CIVE 3331 - ENVIRONMENTAL ENGINEERING
Spring 2003

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Purpose: Lecture #7 CIVE3331

This is a long lecture! The parallels with the text will be apparent near the end. Focus on the IDEAS.

Transport Phenomenon

Transport is encountered in nearly every aspect of environmental engineering. Transport principles must be understood to explain and predict the concentrations and effects of pollutants in the receiving medium, treatment system, and in sampling devices (instruments).

Contaminant Flux

Transport of materials is quantified in terms of flux density or flux. Flux density is the amount of material that passes a point in space per unit area per unit time. Flux is a vector quantity with magnitude and direction. Flux vectors point in the direction of net material motion and their magnitude indicates the rate of motion in that direction.

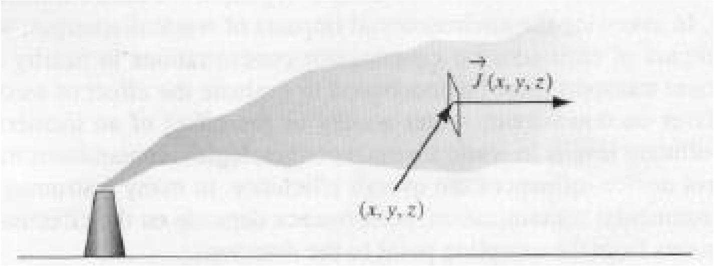

Figure 1. Flux Vector (from:)

Figure 1 depicts how a flux vector is defined. Imagine a frame centered at *(x,y,z)*, oriented perpendicular to the plume time average flow line. The mass of pollutant that passes through this frame per unit time divided by the area of the frame is called the pollutant mass flux. The amount of fluid momentum passing through the frame would be called the momentum flux. Any quantity can be defined in terms of its flux although mass, energy, and momentum are the most common quantities studied in engineering.

Advection

Advection (convection) is the transport of dissolved or suspended material by motion of the host fluid. The prediction of the direction and amount of material transported requires knowledge of the fluid velocity field (the velocity of a fluid particle).

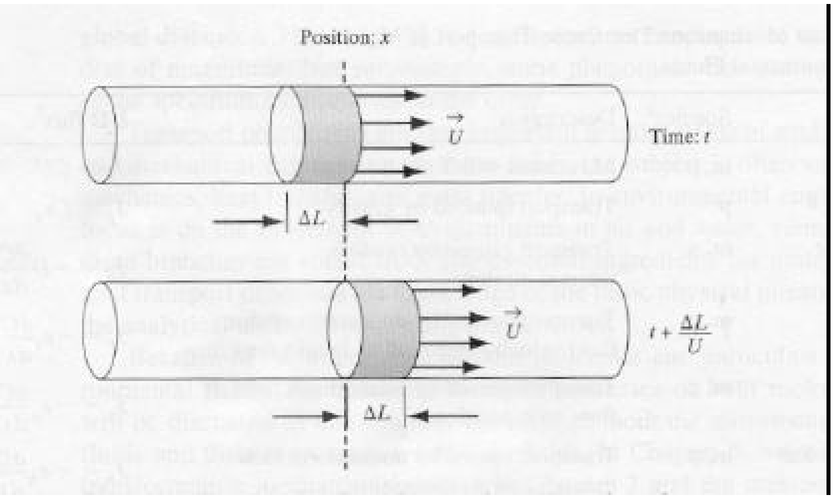

Figure 2: Labeled Fluid Parcel

Figure 2 depicts the flow of a labeled fluid in a tube. One can use the sketch to define various useful properties of the labeled fluid portion as listed.

Table 1. Advection properties

Property	Expression
Mass of labeled fluid	$m = rA\Delta L$
Mass of tracer	$m = CA\Delta L$
Distance traveled by leading (trailing edge)	$x = \Delta L$
Time required to travel distance	$time = \Delta t$
Velocity of leading edge	$u = \frac{x}{time} = \frac{\Delta L}{\Delta t}$
Mass flow through circular frame	$m = rA\Delta L$
Tracer flow through circular frame	$m = CA\Delta L$
Mass through circular frame/unit time	$\frac{m}{time} = \frac{rA\Delta L}{\Delta t}$
Tracer through circular frame/unit time	$\frac{m}{time} = \frac{CA\Delta L}{\Delta t}$
Fluid mass flux	$J = \frac{rUA}{A} = r\frac{Q}{A} = rU$
Tracer mass flux	$J = \frac{CUA}{A} = C\frac{Q}{A} = CU$

The advective flux is the product of the quantity of interest (in this case mass of either host fluid or tracer) and the velocity term. Typically the mean section velocity is used (pipe flow, open channel flow) because fine scale resolution of the velocity field is impossible. In porous media, the pore velocity or average linear velocity is used.

Advection calculations usually use mean section velocity based on discharge measurements.

Discharge

Discharge is the volume rate of flow in a fluid system. It has dimensions of length^3/time.

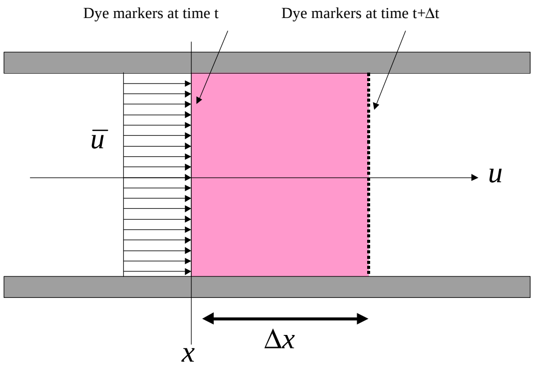

Figure 3: Mean Section Velocity - Uniform Flow Across Section

The figure is a schematic of a conduit completely filled with fluid. Dye markers are placed at location x at some time t. A short period of time later, the position of the dye markers has moved to the location shown on the diagram. The product of the area of the conduit and the distance swept by the dye markers is a volume. The ratio of this volume and time it takes for this volume to be defined is called the volumetric flow rate.

In mathematical terms, the area of the conduit is A. The volume of fluid that passed x in the time interval Δt is $\Delta x A$.

The volumetric flow rate is then

$$Q = \frac{V}{\Delta t} = \frac{\Delta x}{\Delta t} A$$

In the limit this flow rate is defined in terms of the mean section velocity, $Q = \bar{u} A$.

If the velocity varies across the section, the mean sectional velocity is found by integration.

