LECTURE 7

Computer Methods: Well-Mixed Reactors

LECTURE OVERVIEW: I show how computers can be used to obtain solutions for individual reactors and systems of reactors. Three numerical approaches are described: the Euler, Heun, and fourth-order Runge-Kutta methods.

To this point we have used calculus to develop solutions for a number of idealized cases. Although these solutions are extremely useful for obtaining a fundamental understanding of pollutant fate in natural waters, they are somewhat limited in their ability to characterize real problems. There are four reasons why the analytical approaches are limited:

- *Nonidealized loading functions.* To attain closed-form solutions, idealized loading functions must be used. For example the loading must be adequately represented by functions such as the impulse, step, linear, exponential, or sinusoidal forms described in Lec. 4. Although real loadings may sometimes be represented in this way, they are more often arbitrary, with no apparent underlying pattern (recall Fig. 4.1*f*).
- *Variable parameters.* To this point we have assumed that all the model parameters (that is, Q, V, k, v, etc.) are constant. In fact, they may vary temporally.
- *Multiple-segment systems.* As you have learned in the past two chapters, systems of more than two segments require computers for their efficient solution.
- *Nonlinear kinetics.* To this point we have emphasized first-order kinetics. This means that we limited our studies to linear algebraic and differential equations. Although first-order reactions are important, there are a variety of water-quality problems that require nonlinear reactions. In most of these cases analytical solutions cannot be obtained.

All the above problems can be addressed by using the computer and numerical methods. For these reasons you must now begin to learn how computers are used to solve differential equations.

7.1 EULER'S METHOD

Euler's method is the simplest numerical method for solving ordinary differential equations. One way to introduce Euler's method is to derive it to solve the completely mixed lake model,

$$\frac{dc}{dt} = \frac{W(t)}{V} - \lambda c \tag{7.1}$$

where

$$\lambda = \frac{Q}{V} + k + \frac{v}{H} \tag{7.2}$$

The fundamental approach for solving a mathematical problem with the computer is to reformulate the problem so that it can be solved by arithmetic operations. Our one stumbling block for solving Eq. 7.1 in this way is the derivative term dc/dt. However, as we have already shown in Lec. 2, difference approximations can be used to express derivatives in arithmetic terms. For example using a forward difference, we can approximate the first derivative of c with respect to t by

$$\frac{dc_i}{dt} \cong \frac{\Delta c}{\Delta t} = \frac{c_{i+1} - c_i}{t_{i+1} - t_i} \tag{7.3}$$

where c_i and c_{i+1} = concentrations at a present and a future time t_i and t_{i+1}, respectively. Substituting Eq. 7.3 into Eq. 7.1 yields

$$\frac{c_{i+1} - c_i}{t_{i+1} - t_i} = \frac{W(t)}{V} - \lambda c_i \tag{7.4}$$

which can be solved for

$$c_{i+1} = c_i + \left[\frac{W(t)}{V} - \lambda c_i\right](t_{i+1} - t_i) \tag{7.5}$$

Notice that the term in square brackets is the differential equation itself (Eq. 7.1), which provides a means to compute the rate of change or slope of c. Thus the differential equation has been transformed into an algebraic equation that can be used to determine the concentration at t_{i+1} using the slope and a previous value of c. If you are given an initial value for concentration at some time t_i, you can easily compute concentration at a later time t_{i+1}. This new value of c at t_{i+1} can in turn be used to extend the computation to t_{i+2}, and so on. Thus at any time along the way,

$$\text{New value} = \text{old value} + (\text{slope})\,(\text{step}) \tag{7.6}$$

V9

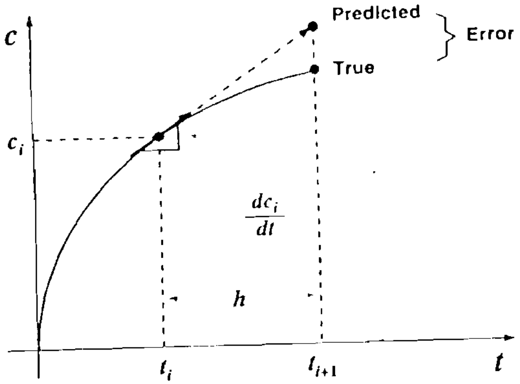

FIGURE 7.1
Graphical depiction of Euler's method.

