7. Water Quality Modeling

Until now we have derived governing equations for and sought solutions to idealized cases where analytical solutions could be found. Many problems in the natural world, however, are complex enough that simplified analytical solutions are inadequate to predict the transport and mixing behavior. In these situations, approximations of the governing transport equations (such as finite difference) must be made so that numerical solutions can be found. These approximations can be simple or complex, but often result in a large number of equations that must be solved to predict the concentration distribution. Hence, computer algorithms are used to make the numerical solutions tractable.

In this chapter, we introduce the field of water quality modeling based on computerized (numerical or digital) tools. This chapter begins by outlining how to select an appropriate numerical tool. The next two section describe common computer approximations. First, simple numerical models based on plug-flow and continuously-stirred tank reactors are introduced. Second, an overview of numerical approximations to the governing equations is presented. Because we are now dealing with approximate solutions, new procedures are needed to assure that our results are acceptable. The final section outlines the crucial steps necessary to test the accuracy of a numerical result. Although computer power is rapidly growing, it remains important to use simple tools and thorough testing in order to understand and synthesize the meaning of numerical results.

7.1 Systematic approach to modeling

A model is any analysis tool that reduces a physical system to a set of equations or a reduced-scale physical model. Moreover, all of the solutions in previous chapters are analytical models of natural systems. Whether analytical or numerical, the main question the modeler must answer is: which model should I use?

7.1.1 Modeling methodology

The ASCE & WPCF (1992) design manual *Design and Construction of Urban Stormwater Management Systems* outlines a four-step selection processes for choosing a water quality analysis tool. These steps are discussed in detail in the following and include (1) defining project goals, (2) describing an acceptable modeling tool, (3) listing the available tools that could satisfy the goals and model description, and (4) selecting the model to be used based on an optimal compromise between goals and available tools.

1. Define project goals. It may sound like an obvious first step, but it is essential and, regrettably, often overlooked: define the project goals before even choosing the model. Fischer et al. (1979) emphasize this step as well, saying that the choice of a model depends crucially on what the model is to do. Modeling goals are quite variable, ranging from the practical (provide the analysis necessary to get the client his discharge permit) to the research oriented (develop a new tool that overcomes some current modeling shortfall).

During this step, as much as possible should be learned about the system to be modeled. Fischer et al. (1979) suggest that if possible, the investigator should become personally familiar with the water body by going out on it in the smallest boat that is safe. Then, before venturing near a computer or a model basin, he or she should make all possible computations, being approximate where necessary, but seeking a feel for what the model will predict. Only after we understand our system can we formulate appropriate project goals. In the words of the famous landscape photographer Ansel Adams, "Visualization is of utmost importance; many failures occur because of our uncertainty about the final image" (quoted in Fischer et al. (1979)). During this stage one begins to formulate the necessary attributes of the model. This leads naturally the next step.

2. Describe an acceptable modeling tool. Before selecting the model for the analysis, formulate a list of abilities and characteristics that the model must have. These can include things like input/output flexibility, common usage in the regulatory community, and physical mixing processes the model must include. Our simplified predictions from step 1 of how the system behaves are used in this step to formulate the model requirements. For instance, if we expect rapid near-field mixing, we may suggest using a one-dimensional model. This step should keep in mind what models are available, but not limit the analysis to known tools if they would be inadequate to meet the project goals. In this stage the project goals may also need to be revised. If the only acceptable modeling tool to meet a particular goal is too costly in terms of computation time and project resources, perhaps that goal can be reformulated within a reasonable project scope. The purpose, therefore, of this step is to optimize the modeling goals by describing practical requirements of the modeling tool.

3. List applicable tools. Once the analysis tool has been adequately described, one must formulate a list of available tools that meet these requirements. In engineering practice, we must often choose an existing model with a broad user base. Appendix D lists several public-domain models. Most of them are available free of charge from government sponsor agencies, but some are also commercial. The purpose of choosing an existing model is that it has been thoroughly tested by many previous users and that the regulatory agencies are accustomed to seeing and interpreting its output. However, available tools may not always be adequate to meet the project goals.

If existing tools are inadequate, then a new tools must be developed, and a list of existing methods is an important step. Methods are the building blocks of models. A one-dimensional finite difference model employs two methods: a one-dimensional approximation and a finite difference numerical scheme. Going a step deeper, the finite-difference

method can have many attributes, such as forward, central, or backward differencing, implicit or explicit formulation, and first-, second-, or higher-order solution algorithms. Section 7.3 describes what some of these terms mean. The point is that, when designing a new tool, there are many existing building blocks from which to choose, and these can be quite helpful. It may turn out that simply adding an unsteady algorithm to an existing steady-state model will meet the project goals. Hence, knowing as much as possible about existing models and methods is essential to implementing and/or designing an analysis tool.