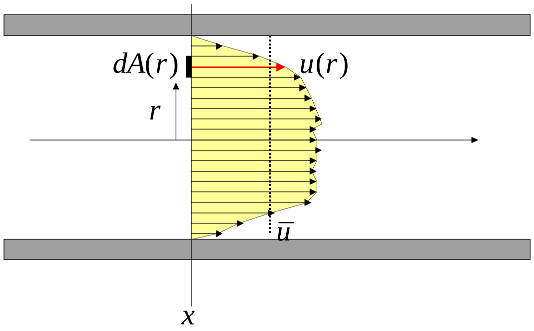

Figure 4: Mean Section Velocity - Non-Uniform Flow Across Section

From calculus we define the differential increment of discharge as, $dQ = udA$. Integration of all the differental elements is expressed as, $\int dQ = \int udA$. From the conceptual definition of average section velocity we can compute its value as the ratio of these two integrals,

$$\bar{u} = \frac{\int udA}{\int dQ}$$

Observe that $Q = \bar{u}A$ is perpendicular to u. For an arbitrary orientation one must compute the scalar product of the velocity vector and the area vector, as depicted in Figure 3.

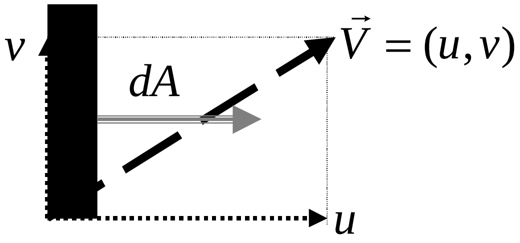

Figure 5: Non-Colinear Velocity and Area Vectors

$$Q = \int \vec{V} \bullet dA = \int u \bullet dA_x + \int v \bullet dA_y$$

Diffusion

Figure 1 represents three snapshots of a closed system with two ideal gasses. Initially the closed system consists of two different ideal gasses at the same pressure separated by a partition (a). When the partition is removed, spontaneous mixing occurs (b). The sharp concentration profiles are rounded. After enough time has elapsed, equilibrium is reached and the concentration of gasses in the system is uniform (c). This mixing process is called molecular diffusion.

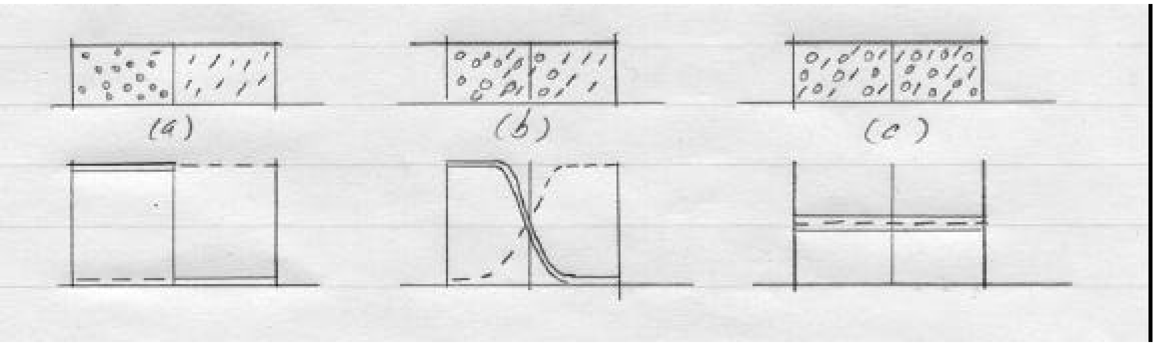

Figure 6. Molecular Diffusion

When the diffusing materials are dilute relative to the host fluid (mole fraction << 1), then the host fluid acts as a conduit and does not need to move for the materials to move. When the materials are not dilute (as in the example above), significant bulk flow occurs of both the diffusing materials and the host fluid. In most civil and environmental engineering problems, the infinite (dilute) dilution condition is appropriate and one ignores the motion effect that the diffusing materials cause on the host fluid.

Figure 7 depicts a physical system with a volatile liquid in contact with the atmosphere through a narrow bore tube. The liquid molecules evaporate to maintain a constant partial pressure equal to the vapor pressure of the liquid. Random motion of these gas molecules takes some of them out of the tube where they are mixed in with the atmosphere.

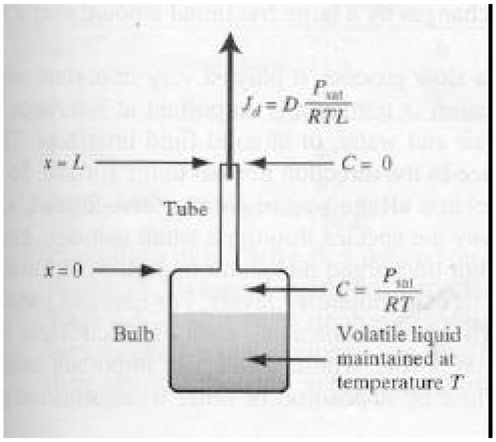

Figure 7. Difussion Experiment

As these molecules leave the tube, more liquid must evaporate to maintain the constant vapor pressure – after a short time the rate of vaporization will become constant. The rate of escape of the molecules is inversely proportional the length of the tube, proportional to the area of the tube, and proportional to the partial pressure of the liquid.

One can incorporate these observations as:

$$\dot{m} \propto -\frac{C_L - C_0}{L} A \,.$$

The constant of proportionality is called the diffusion coefficient and the diffusive flux is expressed as:

$$J = -D\frac{\partial C}{\partial x}$$

This expression is called Fick's first law of diffusion. It can be generalized into three-dimensions as

$$\underline{J} = -D \bullet \left(\frac{\partial C}{\partial x}\underline{i}, \frac{\partial C}{\partial y}\underline{j}, \frac{\partial C}{\partial z}\underline{k}\right) = -D \bullet \nabla(C)$$

The diffusion coefficient is a property of the diffusing species, the host fluid, the temperature, and the pressure.

