Solution 22.5

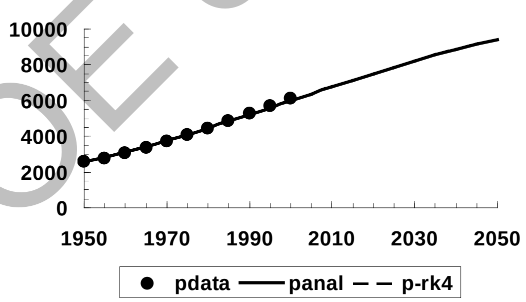
(a) The analytical solution can be used to compute values at times over the range. For example, the value at t = 1955 can be computed as

$$p = 2,555 \frac{12,000}{2,555 + (12,000 - 2,555)e^{-0.026(1955-1950)}} = 2,826.2$$

Values at the other times can be computed and displayed along with the data in the plot below.

(b) The ODE can be integrated with the fourth-order RK method with the results tabulated and plotted below:

t	p-rk4	k_1	t_m	y_m	k_2	t_m	y_m	k_3	t_e	y_e	k_4	ϕ
1950	2555.0	52.29	1952.5	2685.7	54.20	1952.5	2690.5	54.27	1955.0	2826.3	56.18	54.23
1955	2826.2	56.17	1957.5	2966.6	58.06	1957.5	2971.3	58.13	1960.0	3116.8	59.99	58.09
1960	3116.6	59.99	1962.5	3266.6	61.81	1962.5	3271.1	61.87	1965.0	3425.9	63.64	61.83
1965	3425.8	63.64	1967.5	3584.9	65.36	1967.5	3589.2	65.41	1970.0	3752.8	67.06	65.37
1970	3752.6	67.06	1972.5	3920.3	68.63	1972.5	3924.2	68.66	1975.0	4096.0	70.15	68.63
1975	4095.8	70.14	1977.5	4271.2	71.52	1977.5	4274.6	71.55	1980.0	4453.5	72.82	71.52
1980	4453.4	72.82	1982.5	4635.4	73.97	1982.5	4638.3	73.98	1985.0	4823.3	75.00	73.95
1985	4823.1	75.00	1987.5	5010.6	75.88	1987.5	5012.8	75.89	1990.0	5202.6	76.62	75.86
1990	5202.4	76.62	1992.5	5394.0	77.20	1992.5	5395.5	77.21	1995.0	5588.5	77.63	77.18
1995	5588.3	77.63	1997.5	5782.4	77.90	1997.5	5783.1	77.90	2000.0	5977.8	78.00	77.87
2000	5977.7	78.00	2002.5	6172.7	77.94	2002.5	6172.5	77.94	2005.0	6367.4	77.71	77.91
2005	6367.2	77.71	2007.5	6561.5	77.32	2007.5	6560.5	77.32	2010.0	6753.8	76.77	77.29
2010	6753.7	76.77	2012.5	6945.6	76.06	2012.5	6943.9	76.07	2015.0	7134.0	75.21	76.04
2015	7133.9	75.21	2017.5	7321.9	74.21	2017.5	7319.4	74.23	2020.0	7505.0	73.09	74.20
2020	7504.9	73.09	2022.5	7687.6	71.83	2022.5	7684.5	71.85	2025.0	7864.2	70.47	71.82
2025	7864.0	70.47	2027.5	8040.2	68.98	2027.5	8036.5	69.01	2030.0	8209.1	67.43	68.98
2030	8208.9	67.43	2032.5	8377.5	65.75	2032.5	8373.3	65.80	2035.0	8537.9	64.04	65.76
2035	8537.7	64.05	2037.5	8697.8	62.23	2037.5	8693.3	62.28	2040.0	8849.1	60.41	62.25
2040	8849.0	60.41	2042.5	9000.0	58.50	2042.5	8995.2	58.56	2045.0	9141.8	56.61	58.53
2045	9141.6	56.62	2047.5	9283.1	54.65	2047.5	9278.2	54.72	2050.0	9415.2	52.73	54.68
2050	9415.0											



Thus, the RK4 results are so close to the analytical solution that the two results are indistinguishable graphically.