4. Make an optimal compromise between goals and available tools. In the final step of choosing a modeling tool, we seek an optimal compromise between the project goals and the available tools. This is where the decision to proceed with a given modeling tool is made. The project goals are the guide to choosing the model. It sounds simple, but choose the best model to meet the project goals, not just the best available model. As computers become faster, the tendency is to just pick the biggest, boldest model and to force it to meet your needs. However, the enormous amount of output from such a model may be overwhelming and costly and unnecessary in the light of certain project goals. Therefore, choose the most appropriate, simplest model that also satisfies the scientific rigor of the project goals, and when necessary, develop new tools.

7.1.2 Issues of scale and complexity

Throughout the process of choosing a modeling tool one is confronted with issues of system scale and complexity. The world is inherently three-dimensional and turbulent, but with current computer resources, we must often limit our analysis to one- and two-dimensional approximations with turbulence closure schemes that approximate the real world. Hence, we must make trade offs between prototype complexity and model ability.

We can evaluate these trade offs by doing a scale analysis to determine the important scales in our problem. This is the essence of steps one and two, above, where we try to predict what the model will tell us and use this information to characterize the needed tool. For transport problems, we must consider the advective, diffusing reaction equation. For illustration, consider a first-order reaction

$$\frac{\partial C}{\partial t} + \frac{\partial (uC)}{\partial x} + \frac{\partial (vC)}{\partial y} + \frac{\partial (wC)}{\partial z} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} \pm kC. \tag{7.1}$$

This equation has three unit scales: mass, time, and length. It also has three processes: advection, diffusion, and reaction. We would like to formulate typical scales of these three processes from the typical units in the problem. For example, the advection time scale is the time it takes for fluid to move through our system. If we are modeling a river reach of length L with mean velocity U, then the advective time scale is

$$T_a = L/U. \tag{7.2}$$

Processes that occur on time scales much shorter than T_a can neglect advection. We can use these scales to non-dimensionalize the governing equation. To do this, we define the non-dimensional variables using primes as follows

$$\begin{aligned} x &= L_x x'; \quad & y &= L_y y' \\ z &= L_z z'; \quad & u &= U u' \\ v &= V v'; \quad & w &= W w' \\ C &= C_0 C'; \quad & t &= T_0 t' \\ k &= 1/T_r k' \end{aligned} \tag{7.3}$$

where the upper-case variables are typical scales in the problem. For example T_0 is an external time scale, such as a discharge protocol or the diurnal cycle and T_r is the reaction time scale, such as the half-life for a dye-off reaction. The L's are system dimensions and U, V, and W are average velocities. Substituting into (7.1) gives

$$\begin{aligned} \frac{1}{T_0}\frac{\partial C'}{\partial t'} + \frac{U}{L_x}\frac{\partial (u'C')}{\partial x'} + \frac{V}{L_y}\frac{\partial (v'C')}{\partial y'} + \frac{W}{L_z}\frac{\partial (w'C')}{\partial z'} = \\ \frac{D_x}{L_x^2}\frac{\partial^2 C'}{\partial x'^2} + \frac{D_y}{L_y^2}\frac{\partial^2 C'}{\partial y'^2} + \frac{D_z}{L_z^2}\frac{\partial^2 C'}{\partial z'^2} \pm \frac{1}{T_{1/2}} k' C'. \end{aligned} \tag{7.4}$$

Note that to make this equation fully non-dimensional, we must multiple each term by a time scale, for example T_0. We can now determine the relative importance of each term by considering their leading coefficients. Comparing the convective terms

$$\frac{\text{Longitudinal advection}}{\text{Lateral advection}} = \frac{U}{V} \cdot \frac{L_y}{L_x} \tag{7.5}$$

$$\frac{\text{Longitudinal advection}}{\text{Vertical advection}} = \frac{U}{W} \cdot \frac{L_z}{L_x} \tag{7.6}$$

If these ratios are much greater than one, then longitudinal advection is the only advection term that we must keep in the equation. Thus, the importance of a given convection term depends on the velocity scales in our problem and the length of river we are considering. In many river problems, these ratios are much greater than one, and we only keep the longitudinal advection term. Likewise, we can compare the diffusion terms to the advection term. For longitudinal diffusion we have

$$\frac{\text{Longitudinal diffusion}}{\text{Longitudinal advection}} = \frac{D_x}{L_x^2 T_a} \tag{7.7}$$

which is our familiar Peclet number. For large Peclet numbers, we only consider diffusion, and for small Peclet numbers, we only consider advection. Hence, the important terms in the equation again depend on the length of river we are considering.