Kinetic-Molecular Model of Diffusion

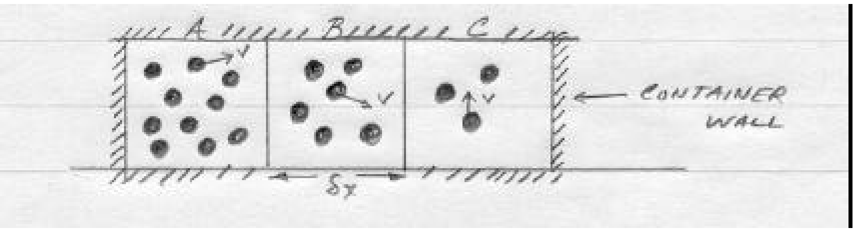

Figure 8. Particles in Closed System

Consider 3 small adjacent cells as depicted in Figure 8. Each particle (molecule) has energy proportional to the square of its molecular velocity – while these velocities might be huge, the particles don't move far before they hit a wall, another particle and their direction changes.

$$E = \frac{1}{2} m|v^2|$$

On average the velocities will have the same magnitude for any species (all tigers run the same speed, all bears run the same speed, but tigers and bears have different speeds). If we consider the energy in each cell we have an energy gradient from cell A to cell C. (We are using the particle number in each cell as a measure of the energy – 10 particles in cell A, 3 in cell C)

$$E_A = \frac{10}{2} m|v^2|; E_B = \frac{6}{2} m|v^2|; E_C = \frac{3}{2} m|v^2|$$

From mechanics principles one can argue that on average more particles will cross from A to B than from B to A in a short time period. Thus cell B will accumulate particles while cell A will tend to lose particles. When the number of particles in each cell is equal, then these will be no further net accumulation in either cell. If we divide each cell by its volume we see that the energy term has dimensions of a concentration multiplied by velocity squared (nearly the same dimension as the diffusion coefficient).

$$\frac{E_A}{dV} = \frac{10}{2}\frac{m|v^2|}{dV} = C_A\frac{|v^2|}{2}$$

Now if we express the difference in energy in adjacent cells as a gradient

$$\nabla E_{A-B} = \frac{C_B - C_A}{dx}\frac{|v^2|}{2} = \frac{\P C}{\P x}\frac{|v^2|}{2}$$

Thus one can conclude that the gradient of energy is proportional to the gradient of concentration. Flux is the flow of energy per unit time from high concentration to low concentration – using this mechanical model it can be expressed as

$$Flux \propto -\frac{\P C}{\P x}\frac{|v^2|}{2}$$

Observe that the flux incorporates the molecular velocity of the molecule relative to the host fluid (a function of molecule size, temperature, and shape). To obtain correct dimensionality we need to express the gradient as energy per unit weight of material (not unit volume) and relate velocity to host fluid properties – ultimately one can arrive at an explanation that matches Fick's law.

In air the diffusion coefficients for a wide range of molecules of various molecular weights and functionalities range from 0.05 cm^2/sec (large volatile organics) to 0.6 cm^2/sec (hydrogen) – a variation of about one order of magnitude. In water the diffusion coefficients range from 0.8 x 10^{-5} cm^2/sec to 4.5 x 10^{-5} cm^2/sec for similar compounds – a variation of about ½ an order of magnitude.

The distance a molecule will travel is proportional to the square root of the product of time and diffusion coefficient – in air 1 meter/per day is reasonable; in water 1 cm/day is reasonable – thus as a process for bulk transport, diffusion is meaningless except at interfaces where it may be the only process. It can achieve huge transport rates at interfaces because of large gradients that occur in these regions.

Dispersion

In actual releases of pollutants into the environment advection based on mean section velocity computations/measurements and diffusion cannot explain observed behavior. As an example, consider the release of smoke particles (0.1 μm) on the left coast of the USA (California) into a westerly wind (wind blowing from west to east) at a speed of 5 meters/sec. Assuming a transcontinental trip, one would expect a spreading of the smoke particles of less than 4 cm over a distance of 5000 meters – thus these two processes alone cannot explain actual behavior.

In actual flows, speeds (velocities) are neither uniform nor steady – the mixing caused by non-uniform flows is called dispersion. Dispersion is a consequence, in modeling, of not being able to accurately describe the velocity field at a small enough scale spatially and temporally to account for the continuous changes in directions and speeds that occurs in real flows. (Read any fluid mechanics textbook – especially the section on turbulent correlation coefficients). There are several processes that arise in fluid flow modeling and measurements that can be called dispersion: shear-induced dispersion; turbulent diffusion; hydrodynamic dispersion.

Shear-Induced Dispersion (Pipe and Open Flows)

Shear-induced dispersion occurs in a flow field where the fluid velocity varies with position in a direction perpendicular to the mean section velocity. If contaminant concentrations in a shearing flow field vary in the direction of mean flow, then a dispersive mixing phenomenon will be observed, producing a net transport of pollutants from regions of high concentration to low concentration.

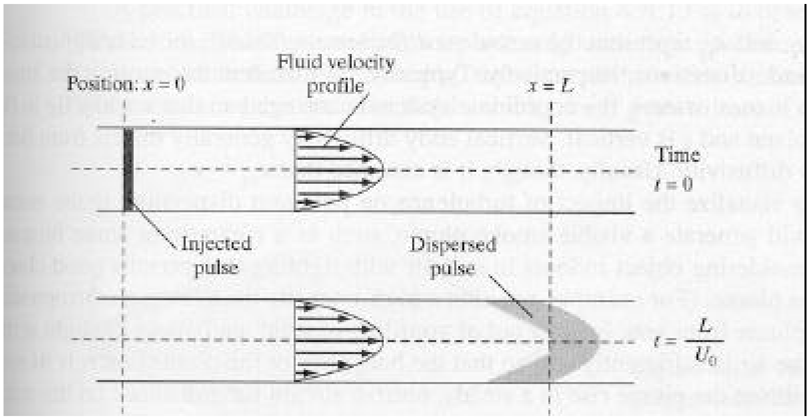

Figure 9. Shear-Induced Dispersion

Typically a Fickian-type model using the section average concentration is used to explain shear-induced dispersion. The diffusion coefficient is called the shear-flow dispersivity.

$$J_{shear} = -\varepsilon_{shear} \frac{\partial \overline{C}}{\partial x}$$

The dispersivity is often estimated from a ratio of velocity variation and a characteristic mixing length based on the dimensions of the flow field.

Turbulent Diffusion (Pipe and Open Flows)

Most flows are turbulent – often we model the flows using ideal (laminar) flow theories and use turbulent flow equations of motion to determine mean velocity values, and turbulent flow variation models to explain the random nature of fluctuations about the mean flow values. In many cases the fluctuations themselves are uninteresting, but their effect on mixing is critical. The mixing caused by the turbulent variations in speed and direction is called turbulent diffusion.

Again a Fickian type model is used, but the point concentration replaces the section average concentration

$$J_{tubulent} = -e_{turbulent} \frac{\partial C}{\partial x}$$

In three dimensions the flux is represented as (isotropic representation – off diagonal terms are not necessarily zero)

$$\underline{J}_{turbulent} = -(e_{xx} \frac{\partial C}{\partial x} \underline{i}, e_{yy} \frac{\partial C}{\partial y} \underline{j}, e_{zz} \frac{\partial C}{\partial z} \underline{k}) = -\begin{pmatrix} e_{xx} & 0 & 0 \\ 0 & e_{yy} & 0 \\ 0 & 0 & e_{zz} \end{pmatrix} \bullet \nabla(C)$$

The diffusion coefficients are known as turbulent diffusion coefficients, or eddy diffusivities. The values of eddy diffusivity vary in space, time, and direction. They are strongly dependent on the nature of the flow field (related to velocity at any location). Closure models (correlations between geometry, flow speed, and eddy diffusivities) are still incomplete, although for many flow systems good predictions are possible.

