 \text{ m}^3/\text{hr}$. From dimensional reasoning, we expect the water in this pond to be replaced every $T_R = V/Q = 10 \text{ hr}$. Similarly, we expect that any chemical constituent dumped into the pond will be flushed out in approximately this time scale. Thus, the spatial scale of the pond constrains the transport behavior observed in the pond. The time-scale, T_R , is commonly known as the *mean hydraulic residence time*. It is the average time that each water parcel entering a system remains in that system. Processes that occur over time-scales much longer than T_R will not be observable in the pond and can be neglected. Alternatively, processes that occur over time-scales much less than T_R will impact the water quality in the pond, and must be considered in any model of the pond. For example, suppose the water entering the pond is an industrial wastewater that is fully depleted of oxygen and polluted with fine sediment. Suppose the time required to reaerate the water through atmospheric exchange is $T_{\text{air}} = 1 \text{ hr}$. The time to remove the sediment from the water column through settling is $T_{\text{settling}} = 100 \text{ hrs}$. By comparing the process time-scales with the residence time, we quickly determine that the effect of settling will be negligible ($T_{\text{settling}} \gg T_R$) but the affect of reaeration will be important ($T_{\text{air}} \ll T_R$) in the pond. Thus, a model of the pond's water quality could neglect settling, but must include reaeration.

Table 1. Summary of Basic Time –Scales

<i>Process</i>	<i>Time Scale</i>
Residence time in volume V with flow rate Q	$T_R \sim V/Q$
Diffusion at rate D over distance L	$T_D \sim L^2/D$
Advection at speed U over distance L	$T_U \sim L/U$
Reaction at rate k	$T_k \sim k^{-1}$

As shown in the above example, the comparison of processes using a single common scale (e.g. time) provides a quick way to identify dominant processes and eliminate negligible ones. Other time-scales can be derived from dimensional constraints. For example, given a length scale, L ,

and a diffusion coefficient, D , with units $[L^2T^{-1}]$, the only combination that yields a unit of time is, $T_D \sim L^2/D$, which is the time scale describing transport by diffusion over a distance L . Similarly, the time-scale for advection by current U over distance L is $T_U \sim L/U$. Here, the tilde, \sim , is read ‘scales upon’. For the advection time scale, it is also true that $T_U = L/U$, because this is the exact time required to travel distance L at speed U .

Now we will use scale analysis to compare each process in the Conservation of Mass equation. If we consider only first-order reactions (see next section), the source term $S = kC$, where $k [s^{-1}]$ is the reaction rate. From dimensional reasoning, one should immediately recognize that the time scale for such a reaction is simply, $T_k \sim k^{-1}$. With homogeneous diffusion the governing equation is,

$$(1) \quad \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} \pm kC.$$

This equation has three units: mass, time, and length. Three processes, advection, diffusion and reaction, contribute to the evolution of (or unsteadiness in) the concentration, $\partial C/\partial t$. To determine which processes are important, we compare the magnitudes of each term. To do this we must recast each variable into a dimensionless form of $O(1)$ using the characteristic scales of the system. Let’s consider a system with dimensions L_x, L_y, L_z . Let T_0 represent the time scale of interest, or the time scale for which we want prediction. C_0 is the initial concentration. We use these characteristic scales to create non-dimensional variables, denoted with an asterisk, which will be $O(1)$ by construction. For example, with L_x the scale of the system in the x -coordinate, $x^* = x/L_x$ will be $O(1)$ within the system domain. The full set of dimensionless variables is given below.

$$(2) \quad (x^*, y^*, z^*) = (x/L_x, y/L_y, z/L_z); \quad C^* = C/C_0; \quad \text{and} \quad t^* = t/T_0$$

We use the new variables to replace C, x, y, z and t in (2), and note that, e.g., $\partial x^2 = \partial x \partial x$. For simplicity in this example, we consider u, v, w, D_x, D_y, D_z , and k to be constants which will not be scaled. Finally cancel C_0 from each term to find

$$(3) \quad \frac{1}{T_0} \frac{\partial C^*}{\partial t^*} + \frac{u}{L_x} \frac{\partial C^*}{\partial x^*} + \frac{v}{L_y} \frac{\partial C^*}{\partial y^*} + \frac{w}{L_z} \frac{\partial C^*}{\partial z^*} = \frac{D_x}{L_x^2} \frac{\partial^2 C^*}{\partial x^{*2}} + \frac{D_y}{L_y^2} \frac{\partial^2 C^*}{\partial y^{*2}} + \frac{D_z}{L_z^2} \frac{\partial^2 C^*}{\partial z^{*2}} \pm kC^*$$

