

## Case Studies: Ordinary Differential Equations

The purpose of this chapter is to solve some ordinary differential equations using the numerical methods presented in Part Seven. The equations originate from practical engineering applications. Many of these applications result in nonlinear differential equations that cannot be solved using analytic techniques. Therefore, numerical methods are usually required. Thus, the techniques for the numerical solution of ordinary differential equations are fundamental capabilities that characterize good engineering practice. The problems in this chapter illustrate some of the trade-offs associated with various methods developed in Part Seven.

Section 28.1 derives from a chemical engineering problem context. It demonstrates how the transient behavior of chemical reactors can be simulated. It also illustrates how optimization can be used to estimate parameters for ODEs.

Sections 28.2 and 28.3, which are taken from civil and electrical engineering, respectively, deal with the solution of systems of equations. In both cases, high accuracy is demanded, and as a consequence, a fourth-order RK scheme is used. In addition, the electrical engineering application also deals with determining eigenvalues.

Section 28.4 employs a variety of different approaches to investigate the behavior of a swinging pendulum. This problem also utilizes two simultaneous equations. An important aspect of this example is that it illustrates how numerical methods allow nonlinear effects to be incorporated easily into an engineering analysis.

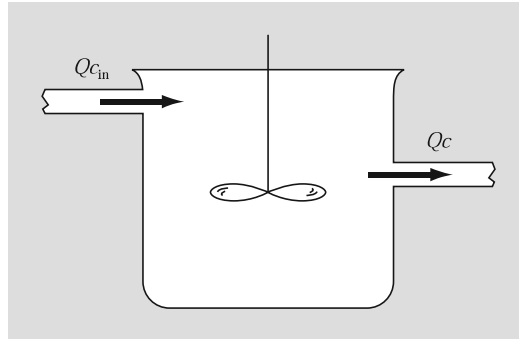
### 28.1 USING ODES TO ANALYZE THE TRANSIENT RESPONSE OF A REACTOR (CHEMICAL/BIO ENGINEERING)

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**Background.** In Sec. 12.1, we analyzed the steady state of a series of reactors. In addition to steady-state computations, we might also be interested in the transient response of a completely mixed reactor. To do this, we have to develop a mathematical expression for the accumulation term in Eq. (12.1).

Accumulation represents the change in mass in the reactor per change in time. For a constant-volume system, it can be simply formulated as

$$\text{Accumulation} = V \frac{dc}{dt} \quad (28.1)$$

**FIGURE 28.1**

A single, completely mixed reactor with an inflow and an outflow.

where  $V$  = volume and  $c$  = concentration. Thus, a mathematical formulation for accumulation is volume times the derivative of  $c$  with respect to  $t$ .

In this application we will incorporate the accumulation term into the general mass-balance framework we developed in Sec. 12.1. We will then use it to simulate the dynamics of a single reactor and a system of reactors. In the latter case, we will show how the system's eigenvalues can be determined and provide insight into its dynamics. Finally, we will illustrate how optimization can be used to estimate the parameters of mass-balance models.

**Solution.** Equations (28.1) and (12.1) can be used to represent the mass balance for a single reactor such as the one shown in Fig. 28.1:

$$V \frac{dc}{dt} = Qc_{\text{in}} - Qc \quad (28.2)$$

Accumulation = inputs – outputs

Equation (28.2) can be used to determine transient or time-variable solutions for the reactor. For example, if  $c = c_0$  at  $t = 0$ , calculus can be employed to analytically solve Eq. (28.2) for

$$c = c_{\text{in}}(1 - e^{-(Q/V)t}) + c_0 e^{-(Q/V)t}$$

If  $c_{\text{in}} = 50 \text{ mg/m}^3$ ,  $Q = 5 \text{ m}^3/\text{min}$ ,  $V = 100 \text{ m}^3$ , and  $c_0 = 10 \text{ mg/m}^3$ , the equation is