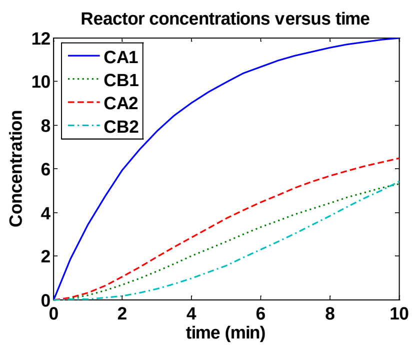
Solution 22.18

Function defining the derivatives:

```
function dc = dCdtReactor(t,C,tau,CA0,k)
dc=[1/tau*(CA0-C(1))-k*C(1); -1/tau*C(2)+k*C(1); ...
    1/tau*(C(1)-C(3))-k*C(3); 1/tau*(C(2)-C(4))+k*C(3)];
```

Script to generate plot using the `rk4sys` function (Fig. 22.8):

```
clear,clc,clf
CA0=20;k=0.12;tau=5;
tspan=[0:1/2:10];y0=[0 0 0 0];
[t,C]=rk4sys(@dCdtReactor,tspan,y0,1/16,tau,CA0,k);
plot(t,C(:,1),t,C(:,2),':',t,C(:,3),'--',t,C(:,4),'-.')
legend('CA1','CB1','CA2','CB2','location','best')
title('Reactor concentrations versus time')
xlabel('time (min)'),ylabel('Concentration')
```



Solution 22.19

The classical 4th order RK method yields

t	*C*	*T*
0	1.0000	15.0000
0.0625	0.9413	60.7968
0.125	0.8858	82.9030
0.1875	0.8336	92.3765
0.25	0.7844	95.1878
0.3125	0.7381	94.5486
0.375	0.6945	92.1809
0.4375	0.6536	89.0041
0.5	0.6150	85.5057
0.5625	0.5788	81.9414
0.625	0.5446	78.4421
0.6875	0.5125	75.0722
0.75	0.4823	71.8606
0.8125	0.4539	68.8176
0.875	0.4272	65.9436
0.9375	0.4021	63.2342
1	0.3784	60.6825

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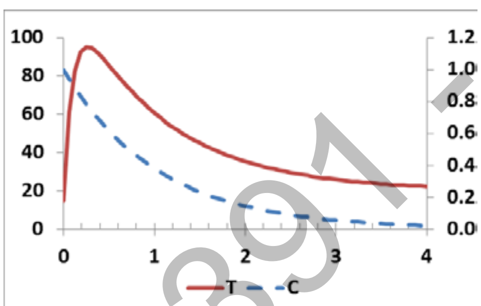
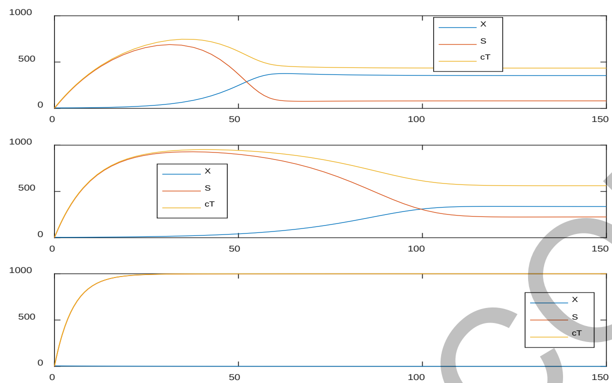


