Solution 23.27

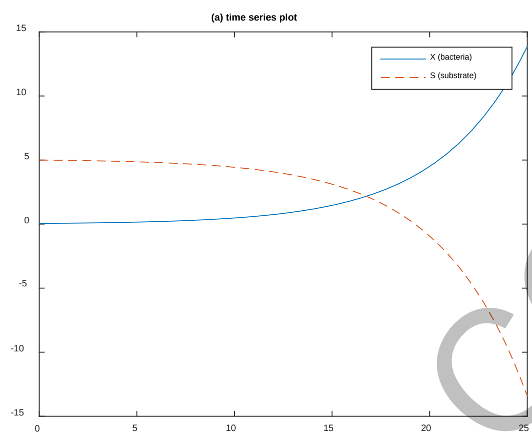
```
clear,clc,clf
Y=0.75;kmax=0.3;ks=1e-4;
tspan=[0 25];y0=[0.05 5];
disp('ode23');
tic;[t, y] = ode23(@bacteria,tspan,y0,[],Y,kmax,ks);toc;
plot(t,y(:,1),t,y(:,2),'--'),legend('X (bacteria)','S (substrate)')
title('(a) time series plot')
pause
disp('ode23 with tol = 1e-6');
options=odeset('RelTol',1e-6);
tic;[t, y] = ode23(@bacteria,tspan,y0,options,Y,kmax,ks);toc;
plot(t,y(:,1),t,y(:,2),'--'),legend('X (bacteria)','S (substrate)')
title('(a) time series plot')
pause
disp('ode45 with tol = 1e-6');
tic;[t, y] = ode45(@bacteria,tspan,y0,options,Y,kmax,ks);toc;
plot(t,y(:,1),t,y(:,2),'--'),legend('X (bacteria)','S (substrate)')
title('(a) time series plot')
pause
disp('ode15s with tol = 1e-6');
tic;[t, y] = ode15s(@bacteria,tspan,y0,options,Y,kmax,ks);toc;
plot(t,y(:,1),t,y(:,2),'--'),legend('X (bacteria)','S (substrate)')
title('(a) time series plot')
pause
disp('ode23s with tol = 1e-6');
tic;[t, y] = ode23s(@bacteria,tspan,y0,options,Y,kmax,ks);toc;
plot(t,y(:,1),t,y(:,2),'--'),legend('X (bacteria)','S (substrate)')
title('(a) time series plot')
pause
disp('ode23t with tol = 1e-6');
tic;[t, y] = ode23t(@bacteria,tspan,y0,options,Y,kmax,ks);;toc;
plot(t,y(:,1),t,y(:,2),'--'),legend('X (bacteria)','S (substrate)')
title('(a) time series plot')
pause
disp('ode23tb with tol = 1e-6');
tic;[t, y] = ode23tb(@bacteria,tspan,y0,options,Y,kmax,ks);toc;
plot(t,y(:,1),t,y(:,2),'--'),legend('X (bacteria)','S (substrate)')
title('(a) time series plot')

function yp = bacteria(t,y,Y,kmax,ks)
yp = [Y*kmax*y(2)/(ks+y(2))*y(1);-kmax*y(2)/(ks+y(2))*y(1)];
end
```

Solution continued on next page...

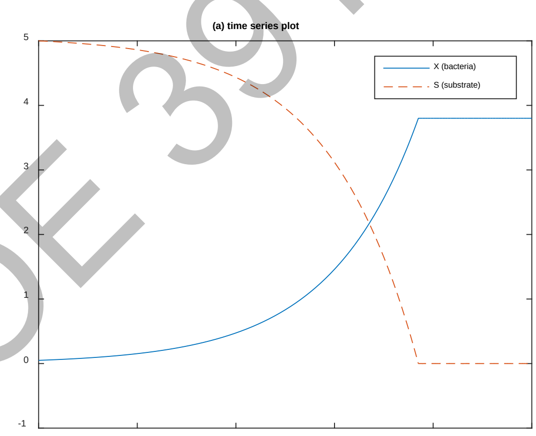
Results:

```
ode23
Elapsed time is 0.024489 seconds.
ode23 with tol = 1e-6
Elapsed time is 1.835925 seconds.
ode45 with tol = 1e-6
Elapsed time is 3.070684 seconds.
ode15s with tol = 1e-6
Elapsed time is 0.077614 seconds.
ode23s with tol = 1e-6
Elapsed time is 0.105561 seconds.
ode23t with tol = 1e-6
Elapsed time is 0.072509 seconds.
ode23tb with tol = 1e-6
Elapsed time is 0.069694 seconds.
```

The first option yields incorrect negative results, but does so quickly.