As an example, when might a one-dimensional steady-state model with dye-off be an acceptable model for a given river reach? The governing model equation would be

$$u\frac{\partial C}{\partial x} = D_x \frac{\partial^2 C}{\partial x^2} - kC. \tag{7.8}$$

By comparing with the non-dimensional equation above, this equation implies several constraints on the river. Consider first the external time-scale. This model implies

$$\frac{UT_0}{L_x} \gg 1. \tag{7.9}$$

For the convective terms, this model implies that

$$\frac{UL_y}{VL_x} \gg 1 \tag{7.10}$$

$$\frac{UL_z}{WL_x} \gg 1 \tag{7.11}$$

or alternatively

$$\frac{\partial C}{\partial y} = \frac{\partial C}{\partial z} = 0. \tag{7.12}$$

Similarly, for diffusion this model implies that

$$\frac{UL_y^2}{L_x D_y} \gg 1 \tag{7.13}$$

$$\frac{UL_z^2}{L_x D_z} \gg 1 \tag{7.14}$$

or, again, alternatively

$$\frac{\partial C}{\partial y} = \frac{\partial C}{\partial z} = 0. \tag{7.15}$$

Finally, for the reaction, this model implies that

$$\frac{UT_{1/2}}{L_x} \approx 1. \tag{7.16}$$

Therefore, by comparing the relevant scales in our problem to the approximations made by models, we can determine just how complex the model must be to approximate our system adequately.

7.1.3 Data availability

As a final comment on the selection and implementation of an analysis tool, we discuss a few points regarding the data that are used to validate the model (Section 7.4 below discusses how to test a model in more detail). The only test available to determine whether the model adequately reproduces our natural system is to compare model output to data (measurements) taken from the prototype system. In general, as the model complexity increases, the number of parameters we can use to adjust the model results to match the prototype also increases, giving us more degrees of freedom. The more degrees of freedom we have, the more data we need to calibrate our model. Hence, the data requirements of a model are directly proportional to the model complexity. If very limited data are available, then complex models should be avoided because they cannot be adequately calibrated or validated.

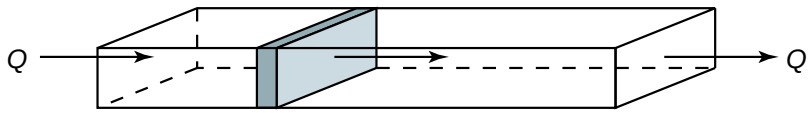

Fig. 7.1. Schematic of a plug-flow reactor.

7.2 Simple water quality models

Some simple water quality models can be developed for special cases where advection or diffusion is dominant. As introduced in Chapter 2, the Peclet number is a measure of diffusion to advection dominance. The Peclet number, Pe, is defined as

$$Pe = \frac{D}{uL} \tag{7.17}$$

$$= \frac{D}{u^2 t} \tag{7.18}$$

where the two definitions are equivalent. The Peclet number is small when advection is dominant and large when diffusion is dominant. Two simple models can be developed for the limiting cases of $Pe \to 0$ and $Pe \to \infty$. A third hybrid model is also introduced in this section for simplified application to arbitrary Pe.

7.2.1 Advection dominance: Plug-flow reactors

For $Pe \to 0$ we can neglect longitudinal diffusion and dispersion, and we have the so-called plug-flow reactor. Shown in Figure 7.1, a slab of marked fluid is advected with the mean flow, perhaps undergoing reactions, but not spreading in the lateral. Taking $D = 0$, the governing reactive transport equation becomes

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = \pm R. \tag{7.19}$$

To solve this equation, we make the familiar coordinate transformation to move our coordinate system with the mean flow. That is,

$$\xi = x - ut \tag{7.20}$$

$$\tau = t. \tag{7.21}$$

As demonstrated in Chapter 2, using the chain rule to substitute this coordinate transformation into (7.19) gives

$$\frac{\partial C}{\partial \tau} = \pm R \tag{7.22}$$

which is easily solved after defining an initial condition and the transformation reaction R.