$$c = 50(1 - e^{-0.05t}) + 10e^{-0.05t}$$

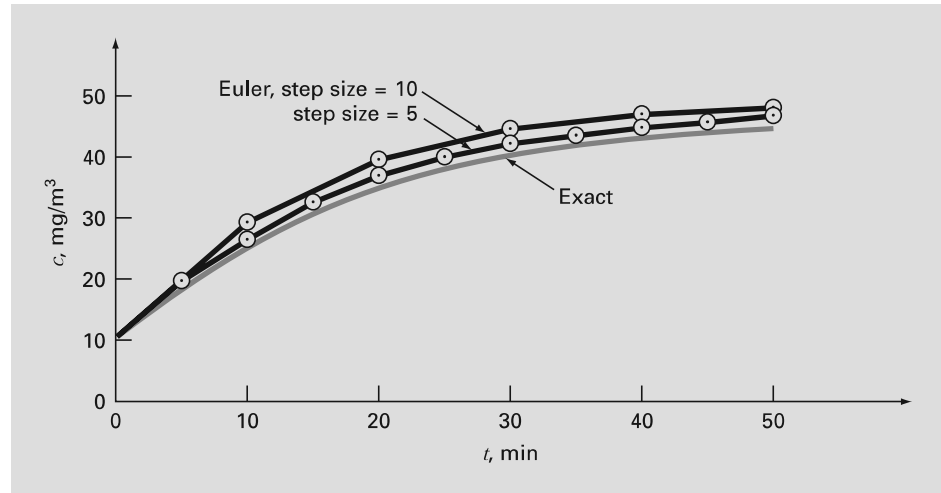
Figure 28.2 shows this exact, analytical solution.

Euler's method provides an alternative approach for solving Eq. (28.2). Figure 28.2 includes two solutions with different step sizes. As the step size is decreased, the numerical solution converges on the analytical solution. Thus, for this case, the numerical method can be used to check the analytical result.

Besides checking the results of an analytical solution, numerical solutions have added value in those situations where analytical solutions are impossible or so difficult that they are impractical. For example, aside from a single reactor, numerical methods have utility when simulating the dynamics of systems of reactors. For example, ODEs can be written

**FIGURE 28.2**

Plot of analytical and numerical solutions of Eq. (28.2). The numerical solutions are obtained with Euler's method using different step sizes.



for the five coupled reactors in Fig. 12.3. The mass balance for the first reactor can be written as

$$V_1 \frac{dc_1}{dt} = Q_{01}c_{01} + Q_{31}c_3 - Q_{12}c_1 - Q_{15}c_1$$

or, substituting parameters (note that  $Q_{01}c_{01} = 50$  mg/min,  $Q_{03}c_{03} = 160$  mg/min,  $V_1 = 50$  m<sup>3</sup>,  $V_2 = 20$  m<sup>3</sup>,  $V_3 = 40$  m<sup>3</sup>,  $V_4 = 80$  m<sup>3</sup>, and  $V_5 = 100$  m<sup>3</sup>),

$$\frac{dc_1}{dt} = -0.12c_1 + 0.02c_3 + 1$$

Similarly, balances can be developed for the other reactors as

$$\frac{dc_2}{dt} = 0.15c_1 - 0.15c_2$$

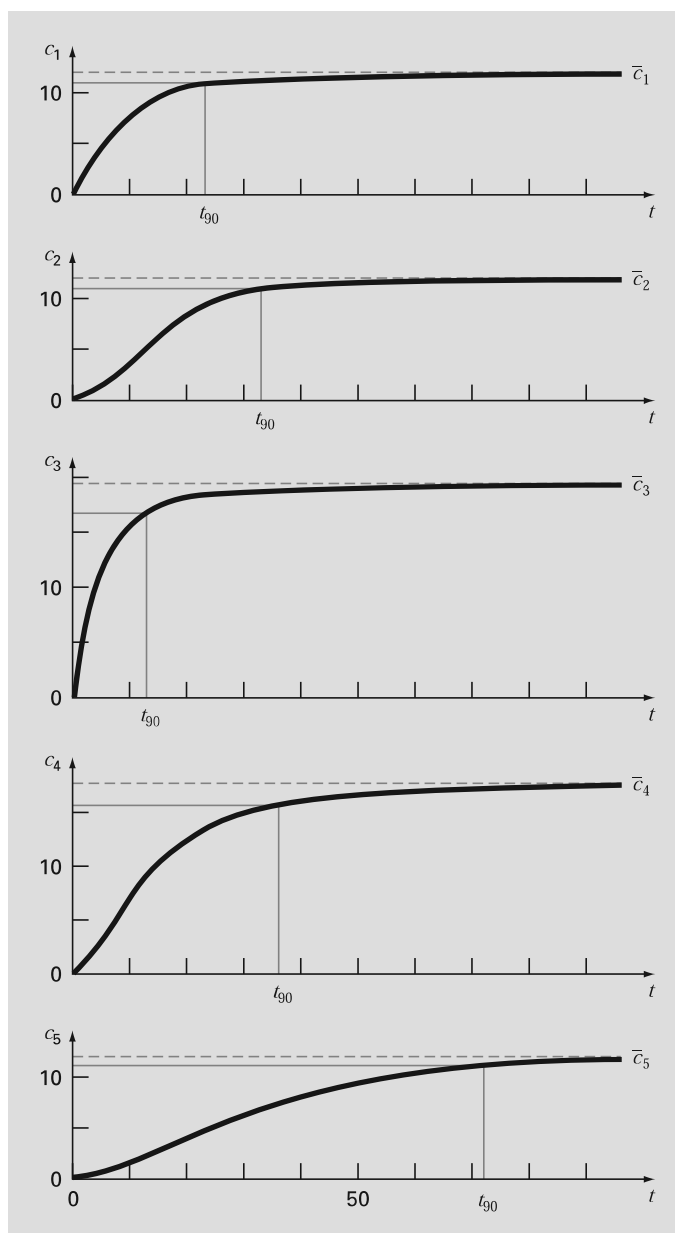
$$\frac{dc_3}{dt} = 0.025c_2 - 0.225c_3 + 4$$