The remaining functions all yield positive results, but the non-stiff solvers (ode23 and ode45) take significantly longer to execute. Notice that the ode45 takes the longest. All the stiff solvers succeed quickly.



Solution 23.32

Scripts and Functions:

```
clc, clear, close all
k = [0.15,0.15,0.15,0.15]';
% adjust parameters to minimize SSE
[ k SSEmin ] = fminsearch(@SSE,k)

function sum=SSE(k)
t=[1,2,3,4,5,6,8,9,10,12,15]';
c1exp=[85.3,66.6,60.6,56.1,49.1,45.3,41.9,37.8,33.7,34.4,35.1]';
c2exp=[16.9,18.7,24.1,20.9,18.9,19.9,20.6,13.9,19.1,14.5,15.4]';
c3exp=[4.7,7.9,20.1,22.8,32.5,37.7,42.4,47,50.5,52.3,51.3]';
c10=100;
c20=0;
c30=0;
tspan=[0;t];
y0=[c10,c20,c30]';
reactanon = @ (t,y) react(t,y,k);
[T Y]=ode45(reactanon,tspan,y0);
e1 = c1exp - Y(2:end,1);
e2 = c2exp - Y(2:end,2);
e3 = c3exp - Y(2:end,3);
sum=e1'*e1 + e2'*e2 + e3'*e3;

function dc=react(t,y,k)
c1=y(1);
c2=y(2);
c3=y(3);
dc(1)=-k(1)*c1+k(2)*c2+k(4)*c3;
dc(2)=k(1)*c1-k(2)*c2-k(3)*c2;
dc(3)=k(3)*c2-k(4)*c3;
dc=dc';
```

Results:

```
k =
    0.2030
    0.1103
    0.4160
    0.0973
SSEmin =
  131.6424
```

Solution 24.11

Several methods could be used to obtain a solution for this problem (e.g., finite-difference, shooting method, finite-element). The finite-difference approach is straightforward:

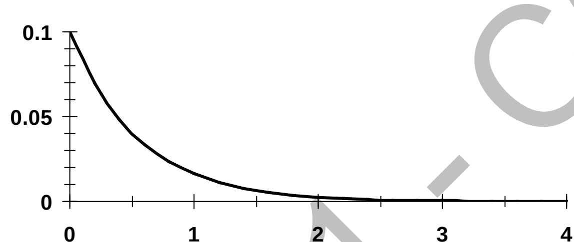
$$D\frac{A_{i-1}-2A_i+A_{i+1}}{\Delta x^2}-kA_i=0$$

Substituting parameter values and collecting terms gives

$$-1.5\times10^{-6}A_{i-1}+(3\times10^{-6}+5\times10^{-6}\Delta x^2)A_i-1.5\times10^{-6}A_{i+1}=0$$

Using a Δx = 0.2 cm this equation can be written for all the interior nodes. The resulting linear system can be solved with an approach like the Gauss-Seidel method. The following table and graph summarize the results.

x	*A*	*x*	*A*	*x*	*A*	*x*	*A*
0	0.1						
0.2	0.069544	1.2	0.011267	2.2	0.001779	3.2	0.000257
0.4	0.048359	1.4	0.007814	2.4	0.001224	3.4	0.000166
0.6	0.033621	1.6	0.005415	2.6	0.000840	3.6	9.93E−05
0.8	0.023368	1.8	0.003748	2.8	0.000574	3.8	4.65E−05
1	0.016235	2	0.002591	3	0.000389	4	0



Solution 24.13

Centered differences can be substituted for the derivatives to give

$$D\frac{c_{a,i+1}-2c_{a,i}+c_{a,i-1}}{\Delta x^2}-U\frac{c_{a,i+1}-c_{a,i-1}}{2\Delta x}-k_1c_{a,i}=0$$
$$D\frac{c_{b,i+1}-2c_{b,i}+c_{b,i-1}}{\Delta x^2}-U\frac{c_{b,i+1}-c_{b,i-1}}{2\Delta x}+k_1c_{a,i}-k_2c_{b,i}=0$$
$$D\frac{c_{c,i+1}-2c_{c,i}+c_{c,i-1}}{\Delta x^2}-U\frac{c_{c,i+1}-c_{c,i-1}}{2\Delta x}+k_2c_{b,i}=0$$