This approach can be represented generally as

$$c_{i+1} = c_i + f(t_i, c_i)h \tag{7.7}$$

where $f(t_i, c_i) = dc_i/dt$ = the value of the differential equation evaluated at t_i and c_i and h = step size ($= t_{i+1} - t_i$). This formula is referred to as ***Euler's*** (or the ***point-slope***) ***method*** (Fig. 7.1).

EXAMPLE 7.1. EULER'S METHOD. A well-mixed lake has the following characteristics:

$Q = 10^5\ m^3\ yr^{-1}$ $\quad V = 10^6\ m^3$
$z = 5$ m $\quad k = 0.2\ yr^{-1}$
$v = 0.25$ m yr^{-1}

At $t = 0$ it receives a step loading of 50×10^6 g yr^{-1} and has an initial concentration of 15 mg L^{-1}. Use Euler's method to simulate the concentration from $t = 0$ to 20 yr using a time step of 1 yr. Compare the results with the analytical solution

$$c = c_0 e^{\lambda t} + \frac{W}{\lambda V}(1 - e^{-\lambda t})$$

Solution: First, the eigenvalue can be computed as

$$\lambda = \frac{10^5}{10^6} + 0.2 + \frac{0.25}{5} = 0.35\ yr^{-1}$$

At the start of the computation ($t_i = 0$) the concentration is 15 mg L^{-1} and the loading is 50×10^6 g yr^{-1}. Using this information and the parameter values, Eq. 7.5 can be employed to compute concentration at t_{i+1}:

$$c(1) = 15 + \left[\frac{50 \times 10^6}{10^6} - 0.35(15)\right]1.0 = 59.75 \text{ mg L}^{-1}$$

For the next interval (from $t = 1$ to 2 yr) the computation is repeated, with the result

$$c(2) = 59.75 + \left[\frac{50 \times 10^6}{10^6} - 0.35(59.75)\right]1.0 = 88.8375 \text{ mg L}^{-1}$$

The calculation is continued in a similar fashion to obtain additional values. The results, along with the analytical solution, are

t(yr)	c (mg L^{-1}) Numerical	Analytical	t(yr)	c (mg L^{-1}) Numerical	Analytical
0	15.00	15.00	6	133.21	127.20
1	59.75	52.75	7	136.59	131.82
2	88.84	79.37	8	138.78	135.08
3	107.74	98.12	9	140.21	137.38
4	120.03	111.33	10	141.14	139.00
5	128.02	120.64	∞	142.86	142.86

The numerical solution is plotted in Fig. 7.2 along with the analytical result. It can be seen that the numerical method accurately captures the major features of the exact solution. However, because we have used straight-line segments to approximate a continuously curving function, there is some discrepancy between the two results. One way to minimize such discrepancies is to use a smaller step size. For example applying Eq. 7.5 at 0.5-yr intervals results in a smaller error, as the straight-line segments track closer to the true solution. Using hand calculations the effort associated with using smaller and smaller step sizes would make such numerical solutions impractical. However, with the aid of the computer large numbers of computations can be performed easily. Thus you can accurately model the concentration without having to solve the differential equation exactly.

The Euler method is a first-order approach. Among other things this means that it would yield perfect results if the underlying solution of the differential equation were a linear polynomial or straight line. The accuracy of Euler's method can be improved by using a smaller time step. Other methods are also available that attain better accuracy by improving the slope estimate used for the extrapolation (see Chapra and Canale 1988 for a review). The following sections describe some of these methods.