$$\frac{dc_4}{dt} = 0.1c_3 - 0.1375c_4 + 0.025c_5$$

$$\frac{dc_5}{dt} = 0.03c_1 + 0.01c_2 - 0.04c_5$$

Suppose that at  $t = 0$  all the concentrations in the reactors are at zero. Compute how their concentrations will increase over the next hour.

The equations can be integrated with the fourth-order RK method for systems of equations and the results are depicted in Fig. 28.3. Notice that each of the reactors shows a different transient response to the introduction of chemical. These responses can be parameterized by a 90 percent response time  $t_{90}$ , which measures the time required for each reactor to reach 90 percent of its ultimate steady-state level. The times range from about

**FIGURE 28.3**

Plots of transient or dynamic response of the network of reactors from Fig. 12.3. Note that all the reactors eventually approach their steady-state concentrations previously computed in Sec. 12.1. In addition, the time to steady state is parameterized by the 90 percent response time  $t_{90}$ .

10 min for reactor 3 to about 70 min for reactor 5. The response times of reactors 4 and 5 are of particular concern because the two outflow streams for the system exit these tanks. Thus, a chemical engineer designing the system might change the flows or volumes of the reactors to speed up the response of these tanks while still maintaining the desired outputs. Numerical methods of the sort described in this part of the book can prove useful in these design calculations.

Further insight into the system's response characteristics can be developed by computing its eigenvalues. First, the system of ODEs can be written as an eigenvalue problem as

$$\begin{bmatrix} 0.12 - \lambda & 0 & -0.02 & 0 & 0 \\ -0.15 & 0.15 - \lambda & 0 & 0 & 0 \\ 0 & -0.025 & 0.225 - \lambda & 0 & 0 \\ 0 & 0 & -0.1 & 0.1375 - \lambda & -0.025 \\ -0.03 & -0.01 & 0 & 0 & 0.04 - \lambda \end{bmatrix} \begin{Bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ e_5 \end{Bmatrix} = \{0\}$$

where  $\lambda$  and  $\{e\}$  = the eigenvalue and the eigenvector, respectively.

A package like MATLAB software can be used to very conveniently generate the eigenvalues and eigenvectors,

```
>> a=[0.12 0.0 -0.02 0.0 0.0;-0.15 0.15 0.0 0.0 0.0;0.0
-0.025 0.225 0.0 0.0; 0.0 0.0 -0.1 0.1375 -0.025;-0.03 -0.01
0.0 0.0 0.04];
```

```
>> [e,l]=eig(a)
```

```
e =
```

```
0 0 -0.1228 -0.1059 0.2490
0 0 0.2983 0.5784 0.8444
0 0 0.5637 0.3041 0.1771
1.0000 0.2484 -0.7604 -0.7493 0.3675
0 0.9687 0.0041 -0.0190 -0.2419
```