Collecting terms gives

$$-50c_{a,i-1}+83c_{a,i}-30c_{a,i+1}=0$$
$$-50c_{b,i-1}+81c_{b,i}-30c_{b,i+1}=3c_{a,i}$$
$$-50c_{c,i-1}+80c_{c,i}-30c_{c,i+1}=c_{b,i}$$

For the inlet node $(i = 1)$, we must use a finite difference approximation for the first derivative. We use a second-order version (recall Table 21.3) so that the accuracy is comparable to the centered differences we employ for the interior nodes. For example, for reactant A,

$$Uc_{a,\text{in}}=Uc_{a,1}-D\frac{-c_{a,3}+4c_{a,2}-3c_{a,1}}{2\Delta x}$$

which can be solved for

$$\left(\frac{3D}{2\Delta x^2}+\frac{U}{\Delta x}\right)c_{a,1}-\left(\frac{2D}{\Delta x^2}\right)c_{a,2}+\left(\frac{D}{2\Delta x^2}\right)c_{a,3}=\frac{U}{\Delta x}c_{a,\text{in}}$$

Because the condition does not include reaction rates, similar equations can be written for the other nodes. Substituting the parameters gives

$$80c_{a,1}-80c_{a,2}+20c_{a,3}=200$$
$$80c_{b,1}-80c_{b,2}+20c_{b,3}=0$$
$$80c_{c,1}-80c_{c,2}+20c_{c,3}=0$$

Solution continued on next page...

For the outlet node $(i = 10)$, the zero derivative condition implies that $c_{11} = c_9$,

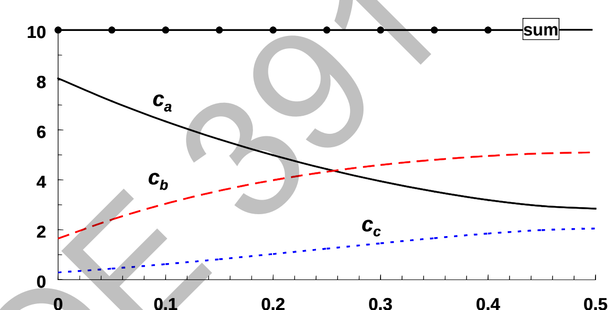
$$-\left(\frac{2D}{\Delta x^2}\right)c_9 + \left(\frac{2D}{\Delta x^2} + k_1\right)c_{10} = 0$$

Again, because the condition does not include reaction rates, similar equations can be written for the other nodes. Substituting the parameters gives

$$-80c_{a,9} + 83c_{a,10} = 0$$
$$-80c_{b,9} + 81c_{b,10} = 3c_{a,10}$$
$$-80c_{c,9} + 80c_{c,10} = c_{b,10}$$

Notice that because the reactions are in series, we can solve the systems for each reactant separately in sequence. The result is

x	c_a	c_b	c_c	**sum**
0	8.0646	1.6479	0.2875	10
0.05	7.1492	2.4078	0.4430	10
0.1	6.3385	3.0397	0.6218	10
0.15	5.6212	3.5603	0.8184	10
0.2	4.9878	3.9846	1.0276	10
0.25	4.4309	4.3258	1.2433	10
0.3	3.9459	4.5955	1.4587	10
0.35	3.5320	4.8035	1.6644	10
0.4	3.1955	4.9572	1.8473	10
0.45	2.9542	5.0591	1.9867	10
0.5	2.8474	5.1021	2.0505	10



Solution 24.14

Centered differences can be substituted for the derivatives to give

$$D\frac{c_{a,i+1}-2c_{a,i}+c_{a,i-1}}{\Delta x^2}=0 \qquad 0 \le x < L$$

$$D_f\frac{c_{a,i+1}-2c_{a,i}+c_{a,i-1}}{\Delta x^2}-kc_{a,i}=0 \qquad L \le x < L+L_f$$

Collecting terms

$$-\frac{D}{\Delta x^2}c_{a,i-1}+\frac{2D}{\Delta x^2}c_{a,i}-\frac{D}{\Delta x^2}c_{a,i+1}=0 \qquad 0 \le x < L$$

$$-\frac{D_f}{\Delta x^2}c_{a,i-1}+\left(\frac{2D_f}{\Delta x^2}+k\right)c_{a,i}-\frac{D_f}{\Delta x^2}c_{a,i+1}=0 \qquad L \le x < L+L_f$$