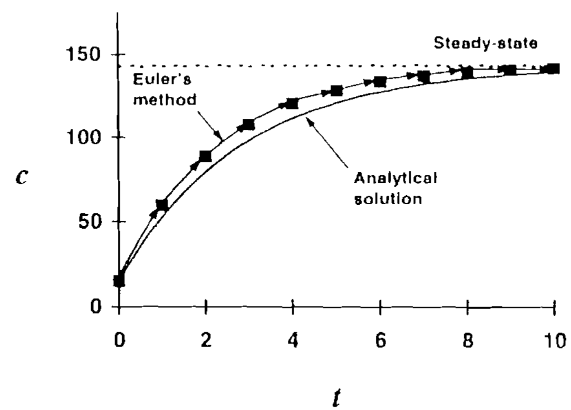

FIGURE 7.2
Comparison of analytical and Euler-method solutions for the well-mixed lake with a step loading.

7.2 HEUN'S METHOD

A fundamental source of error in Euler's method is that the derivative at the beginning of the interval is assumed to apply across the entire interval. One method to improve the estimate of the slope involves the determination of derivatives across the interval—one at the initial point and another at the end point. The two derivatives are then averaged to obtain an improved estimate of the slope for entire interval. This approach, called *Heun's method*, is depicted graphically in Fig 7.3.

Recall that in Euler's method the slope at the beginning of an interval

$$\frac{dc_i}{dt} = f(t_i, c_i) \tag{7.8}$$

is used to extrapolate linearly to c_{i+1}:

$$c_{i+1}^0 = c_i + f(t_i, c_i)h \tag{7.9}$$

For the standard Euler method we would stop at this point. However, in Heun's method the c_{i+1}^0 calculated in Eq. 7.9 is not the final answer but an intermediate prediction. This is why we have distinguished it with a superscript 0. Equation 7.9 provides an estimate of c_{i+1} that allows the calculation of an estimated slope at the end of the interval:

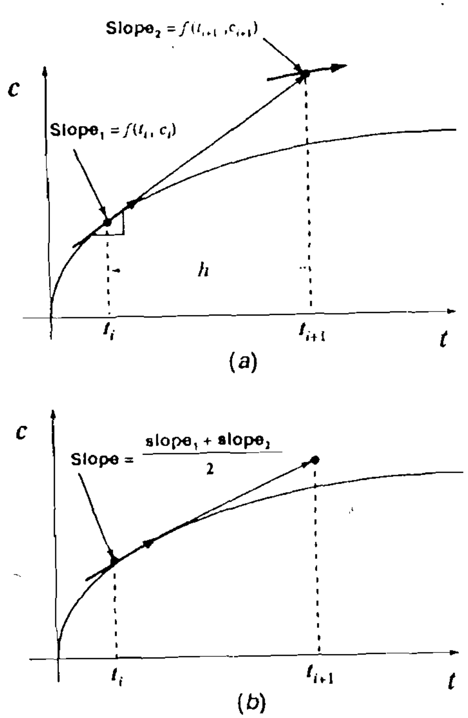

FIGURE 7.3
Graphical depiction of Heun's method. (a) Predictor; (b) corrector.

$$\frac{dc_{i+1}}{dt} = f(t_{i+1}, c_{i+1}^0) \tag{7.10}$$

Thus the two slopes (Eqs. 7.8 and 7.10) can be combined to obtain an average slope for the interval

$$\frac{\overline{dc}}{dt} = \frac{f(t_i, c_i) + f(t_{i+1}, c_{i+1}^0)}{2} \tag{7.11}$$

This average slope is then used to extrapolate linearly from c_i to c_{i+1},

$$c_{i+1} = c_i + \frac{f(t_i, c_i) + f(t_{i+1}, c_{i+1}^0)}{2}h \tag{7.12}$$

The Heun method is called a ***predictor-corrector method***. As derived above it can be expressed concisely as

Predictor: $$c_{i+1}^0 = c_i + f(t_i, c_i)h \tag{7.13}$$

Corrector: $$c_{i+1} = c_i + \frac{f(t_i, c_i) + f(t_{i+1}, c_{i+1}^0)}{2}h \tag{7.14}$$

Note that because Eq. 7.14 has c_{i+1} on both sides of the equal sign, it can be solved iteratively to refine the result. That is, an old estimate can be used repeatedly to provide an improved estimate of c_{i+1}. It should be understood that this iterative process will not necessarily converge on the true answer but will converge on an estimate with a finite truncation error. However, this truncation error will be smaller than for cruder approaches like Euler's method.