unsteadiness three advection terms three diffusion terms reaction

Since each starred variable is $O(1)$ by construction, we can compare the unsteadiness, the advection, the diffusion, and the reaction terms simply by comparing the leading coefficient of each term. Comparing the advection terms,

$$(4) \quad \frac{\text{longitudinal advection}}{\text{lateral advection}} = \frac{uL_y}{vL_x} = \frac{\text{time - scale for lateral advection}}{\text{time - scale for longitudinal advection}} = \frac{T_V}{T_U}$$

$$\frac{\text{longitudinal advection}}{\text{vertical advection}} = \frac{uL_z}{wL_x} = \frac{\text{time - scale for vertical advection}}{\text{time - scale for longitudinal advection}} = \frac{T_W}{T_U}$$

If both ratios are much greater than one (by an order of magnitude or more), then only longitudinal advection is significant, and the other two terms may be dropped. This is a common approximation for channels and rivers, for which typically $u \gg v, w$. As noted in (4), these are ratios of time scales. If longitudinal advection occurs more quickly, $T_U \ll T_V$ and $T_U \ll T_W$, and we neglect lateral and vertical advection. Similarly, compare the relative importance of diffusion and advection.

$$(5) \quad \frac{\text{longitudinal advection}}{\text{longitudinal diffusion}} = \frac{uL_x^2}{D_x L_x} = \frac{uL_x}{D_x} = \frac{T_D}{T_U}$$

This ratio is the Peclet number (Pe). If $Pe \gg 1$, then advection is faster than diffusion ($T_U \ll T_{D_x}$) and transport over domain scale, L_x , is dominated by advection. The contribution of longitudinal diffusion to $\partial C/\partial t$ is negligible. Conversely, if $Pe \ll 1$ then diffusion is faster ($T_{D_x} \ll T_U$) and it dominates transport over L_x ; the impact of advection on $\partial C/\partial t$ is negligible. The Peclet number is discussed further in Chapter 5. Finally, we compare the reaction term to the advection term.

$$(7) \quad \frac{\text{longitudinal advection}}{\text{reaction}} = \frac{u}{L_x k} = \frac{T_k}{T_U}$$

If $T_k \gg T_U$, then very little reaction will occur in the time taken for fluid to advect through the domain of interest (L_x), so the reaction term should be neglected, consistent with the ratio in (7).

Basic Hydraulic Models

Below we describe two simple flow models for the special cases when advection or diffusion dominate the transport in the system. Both models are based on simple box systems with longitudinal dimension, L , longitudinal velocity, U , and longitudinal diffusion, D_x . The Peclet number ($Pe = UL/D_x$) indicates whether advection or diffusion dominates this system. For $Pe \rightarrow 0$, diffusion will dominate. For $Pe \rightarrow \infty$, advection will dominate.

Plug-Flow Reactor [$Pe \rightarrow \infty$] This model assumes that fluid particles pass through and leave the system in the same order than they enter. It assumes that perfect mixing occurs in the lateral and vertical directions, but that no mixing occurs in the longitudinal direction, i.e. $D_x = 0$. This creates slabs of fluid that do not communicate with one another as they pass through the system. With $D_x = 0$, the Peclet number, $Pe = \infty$, indicating that transport through the system is

dominated by advection. For this model to be reasonable, the lateral length-scales must be sufficiently small (or the lateral diffusion sufficiently large) such that the time required to mix a scalar species laterally ($L_{y,z}^2/D_{y,z}$) is much shorter than the time to advect that species over the longitudinal distance L . Considering Figure 1, one can easily recognize that any chemical introduced at $x = 0$ will arrive at $x = L$ at exactly the advection time scale, $T_U = L/U$. Multiplying by the unity ratio A/A , we find $T_U = \forall/Q = T_R$. That is, for a plug-flow model each slab of fluid remains in the system for exactly the residence time, T_R .