Hydrodynamic Dispersion (Porous Flows)

Conceptually hydrodynamic dispersion is similar to shear-induced dispersion in pipe and open flows. It occurs because of sectional velocity variation at the pore scale and because of macroscopic flow variation because of medium non-homogeneity. It is not a consequence of turbulence because it occurs even in laminar flows in porous media. Again the working model is a Fickian type model:

$$\underline{J}_{hydrodynamic} = -(e_{xx} \frac{\partial C}{\partial x} \underline{i}, e_{yy} \frac{\partial C}{\partial y} \underline{j}, e_{zz} \frac{\partial C}{\partial z} \underline{k}) = -\begin{pmatrix} e_{xx} & 0 & 0 \\ 0 & e_{yy} & 0 \\ 0 & 0 & e_{zz} \end{pmatrix} \bullet \nabla(C)$$

In hydrodynamic dispersion the diffusion coefficients are called hydrodynamic dispersion coefficients and are directly proportional to the local average linear velocity.

Dispersion is a mixing process that is modeled using a model that is structurally identical to diffusion. The dispersion coefficients are dependent on the flow field for both magnitude and direction. The dispersion coefficients in most flows are orders of magnitude larger than diffusion coefficients making their accurate representation critical for good predictive modeling of pollutant transport.

To model pollutant transport one must first determine the nature of the flow (velocity) field. The study of flow is the subject of your fluid mechanics course(s), for much of this course the flows will be steady and uniform, but you should be aware that this situation (steady and uniform) is a limiting situation that is often not true for real flows – neverless the analysis and desing concepts are relevant, and the mathematics is manageable, so we study such flows.

Mass Transfer at Fluid Boundaries

Transfer across boundaries is of interest in environmental engineering because many treatment technologies depend of transferring pollutants from one phase to another (ammonia stripping as an example). Transport may occur by a variety of mechanisms, diffusion is always present and is often the reat-limiting process, advection plays a role in controlling the layer thickness through which diffusion can occur, for particles (studied later in the course) other forces can play important roles. For engineering purposes, we seek a description (model) that captures overall effects, does not violate mass conservation principles, and is practical to apply.

Mass Transfer Coefficient

The net rate of mass transfer between a fluid and boundary is represented as

$$J_b = k_m (C - C_i),$$

where the k_m term is called the mass transfer coefficient, C is the concentration far from the boundary and C_i is the concentration near the boundary. If the distance is known then the equation can be recast in a Fickian-type structure as

$$J_b = -D\frac{(C - C_i)}{L}$$

and the relationship between the difussion process and mass-transfer coefficient is apparent. Now the distances are often unknown, but this model is the basis for most models of mass transfer at the boundary – the model is sometimes called a linear-driving force model.

These ideas are used to estimate transfer by film-theory (the interface is a thin film), penetration theory (the “film” penetrates into the bulk), and boundary layer theory (film thinkness varies in space as a function of flow velocity). In this class what is important is that the flux across the boundary is proportional to a concentration gradient at the boundary. In the case of water pollution, we will be concerned with the transfer of gas (oxygen) across the air-water boundary. We will use the saturation concentration as the “far-field” value (we get the numerical value from Henry’s Law) and the mixed concentration as the unknown value. The mass transfer coefficient will be called the re-aeration coefficient.

Idealized River Model

Consider an idealized stream of uniform cross section A, width W and uniform, steady velocity u, as sketched in Figure 10. The waste discharge point is just upstream of x = 0. We will study the concentration of some non-conservative material in the system.

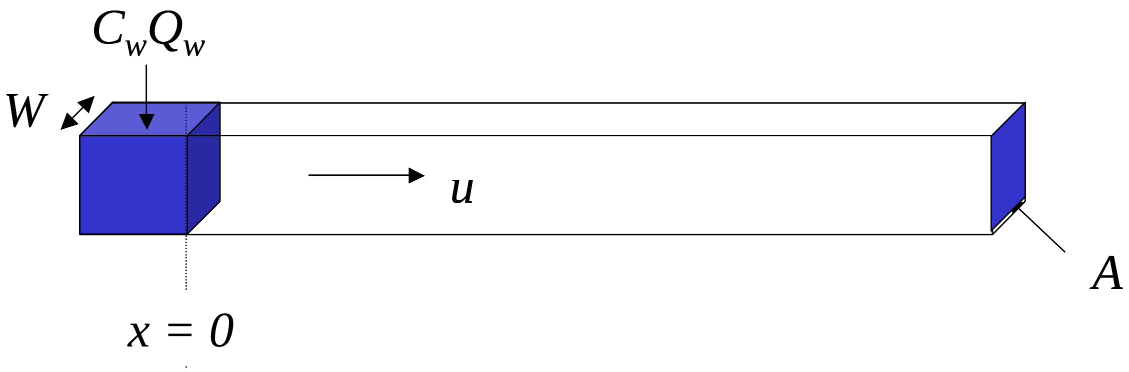

Figure 10. Stream Model

The first step is to study the mixing in the shaded box. In a real system, this mixing occurs over some distance that is governed by the discharge rate, geometry, depth of flow, and waste type. In this case, as a first assumption we assume the mixing occurs over a very short distance and use the principle of conservation of mass to determine the concentration of dissolved O2 or waste in the system.

Now we examine the box more closely. Upstream to the waste the concentration is C_R and the flow is Q_R. After mixing (at x = 0) the concentration is C_o and the flow is Q_o. The relevant sketch and mathematics are shown below.