As with other iterative methods, a termination criterion for convergence of the corrector is provided by

$$\% \text{ error} = \left| \frac{c_{i+1}^j - c_{i+1}^{j-1}}{c_{i+1}^j} \right| (100\%) \tag{7.15}$$

where c_{i+1}^{j-1} and c_{i+1}^j are the results from the prior and the present iteration of the corrector, respectively.

EXAMPLE 7.2. THE HEUN METHOD. Use the Heun method to solve the same problem as in Example 7.1. For the present application do not iterate the corrector.

Solution: At the start of the computation ($t_i = 0$) the concentration is 15 mg L^{-1} and the loading is 50×10^6 g yr^{-1}. Using this information and the parameter values, Eq. 7.1 can be used to compute a slope estimate at t_i:

$$f(0, 15) = 50 - 0.35(15) = 44.75$$

which can then be used to calculate the concentration at the end of the interval

$$c(1) = 15 + (44.75)1.0 = 59.75 \text{ mg L}^{-1}$$

This value can in turn be employed to estimate a slope at the end of the interval

$$f(1, 59.75) = 50 - 0.35(59.75) = 29.0875$$

Then the two slopes can be input into the corrector to calculate the final result

$$c(1) = 15 + \tfrac{1}{2}(44.75 + 29.0875)1 = 51.91875 \text{ mg L}^{-1}$$

which is much closer to the true value than was obtained with Euler's method. The calculation is continued in a similar fashion to obtain additional values. The results, along with the analytical solution, are

t (yr)	c (mg L^{-1}) Numerical	c (mg L^{-1}) Analytical	t (yr)	c (mg L^{-1}) Numerical	c (mg L^{-1}) Analytical
0	15.00	15.00	6	126.30	127.20
1	51.92	52.75	7	131.08	131.82
2	78.18	79.37	8	134.48	135.08
3	96.85	98.12	9	136.90	137.38
4	110.14	111.33	10	138.62	139.00
5	119.58	120.64	∞	142.86	142.86

The Heun method is a second-order approach. Among other things this means that it would yield perfect results if the underlying solution of the differential equation were a quadratic polynomial. Thus it is superior to the Euler approach. However, the fact that two derivative evaluations must be made for each time step means that a computational price is paid for the gain in accuracy.

7.3 RUNGE-KUTTA METHODS

The Runge-Kutta (or RK) methods are a family of numerical methods that are used extensively in water-quality modeling. The RK methods all have the general form

$$c_{i+1} = c_i + \phi h \tag{7.16}$$

where ϕ = a slope estimate (formally called an ***increment function***). Comparison of Eq. 7.16 with Eq. 7.7 indicates that Euler's method is actually a first-order RK method with $\phi = f(t_i, c_i)$. In addition the Heun method (without corrector iteration) is a second-order RK algorithm (Chapra and Canale 1988).

The most commonly used RK method is the classical fourth-order method that has the form

$$c_{i+1} = c_i + \left[\tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)\right]h \tag{7.17}$$

where

$$k_1 = f(t_i, c_i) \tag{7.18}$$

$$k_2 = f\left(t_i + \tfrac{1}{2}h, c_i + \tfrac{1}{2}hk_1\right) \tag{7.19}$$

$$k_3 = f\left(t_i + \tfrac{1}{2}h, c_i + \tfrac{1}{2}hk_2\right) \tag{7.20}$$

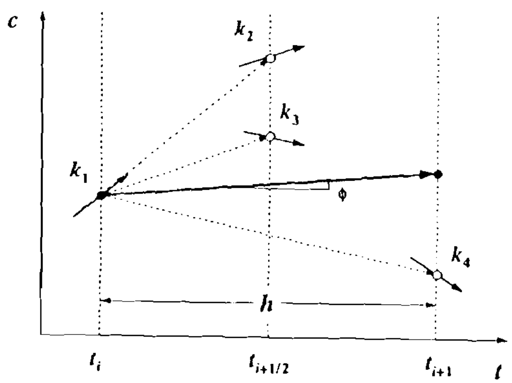

FIGURE 7.4
Graphical depiction of the fourth-order RK method.