For example, consider a first-order die-off reaction for a slab with initial concentration C_0. The solution to (7.22) is

$$C(\tau) = C_0 \exp(-k\tau) \tag{7.23}$$

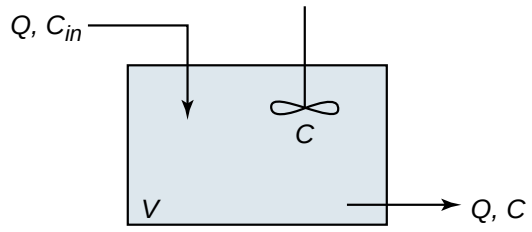

Fig. 7.2. Schematic of a continuously-stirred tank reactor (CSTR).

or in the original coordinate system, we have the interchangeable solutions

$$C(t) = C_0 \exp(-kt) \tag{7.24}$$

$$C(x) = C_0 \exp(-kx/u). \tag{7.25}$$

The residence time for a plug-flow reactor depends on the distance of interest L_0. From the definition of residence time

$$\begin{aligned} t_{res} &= \frac{V}{Q} \\ &= \frac{L_0 A}{Q} \end{aligned} \tag{7.26}$$

where A is the cross-sectional area of the channel and Q is the steady flow rate. The fluid residence time, the travel time for a slab to move the distance L_0, can also be expressed using the same variables

$$\begin{aligned} t_{slab} &= \frac{L_0}{u} \\ &= \frac{L_0 A}{Q} \\ &= t_{res}. \end{aligned} \tag{7.27}$$

Hence, the fluid and species residence times are equal.

7.2.2 Diffusion dominance: Continuously-stirred tank reactors

For $Pe \to \infty$ we can neglect advection and we have the so-called continuously-stirred tank reactor (CSTR). Shown in Figure 7.2, fluid that enters the reactor is assumed to instantaneously mix throughout the full reactor volume. To write the governing equation, consider mass conservation in the tank

$$\frac{dM}{dt} = \dot{m}_{in} - \dot{m}_{out}. \tag{7.28}$$

The inflow provides the mass flux into the control volume, $\dot{m}_{in}$. Loss of mass, $\dot{m}_{out}$ is given by the outflow and possible die-off reactions. Writing the conservation of mass in concentrations and flow rates yields

$$\frac{d(CV)}{dt} = Q(C_{in} - C_{out}) \pm S \tag{7.29}$$

where V is the volume of the tank and $S = VR$ is a source or sink reaction term. Because the tank is well mixed, we can assume that C_{out} is equal to the concentration in the tank C. Taking V as constant, we can move it outside the derivative, and the governing equation becomes

$$\frac{dC}{dt} = \frac{Q}{V}(C_{in} - C) \pm R. \tag{7.30}$$

Substituting the definition of the residence time, we have finally

$$\frac{dC}{dt} = \frac{1}{t_{res}}(C_{in} - C) \pm R \tag{7.31}$$

which is the governing equation for a CSTR.

Consider first the conserving case, where $R = 0$. Taking the initial condition as a clean tank $C_0 = 0$, the solution to (7.31) is

$$C(t) = C_{in}\left[1 - exp\left(-\frac{t}{t_{res}}\right)\right]. \tag{7.32}$$

Thus, the concentration in the tank increases exponentially with a rate constant $k = 1/t_{res}$. The concentration in the tank reaches steady state asymptotically. If we define steady state as the time, t_{ss}, until $C = 0.99C_0$, then

$$t_{ss} = 4.6t_{res}. \tag{7.33}$$

Therefore, without reactions, steady state is reached in about 4.6 residence times.

The solution for the reacting case is slightly more complicated because (7.31) is an inhomogeneous differential equation with forcing function $\pm R$. Consider the case of a first-order die-off reaction and an initial tank concentration of $C_0 = 0$. Assuming a particular solution (see Appendix C for an example of solving an inhomogeneous equation) of the form $C_p = AC_{in}$, the solution is found to be

$$C(t) = \frac{C_{in}}{1 + kt_{res}}\left[1 - \exp\left[-\left(\frac{1 + kt_{res}}{t_{res}}\right)t\right]\right]. \tag{7.34}$$

Because of the reaction, the steady state concentration in the tank is no longer the inflow concentration, but rather

$$C_{ss} = \frac{C_{in}}{1 + kt_{res}} \tag{7.35}$$

and the coefficient $1/(1 + kt_{res})$ is one minus the removal rate. The time to reach steady state, t_{ss}, is the time to reach $0.99C_{ss}$ or

$$t_{ss} = \frac{4.6t_{res}}{1 + kt_{res}}. \tag{7.36}$$

7.2.3 Tanks-in-series models

The simplest type of river-flow model that incorporates some form of diffusion or dispersion is the tanks-in-series model, which is a chain of linked CSTRs. An example tanks-in-series model is shown in Figure 7.3. In the example each tank has the same dimensions,