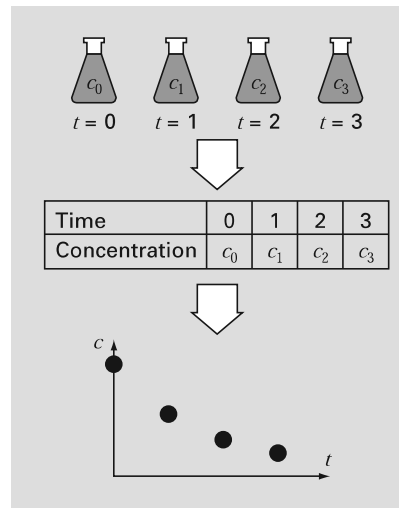
```
l =
```

```
0.1375 0 0 0 0
0 0.0400 0 0 0
0 0 0.2118 0 0
0 0 0 0.1775 0
0 0 0 0 0.1058
```

The eigenvalues can be interpreted by recognizing that the general solution for a system of ODEs can be represented as the sum of exponentials. For example, for reactor 1, the general solution would be of the form

$$c_1 = c_{11}e^{-\lambda_1 t} + c_{12}e^{-\lambda_2 t} + c_{13}e^{-\lambda_3 t} + c_{14}e^{-\lambda_4 t} + c_{15}e^{-\lambda_5 t}$$

where  $c_{ij}$  = the part of the initial condition for reactor  $i$  that is associated with the  $j$ th eigenvalue. Thus, because, for the present case, all the eigenvalues are positive (and hence negative in the exponential function), the solution consists of a series of decaying exponentials. The one with the smallest eigenvalue (in our case, 0.04) will be the slowest. In some

**FIGURE 28.4**

A simple experiment to collect rate data for a chemical compound that decays with time (reprinted from Chapra 1997).

cases, the engineer performing this analysis could be able to relate this eigenvalue back to the system parameters. For example, the ratio of the outflow from reactor 5 to its volume is  $(Q_{55} + Q_{54})/V_5 = 4/100 = 0.04$ . Such information can then be used to modify the system's dynamic performance.

The final topic we would like to review within the present context is *parameter estimation*. One area where this occurs frequently is in *reaction kinetics*, that is, the quantification of chemical reaction rates.

A simple example is depicted in Fig. 28.4. A series of beakers are set up containing a chemical compound that decays over time. At time intervals, the concentration in one of the beakers is measured and recorded. Thus, the result is a table of times and concentrations.

One model that is commonly used to describe such data is

$$\frac{dc}{dt} = -kc^n \quad (28.3)$$

where  $k$  = a reaction rate and  $n$  = the order of the reaction. Chemical engineers use concentration-time data of the sort depicted in Fig. 28.4 to estimate  $k$  and  $n$ . One way to do this is to guess values of the parameters and then solve Eq. (28.3) numerically. The predicted values of concentration can be compared with the measured concentrations and an assessment of the fit made. If the fit is deemed inadequate (for example, by examining a plot or a statistical measure like the sum of the squares of the residuals), the guesses are adjusted and the procedure repeated until a decent fit is attained.

The following data can be fit in this fashion:

$t, d$	0	1	3	5	10	15	20
$c, \text{mg/L}$	12	10.7	9	7.1	4.6	2.5	1.8

	A	B	C	D	E	F	G	H
1	Fitting of reaction rate							
2	data with the integral/least-squares approach							
3	k	0.091528						
4	n	1.044425						
5	dt	1						
6	t	k1	k2	k3	k4	cp	cm	(cp-cm)^2
7	0	-1.22653	-1.16114	-1.16462	-1.10248	12	12	0
8	1	-1.10261	-1.04409	-1.04719	-0.99157	10.83658	10.7	0.018653
9	2	-0.99169	-0.93929	-0.94206	-0.89225	9.790448		
10	3	-0.89235	-0.84541	-0.84788	-0.80325	8.849344	9	0.022697
11	4	-0.80334	-0.76127	-0.76347	-0.72346	8.002317		
12	5	-0.72354	-0.68582	-0.68779	-0.65191	7.239604	7.1	0.019489
13	6	-0.65198	-0.61814	-0.61989	-0.5877	6.552494		
14	7	-0.58776	-0.55739	-0.55895	-0.53005	5.933207		
15	8	-0.53011	-0.50283	-0.50424	-0.47828	5.374791		
16	9	-0.47833	-0.45383	-0.45508	-0.43175	4.871037		
17	10	-0.4318	-0.40978	-0.4109	-0.38993	4.416389	4.6	0.033713
18	11	-0.38997	-0.37016	-0.37117	-0.35231	4.005877		
19	12	-0.35234	-0.33453	-0.33543	-0.31846	3.635053		
20	13	-0.31849	-0.30246	-0.30326	-0.28798	3.299934		
21	14	-0.28801	-0.27357	-0.2743	-0.26054	2.996949		
22	15	-0.26056	-0.24756	-0.24821	-0.23581	2.7229	2.5	0.049684
23	16	-0.23583	-0.22411	-0.22469	-0.21352	2.474917		
24	17	-0.21354	-0.20297	-0.20349	-0.19341	2.250426		
25	18	-0.19343	-0.18389	-0.18436	-0.17527	2.047117		
26	19	-0.17529	-0.16668	-0.16711	-0.1589	1.862914		
27	20	-0.15891	-0.15115	-0.15153	-0.14412	1.695953	1.8	0.010826
28								
29							SSR =	0.155062