$$k_4 = f(t_i + h, c_i + hk_3) \tag{7.21}$$

where the functions are merely the original differential equation evaluated at specific values of t and c. That is,

$$f(t, c) = \frac{dc}{dt}(t, c) \tag{7.22}$$

The fourth-order RK method is similar to the Heun approach in that multiple estimates of the slope are developed to come up with an improved average slope for the interval. As depicted in Figure 7.4, each of the k's represents a slope. Equation 7.17 then represents a weighted average of these to arrive at the improved slope.

EXAMPLE 7.3. THE FOURTH-ORDER RK METHOD. Use the classical fourth-order RK method to solve the same problem as in Example 7.1.

Solution: At the start of the computation (t_i = 0) the concentration is 15 mg L^{-1} and the loading is 50 × 10^6 g yr^{-1}. Using this information and the parameter values, Eqs. 7.17 to 7.21 can be used to compute concentration at t_{i+1}:

$$k_1 = f(0, 15) = 50 - 0.35(15) = 44.750$$

$$k_2 = f\left[0 + \tfrac{1}{2}(1), 15 + \tfrac{1}{2}(1)44.750\right] = f(0.5, 37.375) = 50 - 0.35(37.375) = 36.919$$

$$k_3 = f\left[0 + \tfrac{1}{2}(1), 15 + \tfrac{1}{2}(1)36.919\right] = f(0.5, 33.459) = 50 - 0.35(33.459) = 38.289$$

$$k_4 = f[0 + 1, 15 + 1(38.289)] = f(0.5, 53.289) = 50 - 0.35(53.289) = 31.349$$

$$c(1) = 15 + \left\{\tfrac{1}{6}(44.750 + 2(36.919 + 38.289) + 31.349)\right\}(1) = 52.75 \text{ mg L}^{-1}$$

For the next interval (t = 1 to 2 yr) the computation is repeated, with the result

$$c(2) = 52.75 + \left[\tfrac{1}{6}(31.537 + 2(26.018 + 26.984) + 22.092)\right](1) = 79.36 \text{ mg L}^{-1}$$

The calculation is continued in a similar fashion to obtain additional values. The results, along with the analytical solution, are

۸۲

t (yr)	c (mg L^{-1}) Numerical	Analytical	t (yr)	c (mg L^{-1}) Numerical	Analytical
0	15.00	15.00	6	127.19	127.20
1	52.75	52.75	7	131.82	131.82
2	79.36	79.37	8	135.08	135.08
3	98.11	98.12	9	137.38	137.38
4	111.32	111.33	10	138.99	139.00
5	120.63	120.64	∞	142.86	142.86

Thus, for this example, the numerical method very accurately follows the analytical solution. Discrepancies are limited to a unit quantity in the second decimal place.

7.4 SYSTEMS OF EQUATIONS

All the methods described previously can easily be adapted to simulate systems of differential equations of the form

$$\frac{dc_1}{dt} = f_1(c_1, c_2, \ldots, c_n) \tag{7.23}$$

$$\frac{dc_2}{dt} = f_2(c_1, c_2, \ldots, c_n) \tag{7.24}$$

$$\vdots$$

$$\frac{dc_n}{dt} = f_n(c_1, c_2, \ldots, c_n) \tag{7.25}$$

The solution of such a system requires that n initial conditions be known at the starting point. Then Eqs. 7.23 to 7.25 can be employed to develop slope estimates for each of the unknowns. These slope estimates are used to predict values of concentration at a new time. The process can then be repeated to project out another time step.

EXAMPLE 7.4. SPILL FOR TWO LAKES IN SERIES. A spill of 5 kg of a soluble pesticide takes place in the first of two lakes in series. Note that both lakes are completely mixed. The pesticide is subject to no losses except for flushing. Parameters for the lakes are

	Lake 1	Lake 2
Volume (m^3)	0.5×10^6	0.6×10^6
Outflow (m^3 yr^{-1})	1×10^6	1×10^6

Predict the concentration of both lakes as a function of time using Euler's method. Compare these results with the analytical solution. Present your results graphically.