The boundary conditions can be developed. For the first node $(i=1)$,

$$\frac{2D}{\Delta x^2}c_{a,1}-\frac{D}{\Delta x^2}c_{a,2}=\frac{D}{\Delta x^2}c_{a0}$$

For the last,

$$-\frac{2D_f}{\Delta x^2}c_{a,n-1}+\left(\frac{2D_f}{\Delta x^2}+k\right)c_{a,n}=0$$

A special equation is also required at the interface between the diffusion layer and the biofilm $(x=L)$. A flux balance can be written around this node as

$$D\frac{c_{a,i-1}-c_{a,i}}{\Delta x}+D_f\frac{c_{a,i+1}-c_{a,i}}{\Delta x}-k\frac{\Delta x}{2}c_{a,i}=0$$

Collecting terms gives

$$-\frac{D}{\Delta x}c_{a,i-1}+\left(\frac{D+D_F}{\Delta x}+k\frac{\Delta x}{2}\right)c_{a,i}-\frac{D_f}{\Delta x}c_{a,i+1}=0$$

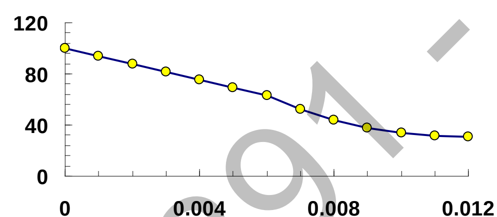
Solution continued on next page...

Substituting the parameters gives

first node:	$160{,}000c_{a,1} - 80{,}000c_{a,2} = 8{,}000{,}000$
interior nodes (diffusion layer):	$-80{,}000c_{a,i-1} + 160{,}000c_{a,i} - 80{,}000c_{a,i+1} = 0$
boundary node (i = 6):	$-80{,}000c_{a,5} + 121{,}000c_{a,6} - 40{,}000c_{a,7} = 0$
interior nodes (biofilm):	$-40{,}000c_{a,i-1} + 82{,}000c_{a,i} - 40{,}000c_{a,i+1} = 0$
last node:	$-80{,}000c_{a,n-1} + 82{,}000c_{a,n} = 0$

The solution is

x	c_a
0	100.0000
0.001	93.8274
0.002	87.6549
0.003	81.4823
0.004	75.3097
0.005	69.1372
0.006	62.9646
0.007	52.1936
0.008	44.0322
0.009	38.0725
0.01	34.0164
0.011	31.6611
0.012	30.8889



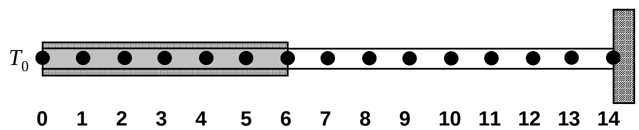
Solution 24.22

Heat balances for the two sections can be written as

rod: $$\frac{d^2T}{dx^2} = 0$$

tube: $$\frac{d^2T}{dx^2} + \frac{2h}{rk_2}(T_\infty - T) = 0$$

The nodes can be set up as shown:



Substituting finite differences for the interior nodes gives

Rod nodes i = 1 through 5: $$\frac{T_{i-1} - 2T_i + T_{i+1}}{\Delta x^2} = 0$$

Tube nodes i = 7 through 13: $$\frac{T_{i-1} - 2T_i + T_{i+1}}{\Delta x^2} + \frac{2h}{rk_2}(T_\infty - T_i) = 0$$

At the left end (node 0), $T = T_0$, so the heat balance for node 1 is

$$2T_1 - T_2 = T_0$$

For nodes 2 through 5:

$$\begin{aligned}
-T_1 + 2T_2 - T_3 &= 0 \\
-T_2 + 2T_3 - T_4 &= 0 \\
-T_3 + 2T_4 - T_5 &= 0 \\
-T_4 + 2T_5 - T_6 &= 0
\end{aligned}$$

For nodes 7 through 13

$$-T_{i+1} + \left(2 + \frac{2h\Delta x^2}{rk_2}\right)T_i - T_{i-1} = \frac{2h\Delta x^2}{rk_2}T_\infty$$

Solution continued on next page...