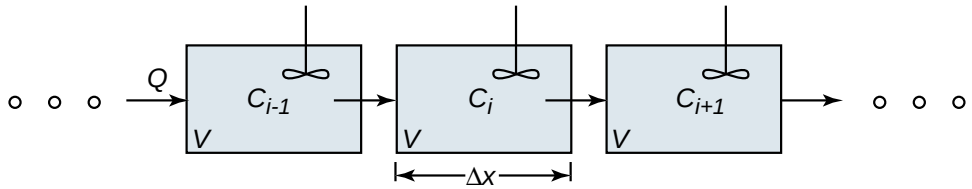

Fig. 7.3. Schematic of a tanks-in-series model. The model is made up of several CSTR linked in series.

and the flow rate is constant. The method also works for variable volume tanks, and under gradually-varied flow conditions, stage-discharge relationships can be used to route variable flows through the tanks. To see why the tanks-in-series model produces diffusion, consider an instantaneous pulse injection in the first tank. The outflow from that tank would be the solution to the CSTR given by (7.32). The outflow from the first tank is, therefore, exponential, clearly not the expected Gaussian distribution. But, this outflow goes into the next tank. At first, that tank is clean, and the little bit of tracer entering the tank in the beginning is quickly diluted; hence, the outflow concentration starts at zero and increases slowly. Eventually, a large amount of the tracer in the first tank has moved on to the second tank and the outflow from the second tank reaches a maximum concentration. The inflow from the first tank becomes increasingly cleaner, and the outflow from the second tank also decreases in concentration. Eventually, all the tracer has flowed through both tanks and the concentration is zero at the outlet of the second tank. The concentration curve over time for the second tank started at zero, increased smoothly to a maximum concentration, then decreased slowly back down to zero. These characteristics are very similar to the Gaussian distribution; hence, we expect that by dimensioning the tanks properly, we should be able to reproduce the behavior of advective diffusion in the downstream tanks.

To find the proper tank dimensions, consider the mass conservation equation for a central tank. Inflow comes from the upstream tank, and outflow goes to the downstream tank; thus, we have

$$\frac{dM_i}{dt} = Q(C_{i-1} - C_i) \pm VR. \tag{7.37}$$

For the remaining analysis we will neglect the reaction term. Assuming each tank has the same length, the tank volume can be written as $V = A\Delta x = A(x_i - x_{i-1})$. Using this definition to write M_i in concentration units gives

$$\frac{dC_i}{dt} = u\frac{C_{i-1} - C_i}{x_i - x_{i-1}} \tag{7.38}$$

which is the discrete equation describing the tanks-in-series model.

The difference term on the right-hand-side of (7.38) is very close to the backward difference approximation to $\partial C/\partial x$:

$$\frac{\partial C}{\partial x} = \frac{C_i - C_{i-1}}{x_i - x_{i-1}} \tag{7.39}$$

which has no error for $\Delta x \to 0$. For finite grid size, the Taylor-series expansion provides an estimate of the error. The second-order Taylor-series expansion of C_{i-1} about C_i is

$$C_{i-1} = C_i + \left.\frac{\partial C_i}{\partial x}\right|_i (x_{i-1} - x_i) + \frac{1}{2}\left.\frac{\partial^2 C_i}{\partial x^2}\right|_i (x_{i-1} - x_i)^2 + \cdots \tag{7.40}$$

as given in Thomann & Mueller (1987). Rearranging this equation, we can obtain

$$\frac{C_i - C_{i-1}}{x_i - x_{i-1}} = \frac{\partial C_i}{\partial x} - \frac{1}{2}\frac{\partial^2 C_i}{\partial x^2}(x_i - x_{i-1}). \tag{7.41}$$

Multiplying this result by -1 gives

$$\frac{C_{i-1} - C_i}{x_i - x_{i-1}} = -\frac{\partial C_i}{\partial x} + \frac{1}{2}\frac{\partial^2 C_i}{\partial x^2}(x_i - x_{i-1}) \tag{7.42}$$

which can be substituted immediately for the right-hand-side of (7.38) leaving

$$\frac{dC_i}{dt} = -u\frac{\partial C_i}{\partial x} + \frac{u(x_i - x_{i-1})}{2}\frac{\partial^2 C_i}{\partial x^2}. \tag{7.43}$$

Dropping the subscripts and recognizing $\Delta x = (x_i - x_{i-1})$ gives the governing equation

$$\frac{dC}{dt} + u\frac{\partial C}{\partial x} = \frac{u\Delta x}{2}\frac{\partial^2 C}{\partial x^2}. \tag{7.44}$$

Thus, our derived governing equation for a tanks-in-series model has the same form as the advective diffusion equation with a diffusion coefficient of $D_n = u\Delta x/2$.