Solution: First, we can develop the mass balances for the system:

$$\frac{dc_1}{dt} = -\lambda_{11}c_1 \qquad \frac{dc_2}{dt} = \lambda_{21}c_1 - \lambda_{22}c_2$$

where

$$\lambda_{11} = \frac{Q_{12}}{V_1} \qquad \lambda_{21} = \frac{Q_{12}}{V_2} \qquad \lambda_{22} = \frac{Q_{23}}{V_2}$$

۸۳

Substituting the parameter values results in

$$\frac{dc_1}{dt} = -2c_1$$

$$\frac{dc_2}{dt} = 1.667c_1 - 1.667c_2$$

If $c_1 = 10\ \mu$g L^{-1} and $c_2 = 0$, then the general solution can be developed as

$$c_1 = 10e^{-2t}$$

$$c_2 = \frac{1.667(10)}{1.667 - 2}(e^{-2t} - e^{-1.667t})$$

Now we can proceed with Euler's method. First, the differential equations are employed to calculate the slopes at $t = 0$,

$$\frac{dc_1}{dt}(0) = -2(10) = -20$$

$$\frac{dc_2}{dt}(0) = 1.667(10) - 1.667(0) = 16.667$$

These values can then be used to extrapolate out to $t = 0.1$ yr,

$$c_1(0.1) = 10 - 20(0.1) = 8\ \mu\text{g L}^{-1}$$

$$c_2(0.1) = 0 + 16.667(0.1) = 1.667\ \mu\text{g L}^{-1}$$

For the next interval ($t = 0.1$ to 0.2 yr) the computation is repeated. First, the slopes are determined at $t = 0.1$ yr:

$$\frac{dc_1}{dt}(0.1) = -2(8) = -16$$

$$\frac{dc_2}{dt}(0.1) = 1.667(8) - 1.667(1.667) = 10.556$$

These values can then be used to extrapolate out to $t = 0.2$ yr,

$$c_1(0.2) = 8 - 16(0.1) = 6.4\ \mu\text{g L}^{-1}$$

$$c_2(0.2) = 1.667 + 10.556(0.1) = 2.722\ \mu\text{g L}^{-1}$$

The calculation is continued in a similar fashion to obtain additional values. The results, along with the analytical solution, are

t (yr)	c_1 (μg L^{-1}) Numerical	Analytical	c_2 (μg L^{-1}) Numerical	Analytical
0.0	10.00	10.00	0.00	0.00
0.1	8.00	8.19	1.67	1.39
0.2	6.40	6.70	2.72	2.31
0.3	5.12	5.49	3.35	2.89
0.4	4.10	4.49	3.63	3.20
0.5	3.28	3.68	3.71	3.34
0.6	2.62	3.01	3.64	3.33
0.7	2.10	2.47	3.47	3.24
0.8	1.68	2.02	3.24	3.09
0.9	1.34	1.65	2.98	2.89
1.0	1.07	1.35	2.71	2.68

The results are plotted in Fig. 7.5 along with the analytical solution. As was the case for the single equation (Example 7.1), one way to minimize the discrepancies is to use a smaller step size.

The Heun and the fourth-order Runge-Kutta methods can also be used to simulate systems of ODEs. However, as illustrated by the following example, care should be taken to sequence the calculation of the slopes prior to computing new concentrations.

EXAMPLE 7.5. SYSTEMS OF ODES WITH THE FOURTH-ORDER RK METHOD. Use the classical fourth-order RK method to solve the same problem as in Example 7.4.