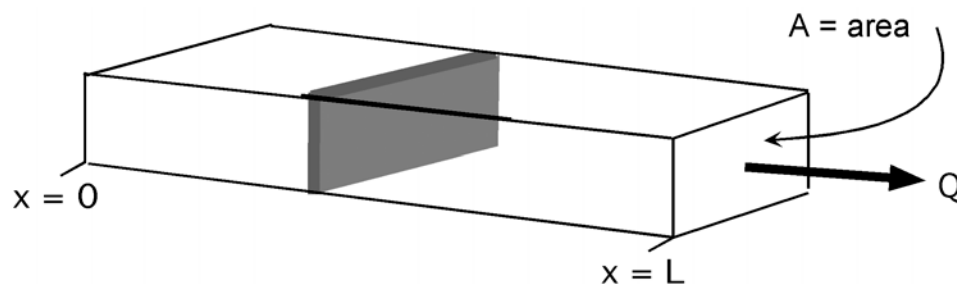


Figure 1. Plug Flow Reactor Model

Stirred Reactor [$Pe \rightarrow 0$] This model assumes that as each fluid parcel enters the reactor it is instantaneously mixed throughout the volume. Effectively, $D \rightarrow \infty$ so that $Pe = UL/D = 0$. If tracer is introduced at $x = 0$, $t = 0$, some fraction of tracer will immediately appear at the exit, $x = L$, so that some fluid remain in the system far less than T_R . But, other parcels remain in far longer than T_R so that T_R is still the mean residence time. This idea is developed mathematically below.

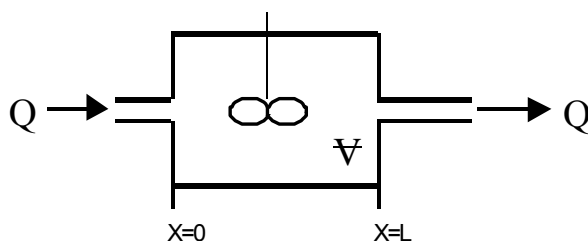


Figure 2. Stirred Reactor Model

To select a Plug-Flow Model or a Stirred Reactor Model we consider the Peclet number of the system. The Peclet number reveals the relative magnitude of the residence time, T_R , and the time-scale, T_D , required to mix the system to uniform concentration through diffusive processes. For plug flow $T_D = \infty$, because it never mixes longitudinally. For a stirred reactor $T_D = 0$, because it mixes instantaneously. Of course these conditions are never perfectly met. But, *relatively speaking*, the mixing time could be approximately infinite (much longer time than other processes), or approximately zero (much less time than other processes). So, to determine what transport model is appropriate, we can compare time scales for advection through the system (T_R) and mixing within the system. If $T_D \ll T_R$ then a stirred reactor is reasonable. If $T_D \gg T_R$ then a plug flow reactor is reasonable. A lake characteristically has a large water volume and low velocity (T_R is long) so we expect $T_R \gg T_D$, such that a lake system approaches a Stirred Reactor. In contrast, a river has characteristically high velocity and limited area, so we expect $T_R \ll T_D$ and the system approaches a Plug-Flow model.

Residence Time Distributions

Because real systems are complicated and do not fit the Plug-Flow or Stirred Reactor models perfectly, we need a more specific way to describe the transport through unique systems. Ultimately we want to know how long each parcel of fluid remains in the system. But tracking each an every parcel of fluid is prohibitive. So, we settle for knowing the statistical distribution of residence times. The residence time distribution function, $RTD(t)$, describes the time spent in the system by different fractions of fluid, *i.e.* it is the probability density function for residence time. By construction, $[RTD(t) \Delta t]$ is the fraction of incoming water that stays in the system for a length of time between t and $t+\Delta t$. To find the $RTD(t)$ for a system, you must release a mass, M , of conservative tracer at the inlet and measure the concentration at the outlet of the system, $C(t)$.

$$(8) \quad RTD(t) = \frac{QC(t)}{\int_0^{\infty} QC(t)dt} = [T^{-1}]$$

The integral in the denominator should equal the total mass released, M . However, some dye may be lost due to adsorption to plant and soil surfaces, degradation by sunlight, or trapping in stagnant regions of the system. Or, the tail of the distribution, the low concentrations at the very end of the sampling, may be too low in concentration to accurately measure. Thus, calculation of the denominator of (10) is an important check of mass recovery. If the denominator is much less than the injected mass, M , the RTD will not be very accurate. Finally, by definition $\int_0^{\infty} RTD(t)dt = 1$. That is, the sum of probabilities must be 1. If the flow is steady, $Q = \text{constant}$, (8) is simplified to

$$(9) \quad RTD(t) = \frac{C(t)}{\int_0^{\infty} C(t)dt}$$

The moments of RTD(t) define the transport behavior of the system. The first moment is called the Detention Time, T_{det} , which is the average time that a particle spends in the system. It may also be called the Effective Residence Time.