The effective diffusion coefficient, D_n, for a tanks-in-series model is actually a numerical error due to the discretization. As the discretization becomes more course, the numerical error increases and the numerical diffusion goes up. For $\Delta x \to 0$, the numerical diffusion vanishes, and we have the plug-flow reactor. Hence, for a tanks-in-series model, we choose the tank size such that D_n is equal to the physical longitudinal diffusion and dispersion in the river reach.

7.3 Numerical models

Although the tank-in-series model was shown to be a special discretization of the advective diffusion equation, other numerical techniques specifically set out to discretize the governing equation. For our purposes, a numerical model is any model that seeks to solve a differential equation by discretizing that equation on a numerical grid.

7.3.1 Coupling hydraulics and transport

To simulate chemical transport, the velocity field, represented by $\boldsymbol{u}$ in the transport equation must also be computed. The model that calculates $\boldsymbol{u}$ is called the hydrodynamic or hydraulic model. Thus, to simulate transport, the hydrodynamic and transport models must be properly coupled.

Whether the hydrodynamic and transport models must be implicitly coupled or whether they can be run in series depends on the importance of buoyancy effects. If the

system is free from buoyancy effects, the hydrodynamics are independent of the transport; hence, they can be run first and their output stored. Then, many transport simulations can be run using the hydrodynamic data without re-running the hydrodynamic code. If buoyancy effects are present in the water body, then the transport of buoyancy (heat or salinity or both) must be coupled with the hydrodynamics, and both models must be run together. Once the output from the coupled model is stored, further transport simulations can be run for constituents that do not influence the buoyancy (these are called passive constituents). Because the hydrodynamic portion of the model is computationally expensive, the goal in transport modeling is to de-couple the two models as much as possible.

7.3.2 Numerical methods

There are probably as many numerical methods available to solve the coupled hydrodynamic and advective transport equations as there are models; however, most models can be classified by a few key words.

There are three main groups of numerical methods: finite difference, finite volume, and finite element. For special selections of basis functions and geometries, the three methods can all be made equivalent, but in their standard applications, the methods are all slightly different. The finite difference method is built up from a series of nodes, the finite volume method is built up from a group of cells, and the finite element method is made up of a group of elements, where each element is comprised of two or more grid points. In the finite difference case, the differential equation is discretized over the numerical grid, and derivatives become difference equations that are functions of the surrounding cells. In the finite volume case, the fluxes through the cell network are tracked and the differential equations are integrated over the cell volume. For finite elements, a basis function is chosen to describe the variation of an unknown over the element and the coefficients of the basis functions are found by substituting the basis functions as solutions into the governing equations. Because finite difference methods are easier to implement and understand, these methods are more widely used.

A numerical method may further be explicit or implicit. An explicit scheme is the easiest to solve because the unknowns are written as functions of known quantities. For instance, the concentration at the new time is dependent on concentrations at the previous time step and at upstream (known) locations. In an implicit scheme, the equations for the unknowns are functions of other unknown quantities. For instance, the concentration at the new time may depend on other concentrations at the new time or on downstream locations not yet computed. In the implicit case, the equations represent a system of simultaneous equations that must be solved using matrix algebra. The advantage of an implicit scheme is that it generally has greater accuracy.

Finally, numerical methods can be broadly categorized as Eulerian or Lagrangian. Eulerian schemes compute the unknown quantities on a fixed grid based on functions of other

grid quantities. Lagrangian methods use the method of characteristics to track unknown quantities along lines of known value. For instance, in a Lagrangian transport model, the new concentration at a point could be found by tracking the hydrodynamic solution backward in time to find the point where the water parcel originated and then simply advecting that concentration forward to the new time. Because the Lagrangian method relies heavily on the velocity field, small errors in the velocity field (particularly for fields with divergence) can lead to large errors in the conservation of mass. The advantage of the Lagrangian method is that it can backtrack over several hydrodynamic time steps; hence, there is no theoretical limitation on the size of the time step in a Lagrangian transport model. An example of a one-dimensional Lagrangian scheme is the Holly-Preissman method. By contrast, for the Eulerian model, the time step is limited by a so-called Courant number restriction, that says that the time step cannot be so large that fluid in one cell advects beyond the next adjacent cell over one time step. Mathematically, this can be written as

$$\Delta t \leq \frac{\Delta x}{u} \tag{7.45}$$

where Δt is the time step and Δx is the grid size.