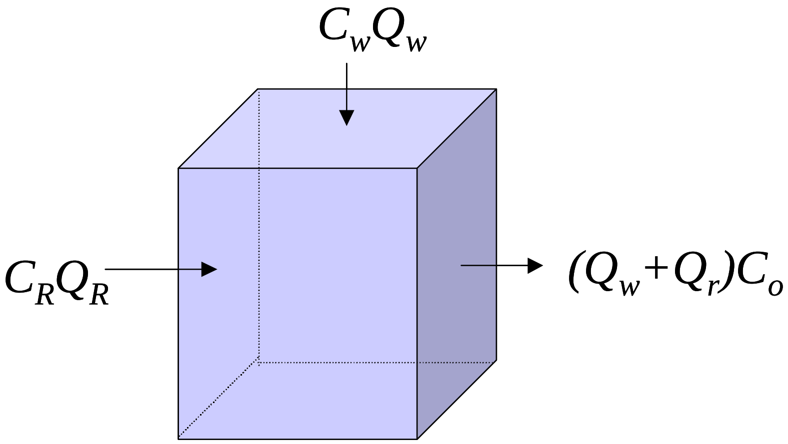

Figure 11. Mixing Zone Properties

Mixing Zone

The mass balance approach is

$$C_0 = \frac{Q_w C_w + Q_R C_R}{Q_W + Q_R}$$

The "C" can be dissolved O2 (which is where we are headed in the present work), L (oxygen demand remaining), or any constituent that can be represented as a concentration. We will be using L and DO shortly, but continue with the generic analysis for now. So now we have the ability to predict the flow and concentration just after mixing. Now we will examine two processes, then combine them. The processes are first-order decay (of BOD) and oxygen transfer across the air-water interface. First the decay.

Decay Downstream of Mixing

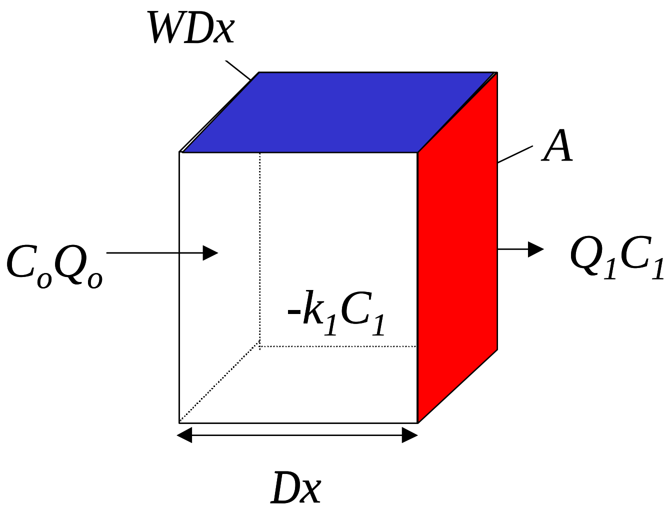

Figure 12. Mass Balance in Section of River

The mass balance principle produces the following equation. The decay term is shown as mass transfer OUT of system.

$$QC_0 - QC_1 - k_1C_1A\Delta x = \frac{d}{dt}C_1A\Delta x$$

Now divide both sides by the volume of the river section.

$$-\frac{Q}{A}\frac{(C_1 - C_0)}{\Delta x} - k_1C_1 = \frac{d}{dt}C_1$$

Now examine the left hand side as the section of the river becomes small (take the limit as Δx becomes infintesimal). We will drop the subscripts 0 and 1, and observe that the left most term is the difference quotient that in the limit becomes a derivative.

$$-\frac{Q}{A}\frac{\partial C}{\partial x} - k_1C = \frac{\partial C}{\partial t}$$

Notice the subtle notation change, the equation is called a partial differential equation. The word partial means that the variable (C in this case) depends partially on x and partially on t. In most engineering problems partial differential equations are typical, equilibrium problems being the notable exception.

As a first step we will examine the case where the time derivative vanishes (equilibrium concentrations). The governing equation is

$$-\frac{Q}{A}\frac{\partial C}{\partial x} - k_1 C = 0$$

This equation can be separated and integrated (treat it as an ODE).

Separate variables: $\frac{dC}{C} = -\frac{k_1 A}{Q} dx$

Integrate:

$$\int \frac{dC}{C} = -\frac{k_1 A}{Q} \int dx =>$$

$$\ln(C) = -\frac{k_1 A x}{Q} + K$$

Simplify: $C(x) = e^K e^{-\frac{k_1 A x}{Q}} = C_0 e^{-\frac{k_1 A x}{Q}} = C_0 e^{-\frac{k_1 x}{u}}$

So the last expression allows us to predict the concentration anywhere downstream of the mixing zone (assuming constant waste discharge into the stream and the other assumptions).

Mass Transfer

Next consider the transfer of mass into the river across the top surface.

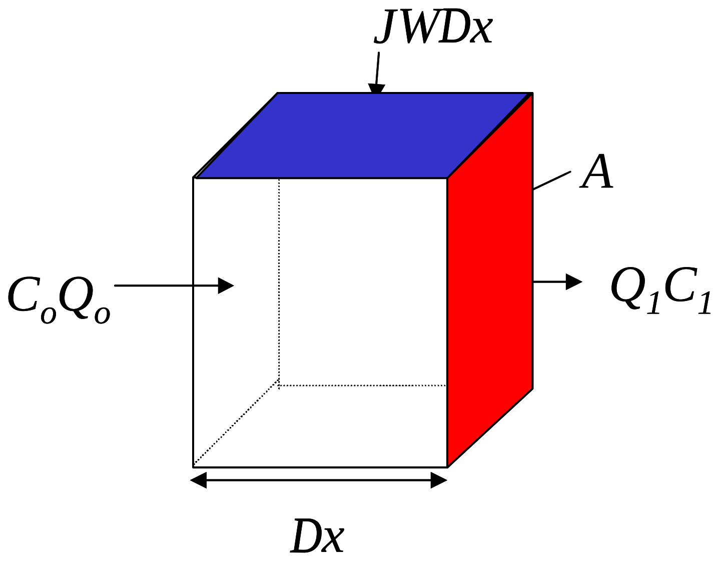

Figure 13. Mass Transfer across Top

The mass balance principle produces the following equation. The interfacial transfer term is shown as mass transfer INTO the system.

$$QC_0 - QC_1 + JW\Delta x = \frac{d}{dt}C_1 A\Delta x$$

Now divide both sides by the volume of the river section.

$$-\frac{Q}{A}\frac{(C_1 - C_0)}{\Delta x} + J\frac{W}{A} = \frac{d}{dt}C_1$$

Now examine the left hand side as the section of the river becomes small (take the limit as Δx becomes infintesimal). We will drop the subscripts 0 and 1, and observe that the left most term is the difference quotient that in the limit becomes a derivative.

$$-\frac{Q}{A}\frac{\partial C}{\partial x} + J\frac{W}{A} = \frac{\partial C}{\partial t}$$

Now examine the case where the time derivative vanishes (equilibrium concentrations). The governing equation is

$$-\frac{Q}{A}\frac{\partial C}{\partial x}+J\frac{W}{A}=0$$

Next insert an expression for the interfacial flux, a linear driving force model is typical so $J=k_2(C_{sat}-C)$

So the expression becomes

$$-\frac{Q}{A}\frac{\partial C}{\partial x}+k_2(C_{sat}-C)\frac{W}{A}=0$$

This equation can be separated and integrated (treat it as an ODE).