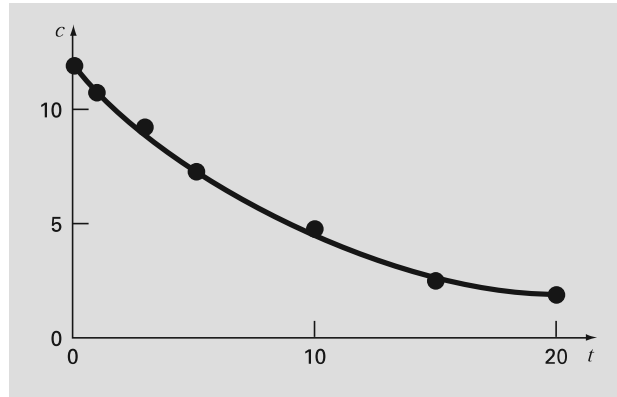
**FIGURE 28.5**

The application of a spreadsheet and numerical methods to determine the order and rate coefficient of reaction data. This application was performed with the Excel spreadsheet.

The solution to this problem is shown in Fig. 28.5. The Excel spreadsheet was used to perform the computation.

Initial guesses for the reaction rate and order are entered into cells B3 and B4, respectively, and the time step for the numerical calculation is typed into cell B5. For this case, a column of calculation times is entered into column A starting at 0 (cell A7) and ending at 20 (cell A27). The  $k_1$  through  $k_4$  coefficients of the fourth-order RK method are then calculated in the block B7..E27. These are then used to determine the predicted concentrations (the  $c_p$  values) in column F. The measured values ( $c_m$ ) are entered in column G adjacent to the corresponding predicted values. These are then used in conjunction with the predicted values to compute the squared residual in column H. These values are then summed in cell H29.

At this point, the Excel Solver can be used to determine the best parameter values. Once you have accessed the Solver, you are prompted for a target or solution cell (H29), queried whether you want to maximize or minimize the target cell (minimize), and prompted for the cells that are to be varied (B3..B4). You then activate the algorithm

**FIGURE 28.6**

Plot of fit generated with the integral/least-squares approach.

[s(olve)], and the results are as in Fig. 28.5. As shown, the values in cells B3..B4 ( $k = 0.0915$  and  $n = 1.044$ ) minimize the sum of the squares of the residuals ( $SSR = 0.155$ ) between the predicted and measured data. A plot of the fit along with the data is shown in Fig. 28.6.

## 28.2 PREDATOR-PREY MODELS AND CHAOS (CIVIL/ENVIRONMENTAL ENGINEERING)

**Background.** Environmental engineers deal with a variety of problems involving systems of nonlinear ordinary differential equations. In this section, we will focus on two of these applications. The first relates to the so-called predator-prey models that are used to study the cycling of nutrient and toxic pollutants in aquatic food chains and biological treatment systems. The second are equations derived from fluid dynamics that are used to simulate the atmosphere. Aside from their obvious application to weather prediction, such equations have also been used to study air pollution and global climate change.

*Predator-prey models* were developed independently in the early part of the twentieth century by the Italian mathematician Vito Volterra and the American biologist Alfred J. Lotka. These equations are commonly called *Lotka-Volterra equations*. The simplest example is the following pair of ODEs:

$$\frac{dx}{dt} = ax - bxy \quad (28.4)$$

$$\frac{dy}{dt} = -cy + dxy \quad (28.5)$$

where  $x$  and  $y$  = the number of prey and predators, respectively,  $a$  = the prey growth rate,  $c$  = the predator death rate, and  $b$  and  $d$  = the rate characterizing the effect of the predator-prey interaction on prey death and predator growth, respectively. The multiplicative terms (that is, those involving  $xy$ ) are what make such equations nonlinear.