Solution 22.25

```
clear,clc,clf
tauw=[20 10 5];
kgmax=0.2; Ks=150; kd=0.01; kr=0.01;
Y=0.5; Sin=1000;
for i = 1:length(tauw)
  [t,c]=ode45(@derivs,[0 150],[5 0],[],tauw(i),kgmax,Ks,kd,kr,Y,Sin);
  cT=c(:,1)+c(:,2);
  subplot(3,1,i)
  plot(t,c,t,cT)
  legend('X','S','cT','location','best')
end

function dy=derivs(t,y,tauw,kgmax,Ks,kd,kr,Y,Sin)
dy=[(kgmax*y(2)./(Ks+y(2))-kd-kr-1/tauw).*y(1);...
    -1/Y*kgmax*y(2)./(Ks+y(2)).*y(1)+kd*y(1)+1/tauw*(Sin-y(2))];
End
```



Solution 23.8

(a) The exact solution is

$$y = Ae^{5t} + t^2 + 0.4t + 0.08$$

If the initial condition at $t = 0$ is 0.08, $A = 0$,

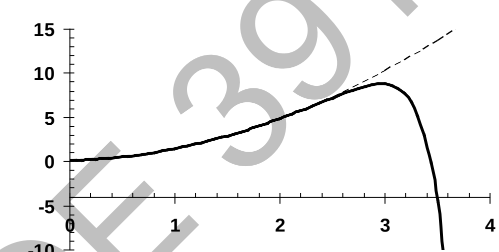
$$y = t^2 + 0.4t + 0.08$$

Note that even though the choice of the initial condition removes the positive exponential terms, it still lurks in the background. Very tiny round off errors in the numerical solutions bring it to the fore. Hence all of the following solutions eventually diverge from the analytical solution.

(b) 4th order RK. Here are the first few steps:

t	*y*
0	0.08
0.03125	0.093476
0.0625	0.108906
0.09375	0.126289
0.125	0.145625
0.15625	0.166914
0.1875	0.190156
0.21875	0.215351
0.25	0.242499

The plot shows the numerical solution (bold line) along with the exact solution (fine line).



Solution continued on next page...

(c)

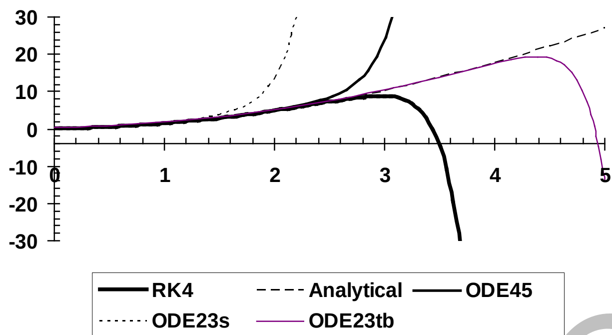
```
function yp = dy(t,y)
yp = 5*(y-t^2);

>> tspan = [0,5];
>> y0 = 0.08;
>> [t,y] = ode45(@dy,tspan,y0);
```

(d)

```
>> [t,y] = ode23s(@dy,tspan,y0);
```

(e)

```
>> [t,y] = ode23tb(@dy,tspan,y0);
```



Solution 23.13

In MATLAB, the first step is to set up a function to hold the differential equations:

```
function dc = dcdtstiff(t, c)
dc = [-0.013*c(1)-1000*c(1)*c(3);-2500*c(2)*c(3);-0.013*c(1)-1000*c(1)*c(3)-2500*c(2)*c(3)];
```

Then, an ODE solver like the function `ode45` can be implemented as in

```
>> tspan=[0,50];
>> y0=[1,1,0];
>> [t,y]=ode45(@dcdtstiff,tspan,y0);
```

If this is done, the solution will take a relatively long time to compute the results. In contrast, because it is expressly designed to handle stiff systems, a function like `ode23s` yields results almost instantaneously.

```
>> [t,y]=ode23s(@dcdtstiff,tspan,y0);
```

In either case, a plot of the results can be developed as

```
>> plot(t,y)
```

Both plots will be identical as shown here