7.3.3 Role of matrices

In the case of explicit models, matrices are not a necessity, but for implicit models and models simulating many contaminant, matrices provide a comfortable (and often necessary) means of solving the governing equations. For an implicit scheme, the equations for a given node at the new time are dependent on the solutions at other nodes at the same time. This means that implicit schemes are inherently a system of equations (sometimes non-linear), which are best solves with matrices. The general matrix equation is

$$\underline{A}\boldsymbol{x} = \boldsymbol{b} \tag{7.46}$$

where $\underline{A}$ is an n x n matrix of equation coefficients, x is an n x 1 vector of unknowns (for example, flow rates), and b is an n x 1 vector of forcing functions. Writing the equations in such a way makes derivation of the model equations manageable and implementation in the computer algorithm straightforward. The solution of (7.46) is

$$\boldsymbol{x} = \underline{A}^{-1}\boldsymbol{b} \tag{7.47}$$

where $\underline{A}^{-1}$ is the matrix inverse. Most computer languages have built-in methods for solving matrices. For the non-linear case, an iteration technique must be employed. A common method is the Newton-Raphson method.

7.3.4 Stability problems

One limitation already mentioned for an Eulerian transport scheme is the Courant number restriction. In general, all schemes have a range of similar restrictions that limit the

allowable spatial grid size and time step such that the scheme remains stable. If the time step is set longer than such a constraint, the model is unstable and will give results with large errors that eventually blow up. The full hydrodynamic equations are hyperbolic and generally have more stringent limitations than the parabolic transport equation. Before implementing a model, it is advised to seek out the published stability criteria for the model; this can save a lot of time in getting the model to run smoothly.

7.4 Model testing

An unfortunate fact of numerical modeling is that implementation and calibration is very time consuming, and little time is available for a thorough suite of model tests. This does not excuse the fact that model testing is necessary, but rather explains why it is often neglected. Even when using well-known tools, the following suite of tests is imperative to ensure that the model is working properly for your application. The following tests are specific to transport models, but apply in a generalized sense to all models.

7.4.1 Conservation of mass

All transport (water quality models) must conserve mass! This is a zeroth-order test that confirms whether the zeroth-moment of the concentration distribution is accurately reproduced in the solution. Clearly, when reactions are present, a given species may be loosing or gaining mass due to the reaction. This test must confirm, then, that the total system mass remains constant and that a species only gains mass at the rate allowed by the reaction equation. This test is often conducted in conjunction with the next test. However, it should always also be conducted for the complex real-world case being simulated, where analytical solutions are not available.

7.4.2 Comparison with analytical solutions

The model should be tested in idealized conditions to compare its results to known analytical solutions. This test confirms whether the model actually solves the governing equation that it was designed to solve. Deviations may be caused by many sources, most notably programming errors and numerical inaccuracy. Although most widely used models are free from programming errors, this cannot be tacitly assumed. In this author's experience, programming errors have been found in well-known, government-supported models by running this test. The issue of numerical inaccuracy arises due to the discretization, as in the case of numerical diffusion mentioned for the tanks-in-series model described above. Hence, the idealized case should have length and time scales as close to the prototype as possible in order to accurately assess the importance of numerical inaccuracy arising from the numerical method and the discretization.

This step can save a lot of time in applying the model to the prototype because the source of errors can often be identified faster in idealized systems. First, the analytical

solution is a known result. If the model gives another result, the model must be wrong. Second, the complexity of the real-world case makes it difficult to assess the importance of deviations from measured results. Once the model has been thoroughly tested against analytical results, deviations can be explained by physical phenomena in the prototype not present or falsely implemented in the model. Third, this test helps determine the stability requirements for complex models.

7.4.3 Comparison with field data

Only after it is certain that the model is solving the equations properly and within a known level of error can the model be compared to field or laboratory measurements of the prototype. The comparison of model results with these date serves two purposes. First, the model must be calibrated; that is, its parameters must be adjusted to match the behavior of the prototype. Second the model must be validated. This means that a calibrated model must be compared to data *not* used in the calibration to determine whether the model is applicable to cases outside the calibration data set. These prototype measurements fall into two categories: tracer studies and data collection of natural events.

Tracer studies. In a tracer study, dye is injected into the natural system, and concentrations are measured in time and space to record how the dye is transported and diluted. The advantage of a tracer study is that the source injection rate and location are known with certainty and that reactions can (often) be neglected. Tracer studies help calibrate the model parameters (such as diffusion and dispersion coefficients and turbulent closure schemes) to the real-world case. These studies also help to confirm whether the model assumptions are met (such as the one-dimensional approximation) and are good tests of both the hydrodynamic and water quality models.

Water quality data. The final set of data available for model testing is actual measurements of the modeled constituents in the prototype under natural conditions. These measurements represent true values, but are difficult to interpret because of our incomplete description of the prototype itself. We often do not know the total loading of constituent, and all the model equations are approximations of the actual physical processes in the prototype. These measurements further help to confirm whether the model assumptions are valid and to calibrate model parameters. Once the tests listed above are completed, the modeler should have a good understanding of how the complex physical processes in the model combine to give the model results. Deviations between the model and the field measurements should then be explained through the physical insight available in the model.