Solution: The important feature of this computation is that all the k's must be computed for the entire system of ODEs before computing the next set of concentrations. For example

$$k_{1,1} = -20 \qquad k_{2,1} = -18 \qquad k_{3,1} = -18.2 \qquad k_{4,1} = -16.36$$
$$k_{1,2} = 16.667 \qquad k_{2,2} = 13.611 \qquad k_{3,2} = 14.032 \qquad k_{4,2} = 11.295$$

These can then be used to compute the two increment functions

$$\phi_1 = \frac{1}{6}[-20 + 2(-18 - 18.2) - 16.36] = -18.127$$
$$\phi_2 = \frac{1}{6}[16.667 + 2(13.611 + 14.032) + 11.295] = 13.875$$

These can be used to extrapolate out in time,

$$c_1(0.1) = 10 - 18.127(0.1) = 8.19 \text{ mg L}^{-1}$$
$$c_2(0.1) = 0 + 13.875(0.1) = 1.39 \text{ mg L}^{-1}$$

The calculation is continued in a similar fashion to obtain additional values. The results match the analytical solution to two decimal places of accuracy. Thus, for this example, the numerical method very accurately follows the analytical solution.

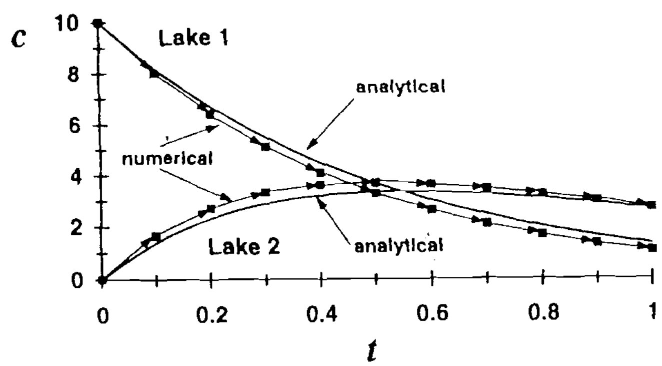

FIGURE 7.5
Comparison of analytical and Euler-method solutions for a system of well-mixed lakes.

PROBLEMS

7.1. Population-growth dynamics is important in a variety of engineering planning studies. One of the simplest models of such growth incorporates the assumption that the rate of change of the population p is proportional to the existing population at any time t:

$$\frac{dp}{dt} = Gp \qquad \text{(P7.1)}$$

where G = a growth rate (yr^{-1}). This model makes intuitive sense because the greater the population, the greater the number of potential parents.

At time $t = 0$ an island has a population of 10,000 people. If $G = 0.075$ yr^{-1}, use Euler's method to predict the population at $t = 20$ yr using a step size of 0.5 yr. Plot p versus t on standard and semi-log graph paper. Determine the slope of the line on the semi-log plot. Discuss your results.

7.2. Although the model in Prob. 7.1 works adequately when population growth is unlimited, it breaks down when factors such as food shortages, pollution, and lack of space inhibit growth. In such cases the growth rate itself can be thought of as being inversely proportional to population. One model of this relationship is

$$G = G'(p_{max} - p) \qquad \text{(P7.2)}$$

where G' = a population-dependent growth rate [(people-yr)$^{-1}$] and p_{max} = the maximum sustainable population. Thus when population is small ($p \ll p_{max}$), the growth rate will be at a high, constant rate of $G'p_{max}$. For such cases growth is unlimited and Eq. P7.2 is essentially identical to Eq. P7.1. However, as population grows (that is, as p approaches p_{max}), G decreases until at $p = p_{max}$ it is zero. Thus the model predicts that when the population reaches the maximum sustainable level, growth is nonexistent, and the system is at a steady-state. Substituting Eq. P7.2 into Eq. P7.1 yields

$$\frac{dp}{dt} = G'(p_{max} - p)p$$

For the same island studied in Prob. 7.1 use Euler's method to predict the population at $t = 20$ yr using a step size of 0.5 yr. Use values of $G' = 10^{-5}$ (people-yr)$^{-1}$ and $p_{max} = 20{,}000$ people. At time $t = 0$ the island has a population of 10,000 people. Plot p versus t and interpret the shape of the curve.

7.3. Recall that in Prob. 4.8 we studied a lake having the following characteristics:

Inflow = outflow = 20×10^6 m^3
Mean depth = 10 m
Surface area = 10×10^6 m^2

A canning plant discharges a pollutant to the system that decays at a rate of 1.05 yr^{-1}. In Prob. 4.8 you were asked to approximate the seasonal loading from a cannery as a sinusoidal input. The following measurements provide a better estimate of the loading pattern over the course of a year.