Separate variables: $$\frac{Q}{A}\frac{\partial C}{\partial x}=k_2(C_{sat}-C)\frac{W}{A}$$

$$\frac{Q}{A}\frac{\partial C}{(C_{sat}-C)}=k_2\frac{W}{A}dx$$

$$\frac{\partial C}{(C_{sat}-C)}=k_2\frac{WA}{AQ}dx$$

Integrate: $$\int\frac{dC}{C_{sat}-C}=\frac{k_2W}{Q}\int dx$$

Variable substitution to integrate

$$h=C_{sat}-C$$
$$dh=-dC$$

substitute: $$\int\frac{dh}{h}=-\frac{k_2W}{Q}\int dx$$

Integrate: $$\ln(h)=-\frac{k_2W}{Q}x+K$$

Simplify: $h = e^{K} e^{-\frac{k_2 W x}{Q}} = h_0 e^{-\frac{k_2 W x}{Q}}$

Replace original variables

$$C_{sat} - C = (C_{sat} - C_0) e^{-\frac{k_{21} W x}{Q}}$$

Rearrange

$$C(x) = C_{sat} - (C_{sat} - C_0) e^{-\frac{k_{21} W x}{Q}}$$

So the last expression allows us to predict the concentration anywhere downstream of the mixing zone where material is transferring across the interface. Henry's law is used to determine the value of the C_{sat}.

Now put both processes together:

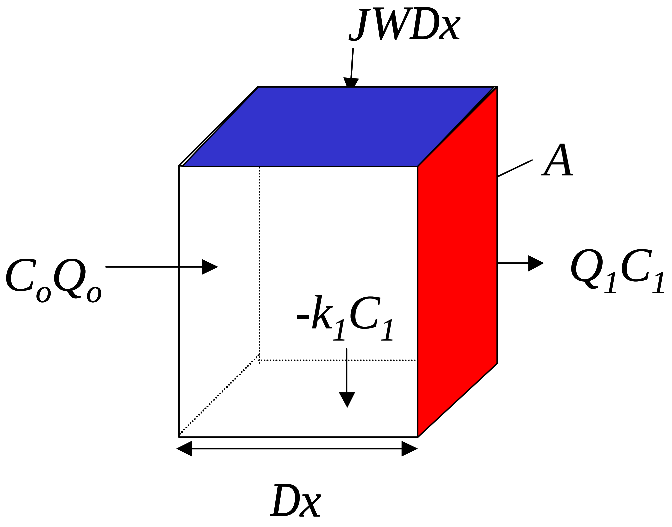

Figure 14. Mass Flux and Decay

The analysis is the same, except both processes are included. Skipping a few steps the combined PDE is:

$$-\frac{Q}{A}\frac{\partial C}{\partial x}+k_2(C_{sat}-C)\frac{W}{A}-k_1C=\frac{\partial C}{\partial t}$$

Considering the time-invariant case:

$$-\frac{Q}{A}\frac{\partial C}{\partial x}+k_2(C_{sat}-C)\frac{W}{A}-k_1C=0$$

Separate and Integrate (it is complicated in this case, but here is how)

Rearrange: $$\frac{\partial C}{\partial x}=k_2(C_{sat}-C)\frac{W}{Q}-k_1\frac{A}{Q}C$$

Group terms: $$\frac{\partial C}{\partial x}=k_2\frac{W}{Q}C_{sat}-k_2\frac{W}{Q}C-k_1\frac{A}{Q}C$$

Group constants: $$\frac{\partial C}{\partial x}=k_2\frac{W}{Q}C_{sat}-(k_2\frac{W}{Q}+k_1\frac{A}{Q})C$$

Substitute: $$a=k_2\frac{W}{Q}C_{sat};b=(k_2\frac{W}{Q}+k_1\frac{A}{Q})$$

ODE in C and x: $$\frac{\partial C}{\partial x}=a-bC$$

Separate: $$\frac{\partial C}{a-bC}=dx$$

Another substitution:

$$\frac{\partial C}{a-bC}=dx;$$
$$U=a-bC;$$
$$dU=-bdC$$
$$\frac{dU}{U}=-bdx$$

Integrate and evaluate:

$$\ln(U)=-bx+K;$$
$$U=U_0e^{-bx}$$

Now substitute back into original variables:

$$(\frac{k_2W}{Q}C_{sat} - \frac{k_2W}{Q}C(x) - \frac{k_1A}{Q}C(x)) = (\frac{k_2W}{Q}C_{sat} - \frac{k_2W}{Q}C_0 - \frac{k_1A}{Q}C_0)e^{-(\frac{k_2W}{Q}+\frac{k_1A}{Q})x}$$

Simplify some more

$$C(x) = [\frac{k_2W}{Q}C_{sat} - (\frac{k_2W}{Q}C_{sat} - \frac{k_2W}{Q}C_0 - \frac{k_1A}{Q}C_0)e^{-(\frac{k_2W}{Q}+\frac{k_1A}{Q})x}]/[\frac{k_2W}{Q} + \frac{k_1A}{Q}]$$

Now this model assumes that the decay of C is proportional to the amount of C still in the river at some location. Such a model might be appropriate for a waste material that undergoes some kind first-order decay – say bio-degredation.

The classical dissolved oxygen model, however, assumes that the decay of DO is proportional to the amount of oxygen demand remaining, not the amount of waste or oxygen itself, so the expression is arrived at slightly differently – the above ideas are useful in helping us find the solution to the classic case

Classical DO Sag Model

Now lets repeat the analysis, only in this case we will consider dissolved oxygen explicitly.

First, in the mixing zone

$$DO_0 = \frac{Q_wDO_w + Q_RDO_R}{Q_W + Q_R} \qquad L_0 = \frac{Q_wL_w + Q_RL_R}{Q_W + Q_R}$$

The decay reaction is

$$\frac{dDO}{dt} = -k_1L = -k_1L_0e^{-k_1t}$$

Observe that the decay of DO is dependent on the amount of L remaining, not the amount of DO, so the situation is not quite as simple as above.