$$(10) \quad T_{det} = \int_0^{\infty} t \text{RTD}(t) dt = \text{detention time.}$$

A natural system may have regions that are excluded from the flow, *e.g.* regions of dense vegetation and stagnant water, or wake regions behind obstruction or bathymetric features. If excluded zones exist, then the detention time will be less than the theoretical Residence Time, T_R , for that system. This follows directly from the fact that with excluded zones present the effective flow volume is reduced, and the effective residence is similarly reduced. If no zones are excluded from the flow, then $T_{det}=T_R$. This is true for any circulation and any level of internal mixing within the system.

The second moment of the RTD is the variance, σ^2 , and it represents the spread of observed residence times around the mean, T_{det} . The variance in the RTD results from mixing or from a distribution of flow paths and flow speeds through the system. The variance is calculated as,

$$(11) \quad \sigma^2 = \int_0^{\infty} (t - T_{det})^2 \text{RTD}(t) dt.$$

Plug Flow RTD

As described with Figure 2, when a slug of tracer is injected at $t = 0$ at the inlet of a Plug Flow system, every particle of tracer will arrive at the outlet at exactly $t = T_R$. The Residence Time Distribution is described mathematically by a Dirac delta function, defined as $\delta(a) = \infty$ at $a = 0$ and $\delta(a) = 0$ at $a \neq 0$. By definition, $\int_{-\infty}^{\infty} \delta(t) dt = 1$. The Plug Flow RTD is then given by,

$$(12) \quad \text{RTD}(t) = \delta(t - T_R) \quad \text{with implied units of } t^{-1}.$$

From (10) the detention time is

$$(15) \quad T_{det} = \int_0^{\infty} t \delta(t - T_R) dt = T_R$$

Note $T_D = T_R$, consistent with the fact that the Plug-Flow circulation has no exclusion zones.

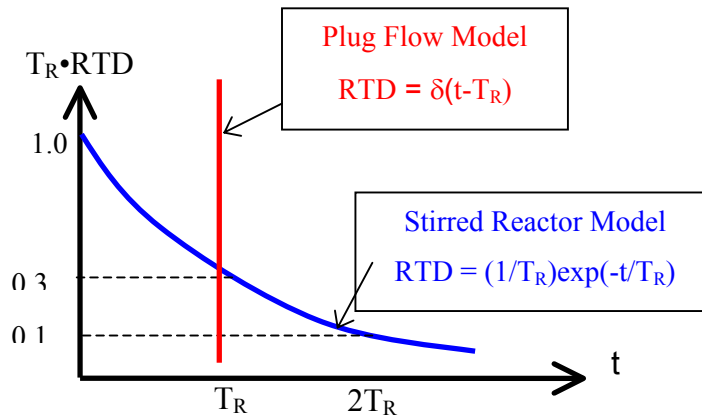


Figure 3. Residence Time Distributions for Plug-Flow and Stirred Reactor Models.

Stirred Reactor RTD

Now consider the stirred reactor shown in Figure 2. We release mass, M , at the inlet at $t = 0$. According to this model, the mass mixes instantaneously producing an initial concentration in the system $C = C_0 = M_0/V$, that is uniform throughout the system. Using a control volume description (see Chapter 2), the evolution of mass within the system follows,

$$(14) \quad \frac{\partial M}{\partial t} = QC_{x=0} - QC_{x=L}$$

After the initial release, the inflow contains no tracer, so $C_{x=0} = 0$. If the system is always mixed, then $C_{x=L} = C$, the concentration everywhere in the volume. Then, using $M = CV$, (14) becomes

$$(15) \quad \frac{\partial C}{\partial t} = -\frac{Q}{V}C = -\frac{1}{T_R}C.$$

With $C = C_0$ at $t = 0$,

$$(16) \quad C(t) = C_0 \exp(-t/T_R)$$

Then from (9),

$$(19) \quad \text{RTD}(t) = \frac{C_0 \exp(-t/T_R)}{\int_0^\infty C_0 \exp(-t/T_R) dt} = \frac{C_0 \exp(-t/T_R)}{T_R C_0} = \frac{\exp(-t/T_R)}{T_R}$$

For (19), the zeroth moment properly yields one.