Month	J	F	M	A	M	J	J	A	S	O	N	D
Load (mta)	29	26	11	0	0	9	23	43	44	64	53	50

If the initial condition is $c = 0$ at $t = 0$,

AK

(*a*) Use the numerical method of your choice to compute the concentration in the system from $t = 0$ to 10 yr.
(*b*) After sufficient time the concentration will approach a dynamic steady-state. At this point, on what day of the year will the in-lake concentration be at a maximum value?

7.4. A small pond has the following characteristics:

Surface area = 0.2×10^6 m^2
Mean depth = 5 m
Outflow = 1×10^6 m^3 d^{-1}

The temperature in the pond varies diurnally as

Time	Midnight	2:00	4:00	6:00	8:00	10:00
Temp. (°C)	21	20	17	16	18	21
Time	Noon	2:00	4:00	6:00	8:00	10:00
Temp. (°C)	25	27	28	26	23	21

Determine the response of the system to a 2-kg spill of a pollutant that decays at a rate $k = 2$ d^{-1}. Calculate the response if the spill takes place (*a*) at midnight or (*b*) at noon. Plot the responses on the same graph. Note that the reaction has a temperature dependence characterized by $\theta = 1.08$.

7.5. Lake Washington, a beautiful lake located in Seattle, Washington, has the following general characteristics:

Volume = 2.9×10^9 m^3
Mean depth = 33 m
Outflow = 1.25×10^9 m^3 yr^{-1}

In the 1950s and 1960s it began to deteriorate because of increased loadings of the nutrient phosphorus. As a consequence, in the late 1960s, sewage inputs were greatly curtailed. The loading pattern from 1930 through the late 1970s can be summarized as in the following table:

Year	Load (mta)	Year	Load (mta)	Year	Load (mta)
1930	40	1961	137.4	1972	103.4
1940	40	1962	148.5	1973	42.9
1941	55	1963	156.5	1974	58.5
1949	55	1964	204.2	1975	99.3
1950	84.8	1965	142.8	1976	42.9
1951	81	1966	124.8	1977	60.3
1956	81	1967	54.3	1978	48.6
1957	93.2	1968	59.1	1979	60.5
1958	104.3	1969	48.2	≥ 1980	60.5
1959	115.3	1970	59.0		
1960	126.4	1971	53.8		

Total phosphorus settles at a rate of about 12 m yr^{-1}.
(*a*) Use the Heun method to compute the lake's response from 1930 through 1990. *Note:* Set the initial condition in 1930 at 17.4 μg L^{-1}.
(*b*) Compare your results with Euler's method.
(*c*) Compare your results with the fourth-order RK method.

7.6. A spill of 5 kg of a soluble pesticide takes place in the first of two lakes in series. The pesticide is subject to volatilization that can be characterized by first-order decay rates $k_1 = 0.002$ d^{-1} and $k_2 = 0.00333$ d^{-1}. Other parameters for the lakes are

	Lake 1	Lake 2
Surface area (m^2)	0.1×10^6	0.2×10^6
Mean depth (m)	5	3
Outflow (m^3 yr^{-1})	1×10^6	1×10^6

Using the fourth-order RK method,
(*a*) Predict the concentration in both lakes as a function of time; present your results as a plot.
(*b*) Determine the time required for the second lake to reach its maximum concentration.

7.7. Aside from the Heun method, there is another second-order approach for solving ordinary differential equations called the ***midpoint*** or ***improved polygon method***. It can be represented mathematically by

$$c_{i+\frac{1}{2}} = c_i + f(t_i, c_i)\frac{h}{2}$$

$$c_{i+1} = c_i + f(t_{i+\frac{1}{2}}, c_{i+\frac{1}{2}})h$$

Thus the first equation uses Euler's method to make a prediction for c at the midpoint of the interval. This value is then used to generate a centered slope estimate that is applied to predict the value at the end of the interval with the second equation. Employ this approach to solve the ODE described in Example 7.2.