Now write the mass balance for DO in the river cell

$$QDO_0 - QDO_1 + k_2 W\Delta x(DO_{sat} - DO_1) = \frac{dDO_1}{dt}A\Delta x$$

Divide and take limits as before

$$-\frac{Q}{A}\frac{dDO}{dx} + \frac{k_2 W}{A}(DO_{sat} - DO) = \frac{dDO}{dt} = -k_1 L_o e^{-k_1 t}$$

Make the variable substitution for time and space (recall the assumptions for the river)

$$-\frac{Q}{A}\frac{dDO}{dx} + \frac{k_2 W}{A}(DO_{sat} - DO) = -k_1 L_o e^{-\frac{k_1 A}{Q}x}$$

Separate, integrate and simplify (note the presence of the exponential term is a complication, but the result is integrated in the same fashion as before).

$$DO(x) = DO_{sat} - [\frac{k_2 L_0}{k_2 - k_1}(e^{-\frac{k_1 A}{Q}x} - e^{-\frac{k_2 A}{Q}x}) + (DO_{sat} - DO_0)e^{-\frac{k_2 A}{Q}x}]$$

In the text the k_1 is called the de-aeration coefficient and k_2 is called the re-aeration coefficient. Thus re-aeration is dependent on flow width and de-aeration on flow velocity. In the context (and variables of the text) we often use the O'Conner and Dobbins model for k_r.

$$k_R = 3.9(\frac{1}{H})^{3/2}(\frac{Q}{A})^{1/2}$$

H is the depth of flow (A/W). The DO Sag equation is:

$$DO(x) = DO_{sat} - [\frac{k_D L_0}{k_D - k_R}(e^{-\frac{k_D A}{Q}x} - e^{-\frac{k_R A}{Q}x}) + (DO_{sat} - DO_0)e^{-\frac{k_R A}{Q}x}]$$

Now once the equation is established we can study a critical point – the location where DO is the smallest. The critical location is determined from

$$\frac{dDO(x)}{dx} = 0$$

And solve for x_c

The result of setting the derivative to zero and solving for x is

$$x_c = \frac{Q}{A}\{\frac{1}{k_R - k_D}\ln(\frac{k_R}{k_D}[1 - \frac{(DO_{sat} - DO_0)(k_R - k_D)}{k_D L_0}])\}$$

The classic convention calls the value (DO_{sat}-DO) the oxygen deficit and actually solved for deficit then back-computes the DO. When doing the work by hand it is easier.

A typical DO profile is sketched below

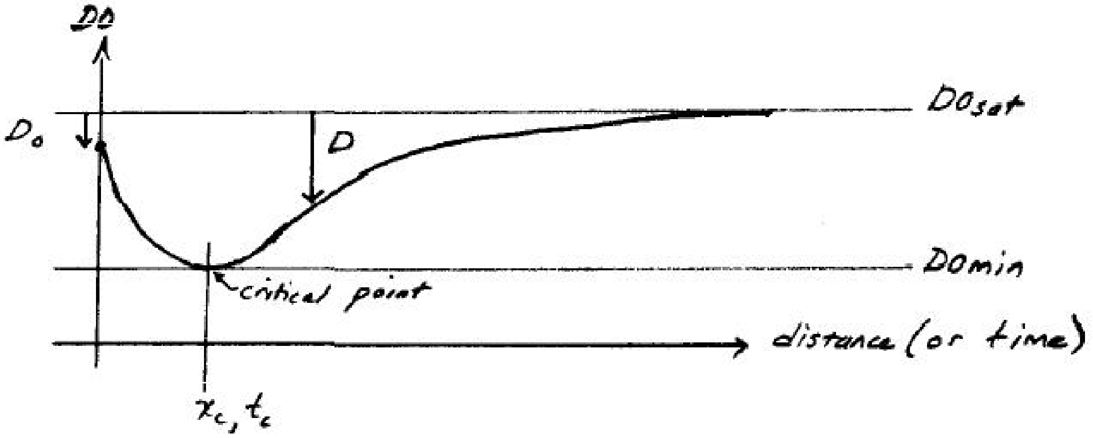

Figure 15. DO Sag Curve

Example (Hand calculations)

1.10 cubic meters per second with BOD=50 mg/L; DO = 2 mg/L is discharged into a stream with flow = 8.7 cubic meters per second with BOD = 6 mg/L ; DO = 8.3 mg/L. Deoxygenation constant is kd = 0.2/day. Average flow depth is 3.0 meters. Average flow width is 10.85 meters. Plot the DO in the stream at 20oC as a function of distance downstream from the discharge point. Locate the critical point and the minimum DO value.

Sketch

Mixing

$$L_o = \frac{(1.1 m^3/s)(50 mg/L) + (8.7 m^3/s)(6 mg/L)}{(1.1 + 8.7 m^3/s)} = 10.9 mg/L$$

$$DO_o = \frac{(1.1 m^3/s)(2 mg/L) + (8.7 m^3/s)(8.3 mg/L)}{(1.1 + 8.7 m^3/s)} = 7.6 mg/L$$

Reaeration

$$DO_{sat} (@20°C) = 9.09 mg/L \quad \therefore \quad D_o = DO_{sat} - D_o = 9.09 - 7.6 = 1.5 mg/L$$

$$k_r \text{ (O'Connor + Dobbins)} = \frac{3.9 u^{1/2}}{H^{3/2}}$$

$$u = \frac{Q}{A} = \frac{1.1 + 8.7 m^3/s}{(3.0)(10.85)} = 0.301 m^3/s$$

$$k_r = \frac{(3.9)(0.3)^{1/2}}{(3.0)^{3/2}} = 0.41/day$$

Critical Point(s)

$$t_c = \frac{1}{(0.41 - 0.20)} \ln\left(\frac{0.41}{0.20}\left[1 - \frac{1.5(0.41-0.20)}{0.20 \times 10.9}\right]\right) =$$