$$\int_0^{\infty} \text{RTD}(t) dt = \int_0^{\infty} \frac{\exp(-t/T_R)}{T_R} dt = -T_R \left[\frac{\exp(-t/T_R)}{T_R} \right]_0^{\infty} = 1$$

The first moment gives the mean detention time. Sidebar: $\int x e^{ax} dx = \frac{e^{ax}}{a^2} (ax - 1)$

$$(18) \quad T_{\text{det}} = \int_0^{\infty} t \text{RTD}(t) dt = \int_0^{\infty} t \frac{\exp(-t/T_R)}{T_R} dt = \frac{1}{T_R} \left[\frac{\exp(-t/T_R)}{1/T_R^2} (-t/T_R - 1) \right]_0^{\infty} = T_R$$

Again, $T_D = T_R$, because the entire volume communicates with no exclusion zones.

Combining Residence Time and Reactions

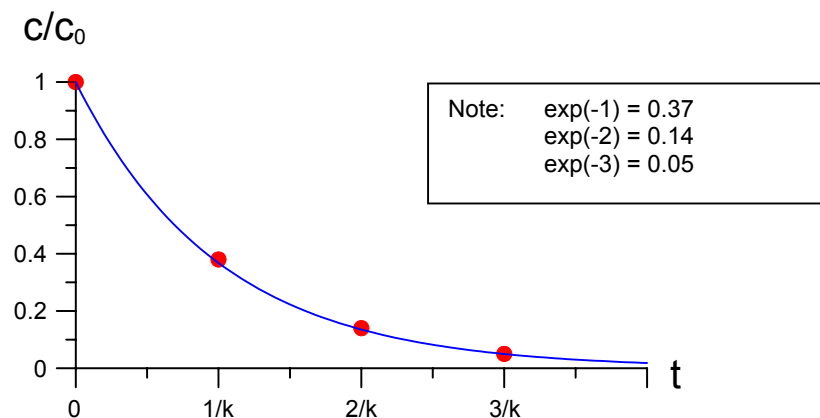
If the rate of loss or gain of mass, dM/dt , is proportional to the amount of substance present, M , to the first power, the reaction is said to be 'first-order'. It is a dirty little secret of environmental engineering that we assume first-order reactions even if we don't really know. But, it is quite often accurate. For a discrete volume, the first-order reaction can also be written $dC/dt \sim C$, or

$$(19) \quad dC/dt = kC$$

where $k [s^{-1}]$ is the reaction rate coefficient. If at $t = 0$, $C = C_0$, then

$$(20) \quad C(t) = C_0 \exp(-kt) \quad \text{or} \quad C/C_0 = \exp(-kt).$$

The decay of C due to a first-order reaction is shown below.



37% of the species remains after the nominal reaction time-scale, $T_k = 1/k$. By convention, a better estimate of the time required for total removal is $T_{95} = 3/k$. But, acceptable removal depends on the toxicity of the chemical. If five percent remains, is it safe?

Finally, to predict the fate of a substance in a particular system we must combine the above model for reaction with the model for transport. If we could follow a discrete packet of fluid through the system, we would observe that the concentration in that little packet decays at the rate $k[T^{-1}]$. If we could follow every single packet that enters the system, we could ultimately predict the concentration at every point (within every packet) in the system for all time. But, this would be prohibitively time consuming. Instead, we describe the range of packet behavior using the range of possible residence times in the system, *i.e.* using the residence time distribution.

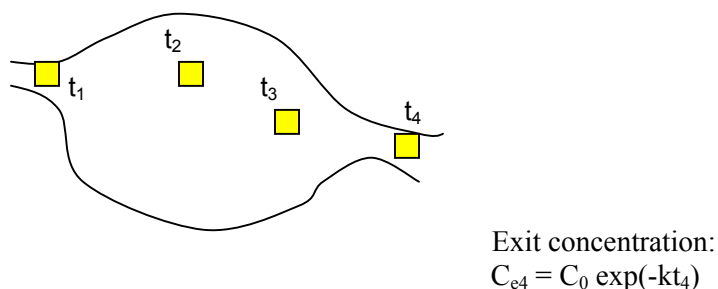


Figure 4a. For a 1st-order reaction, $C(t) = C_0 \exp(-kt)$ governs the chemical evolution within a specific packet of water entering the system. If this packet remains in the system for time t_4 , then the concentration in the packet at the exit will be $C_0 \exp(-kt_4)$.