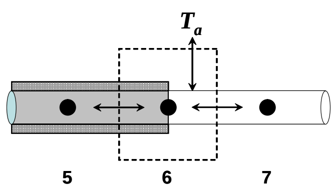
or substituting the parameters,

$$-T_{i-1} + \left(2 + \frac{2\times 3000\ \text{J/(s m}^2\text{K)}(0.1\ \text{m})^2}{0.03\ \text{m}\times 0.615\ \text{J/(s m K)}}\right)T_i + T_{i+1} = \frac{2\times 3000\ \text{J/(s m}^2\text{K)}(0.1\ \text{m})^2}{0.03\ \text{m}\times 0.615\ \text{J/(s m K)}}T_\infty$$

which gives

$$-T_{i-1} + 3254T_i - T_{i+1} = 975{,}610$$

To write a heat balance at the node between the rod and the tube, a heat balance can be written for the element enclosed by the dashed line depicted below:



The steady-state heat balance for this element is

$$0 = -k_1 \frac{T_6 - T_5}{\Delta x} A_c - k_2 \frac{T_6 - T_7}{\Delta x} A_c + h(T_\infty - T_6)A_s$$

where A_c = the cross-sectional area (m^2) = πr^2, and A_s = the surface area (m^2) of the tube within the element boundary = $\pi r \Delta x$. Substituting these areas gives

$$0 = -k_1 \frac{T_6 - T_5}{\Delta x} \pi r^2 - k_2 \frac{T_6 - T_7}{\Delta x} \pi r^2 + h(T_\infty - T_6)\pi r \Delta x$$

or collecting terms

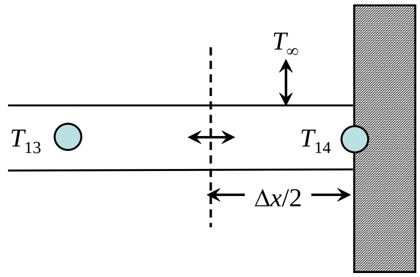
$$-k_1 T_5 + \left(k_1 + k_2 + \frac{h}{r}\Delta x^2\right)T_6 - k_2 T_7 = \frac{h}{r}\Delta x^2 T_\infty$$

Substituting the parameters gives

$$-80.2T_5 + 1080.8T_6 - 0.615T_7 = 300{,}000$$

Solution continued on next page...

At the right end $(i = 14)$, a heat balance is written as



$$0 = -k_2 \frac{T_{14} - T_{13}}{\Delta x} A_c + h(T_\infty - T_{14}) A_s$$

Substituting the areas and collecting terms gives

$$-T_{13} + \left(1 + \frac{h\Delta x^2}{k_2 r}\right) T_{14} = \frac{h\Delta x^2}{k_2 r} T_\infty$$

Substituting parameters yields

$$-T_{13} + 1627 T_{14} = 487805$$

The foregoing equations can be assembled in matrix form as

$$\begin{bmatrix}
2 & -1 & & & & & & & & & & & & \\
-1 & 2 & -1 & & & & & & & & & & & \\
 & -1 & 2 & -1 & & & & & & & & & & \\
 & & -1 & 2 & -1 & & & & & & & & & \\
 & & & -1 & 2 & -1 & & & & & & & & \\
 & & & & -80.2 & 1080.8 & -0.615 & & & & & & & \\
 & & & & & -1 & 3254 & -1 & & & & & & \\
 & & & & & & -1 & 3254 & -1 & & & & & \\
 & & & & & & & -1 & 3254 & -1 & & & & \\
 & & & & & & & & -1 & 3254 & -1 & & & \\
 & & & & & & & & & -1 & 3254 & -1 & & \\
 & & & & & & & & & & -1 & 3254 & -1 & \\
 & & & & & & & & & & & -1 & 3254 & -1 \\
 & & & & & & & & & & & & -1 & 1627
\end{bmatrix}
\begin{Bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \\ T_7 \\ T_8 \\ T_9 \\ T_{10} \\ T_{11} \\ T_{12} \\ T_{13} \\ T_{14} \end{Bmatrix}
=
\begin{Bmatrix} 400 \\ 0 \\ 0 \\ 0 \\ 0 \\ 300000 \\ 975610 \\ 975610 \\ 975610 \\ 975610 \\ 975610 \\ 975610 \\ 975610 \\ 487805 \end{Bmatrix}$$

Solution continued on next page...

These can be solved for

$T_1 = 383.553$ $T_2 = 367.106$ $T_3 = 350.659$ $T_4 = 334.212$ $T_5 = 317.765$
$T_6 = 301.318$ $T_7 = 300.0004$ $T_8 = 300$ $T_9 = 300$ $T_{10} = 300$
$T_{11} = 300$ $T_{12} = 300$ $T_{13} = 300$ $T_{14} = 300$

A plot of the results can be developed as