$$2.67 \text{ days} * \frac{86400 sec}{day} = 230,688 sec.$$

$$x_c = u t_c = (0.30 m/sec)(230,688 sec) = 64300 \text{ meters}$$

Plot

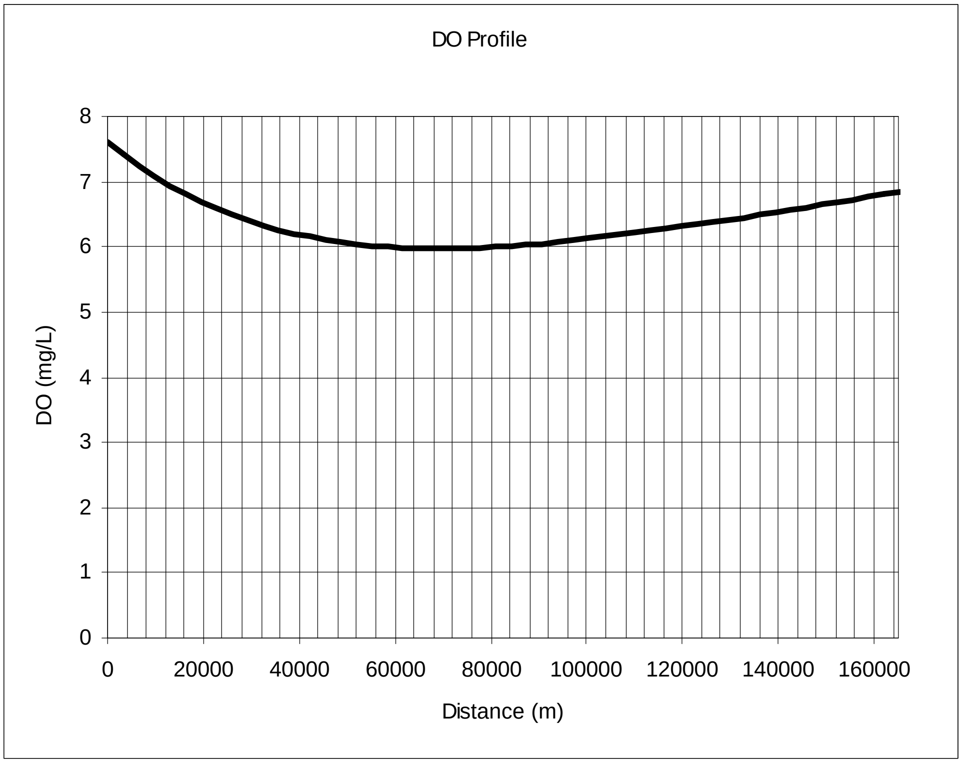

Figure 16. DO Profile – Example

Spreadsheet (Formulas)

	A	B	C	D	E	F
1	Lo	10.9	mg/L			
2	Do	1.5	mg/L			
3	DOsat	9.09	mg/L			
4						
5	u	0.3	m/sec			
6	kd	0.2	/day	=B6/86400	/sec	
7	kr	0.41	/day	=B7/86400	/sec	
8						
9	kdLo/(kr-kd)	=D6*B1/(D7-D6)				
10	Δt	=3600*3				
11						
12	t(sec)	x(meters)	exp(-kdt)	exp(-krt)	D	DO
13	0	=$B$5*A13	=EXP(-$D$6*A13)	=EXP(-$D$7*A13)	=$B$9*(C13-D13)+$B$2*D13	=$B$3-E13
14	=A13+$B$10	=$B$5*A14	=EXP(-$D$6*A14)	=EXP(-$D$7*A14)	=$B$9*(C14-D14)+$B$2*D14	=$B$3-E14
15	=A14+$B$10	=$B$5*A15	=EXP(-$D$6*A15)	=EXP(-$D$7*A15)	=$B$9*(C15-D15)+$B$2*D15	=$B$3-E15
16	=A15+$B$10	=$B$5*A16	=EXP(-$D$6*A16)	=EXP(-$D$7*A16)	=$B$9*(C16-D16)+$B$2*D16	=$B$3-E16
17	=A16+$B$10	=$B$5*A17	=EXP(-$D$6*A17)	=EXP(-$D$7*A17)	=$B$9*(C17-D17)+$B$2*D17	=$B$3-E17
18	=A17+$B$10	=$B$5*A18	=EXP(-$D$6*A18)	=EXP(-$D$7*A18)	=$B$9*(C18-D18)+$B$2*D18	=$B$3-E18
19	=A18+$B$10	=$B$5*A19	=EXP(-$D$6*A19)	=EXP(-$D$7*A19)	=$B$9*(C19-D19)+$B$2*D19	=$B$3-E19
20	=A19+$B$10	=$B$5*A20	=EXP(-$D$6*A20)	=EXP(-$D$7*A20)	=$B$9*(C20-D20)+$B$2*D20	=$B$3-E20
21	=A20+$B$10	=$B$5*A21	=EXP(-$D$6*A21)	=EXP(-$D$7*A21)	=$B$9*(C21-D21)+$B$2*D21	=$B$3-E21
22	=A21+$B$10	=$B$5*A22	=EXP(-$D$6*A22)	=EXP(-$D$7*A22)	=$B$9*(C22-D22)+$B$2*D22	=$B$3-E22
23	=A22+$B$10	=$B$5*A23	=EXP(-$D$6*A23)	=EXP(-$D$7*A23)	=$B$9*(C23-D23)+$B$2*D23	=$B$3-E23
24	=A23+$B$10	=$B$5*A24	=EXP(-$D$6*A24)	=EXP(-$D$7*A24)	=$B$9*(C24-D24)+$B$2*D24	=$B$3-E24
25	=A24+$B$10	=$B$5*A25	=EXP(-$D$6*A25)	=EXP(-$D$7*A25)	=$B$9*(C25-D25)+$B$2*D25	=$B$3-E25
26	=A25+$B$10	=$B$5*A26	=EXP(-$D$6*A26)	=EXP(-$D$7*A26)	=$B$9*(C26-D26)+$B$2*D26	=$B$3-E26
27	=A26+$B$10	=$B$5*A27	=EXP(-$D$6*A27)	=EXP(-$D$7*A27)	=$B$9*(C27-D27)+$B$2*D27	=$B$3-E27

Spreadsheet (Numbers)

	A	B	C	D	E	F
1	Lo	10.9	mg/L			
2	Do	1.5	mg/L			
3	DOsat	9.09	mg/L			
4						
5	u	0.3	m/sec			
6	kd	0.2	/day	2.31E-06	/sec	
7	kr	0.41	/day	4.75E-06	/sec	
8						
9	kdLo/(kr	10.381				
10	Δt	10800				
11						
12	t(sec)	x(meters	exp(-kdt)	exp(-krt)	D	DO
13	0	0	1	1	1.5	7.59
14	10800	3240	0.97531	0.950041	1.687375713	7.40262429
15	21600	6480	0.951229	0.902578	1.858913791	7.23108621
16	32400	9720	0.927743	0.857486	2.015565371	7.07443463
17	43200	12960	0.904837	0.814647	2.158230125	6.93176988
18	54000	16200	0.882497	0.773948	2.287758926	6.80224107
19	64800	19440	0.860708	0.735283	2.404956384	6.68504362
20	75600	22680	0.839457	0.698549	2.510583249	6.57941675
21	86400	25920	0.818731	0.66365	2.605358691	6.48464131
22	97200	29160	0.798516	0.630495	2.68996247	6.40003753
23	108000	32400	0.778801	0.598996	2.765036983	6.32496302
24	118800	35640	0.759572	0.569071	2.831189223	6.25881078
25	129600	38880	0.740818	0.540641	2.888992625	6.20100737
26	140400	42120	0.722527	0.513631	2.938988823	6.15101118
27	151200	45360	0.704688	0.487971	2.981689317	6.10831068