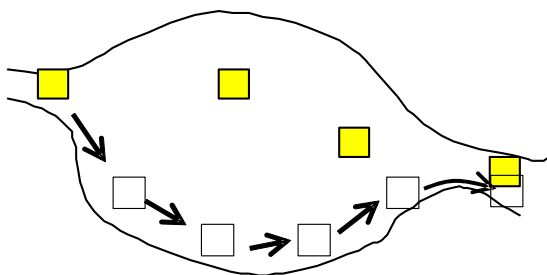
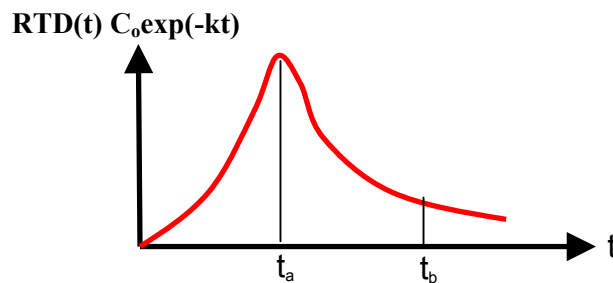


Figure 4b. Consider a different parcel [white boxes], taking a longer route. The concentration in this packet at the exit will be $C_{e6} = C_0 \exp(-kt_6)$ where $t_6 > t_4$, and thus $C_{e6} < C_{e4}$.

The RTD gives the probability of a fluid parcel having a particular residence time. Because each parcel has a different residence time, each parcel will have a different exit concentration. If each parcel entering has concentration C_0 , *i.e.* inlet conditions are steady, then, using a *weighted* average, the steady, mean exit concentration will be

$$(21) \quad \bar{C}_e = \int_0^{\infty} \text{RTD}(t) C(t) dt = \int_0^{\infty} \text{RTD}(t) C_0 \exp(-kt) dt .$$

The first integral is the general expression for any reaction history $C(t)$, and the second integral is specific to first-order reactions. The second integral is represented graphically below. In a parcel with residence time t_a , $C_e = C_0 \exp(-kt_a)$. In a parcel with residence time t_b , $C_e = C_0 \exp(-kt_b)$. The $\text{RTD}(t)$ gives the fraction of water with each residence time, i.e. the average weighting function.



As a simple example, if exactly 50% of the water has a residence time of t_1 and 50% has a residence time of t_2 , then $C_e = 0.5 C_0 \exp(-kt_1) + 0.5 C_0 \exp(-kt_2)$.

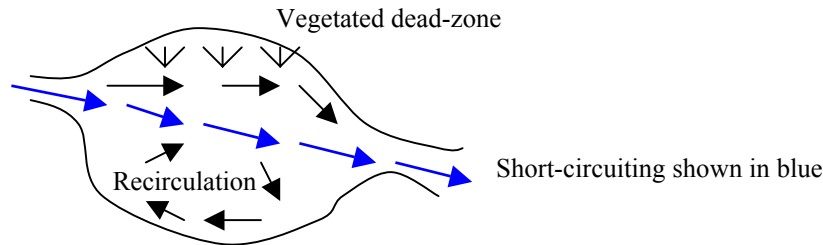
From (21) and assuming a first-order reaction we can calculate the steady exit concentration for a Plug-Flow and Stirred Reactor model with mean residence time, T_R . The mathematical details are given in the first example problem.

Steady Exit Concentration for Plug-Flow: $C_e = C_0 \exp(-kT_R)$

Steady Exit Concentration for Stirred -Reactor: $C_e = C_0 / (1 + kT_R)$

Residence Time Distribution for Real Systems

In real systems, the circulation can never be perfectly described by a plug-flow or stirred reactor model. Real circulation patterns have short-circuiting and dead-zones. Short-circuiting describes a portion of flow that traverses the system in much less than the mean residence time, T_R . Dead-zones are regions of zero mean velocity. The presence of dead-zones can reduce the effective flow volume, so that the detention time, T_{det} , defined by the observed RTD will be less than the ideal residence time, T_R . If there are no exclusion zones, then $T_{det}=T_R$, as is true for both models described above.



A tracer study in the wetland shown above reveals an RTD that is not like Plug Flow or a Stirred Reactor. The presence of dead-zones (exclusion zones) makes the detention time (effective mean residence time) shorter than the ideal value, $T_R = V/Q$. The short-circuiting produces a peak in the RTD at a time less than the detention time, T_{det} .