It is important to point out that the water quality measurement campaign should compliment the output available from the model. That is, the data should be collected such that they can be used to calibrate and test the model. If the model only outputs daily predictions, then the measurements should be able to predict daily values; instantaneous point measurements are only useful for a parameter that does not vary much over the

diurnal cycle. In summary, the model is only as good as the data that support it, and the data must be compatible with the model and flex the parts of the model that are the most uncertain.

Summary

This chapter introduced the concept of water quality modeling. A model is defined as any analysis tool that reduces a physical system to a set of equations or a reduced-scale physical model. A four-step procedure was suggested to help select the appropriate model: (1) define project goals, (2) describe an acceptable modeling tool, (3) list the available tools that could satisfy the goals and model description, and (4) select the model to be used based on an optimal compromise between goals and available tools. Because analytical solutions are not always adequate, numerical techniques were introduced. These included tank reactor models and numerical solution methods for differential equations, such as finite difference and finite element. Because numerical solutions result in a large number of calculations, a rigorous procedure for testing a numerical model was also suggested. These steps include (1) confirming that model conserves mass, (2) testing the model in idealized cases against analytical solutions, and (3) comparing the model to field data in the form of dye studies and the collection of water quality data. Good modeling projects should follow all of these suggested procedures.

Exercises

7.1 Equation scaling. Non-dimensionalize the one-dimensional momentum equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \frac{1}{\rho}\frac{\partial p}{\partial x} + \nu\frac{\partial^2 u}{\partial x^2} \tag{7.48}$$

using the non-dimensional variable definitions

$$u = U_0 u' \; ; \qquad x = Lx' \tag{7.49}$$

$$t = (L/U_0)t' \; ; \qquad p = \rho U_0^2 p' \tag{7.50}$$

Divide the equation by the coefficient in front of $\partial u'/\partial t'$. What familiar non-dimensional number becomes the leading coefficient of the viscous term? When is the viscous term negligible?

7.2 Finite difference. Write the explicit backward-difference approximation to the reaction equation

$$\frac{dC}{dt} = kC. \tag{7.51}$$

Program this solution in a computer and suggest a criteria for selecting the appropriate time step Δt by comparing to the analytical solution

$$C(t) = C_0 \exp(kt). \tag{7.52}$$

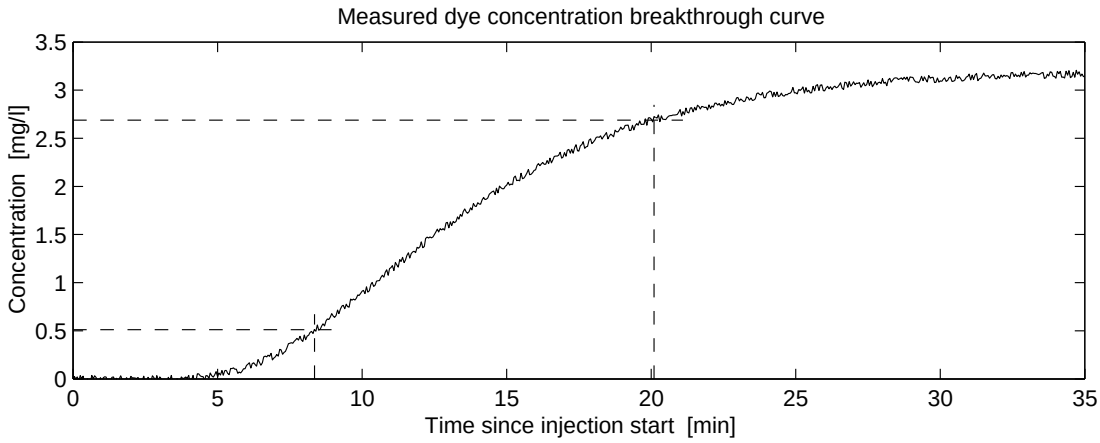

Fig. 7.4. Measured dye concentration for example dye study. Dye fluctuations are due to instrument uncertainty, not due to turbulent fluctuations.

7.3 Tanks-in-series model. A river has a cross-section of $h = 1$ m deep and $B = 10$ m wide. The mean stream velocity is 22.5 cm/s. A dye study was conducted my injecting 2.25 g/s of dye uniformly across the cross-section 150 m upstream of a measurement point. The measurements of dye concentration at $L = 150$ m are given in Figure 7.4. From the figure, determine the value of the dispersion coefficient. Based on this value, how many tanks in a tanks-in-series model would be needed to reproduce this level of dispersion in the numerical model?