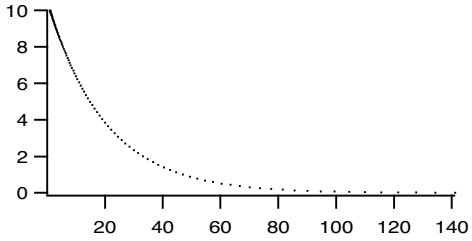

Note that throughout these examples the initial value of YY has remained at 10.

A System of Coupled First-Order Equations

While many interesting systems are described by simple (possibly nonlinear) first-order equations, more interesting behavior results from systems of coupled equations.

The next example comes from chemical kinetics. Suppose you mix two substances A and B together in a solution and they react to form intermediate phase C. Over time C transforms into final product D:

$$A + B \underset{k_2}{\overset{k_1}{\rightleftarrows}} C \qquad C \xrightarrow{k_3} D$$

Here, k_1, k_2, and k_3 are rate constants for the reactions. The concentrations of the substances might be given by the following coupled differential equations:

$$\frac{dA}{dt} = \frac{dB}{dt} = -k_1 \cdot A \cdot B + k_2 \cdot C \qquad \frac{dC}{dt} = k_1 \cdot A \cdot B - k_2 \cdot C - k_3 \cdot C \qquad \frac{dD}{dt} = k_3 \cdot C$$

To solve these equations, first we need a derivative function:

```
Function ChemKinetic(pw, tt, yw, dydt)
   Wave pw           // pw[0] = k1, pw[1] = k2, pw[2] = k3
   Variable tt       // time value at which to calculate derivatives
   Wave yw           // yw[0]-yw[3] containing concentrations of A,B,C,D
   Wave dydt         // wave to receive dA/dt, dB/dt etc. (output)
   dydt[0] = -pw[0]*yw[0]*yw[1] + pw[1]*yw[2]
   dydt[1] = dydt[0]  // first two equations are the same
   dydt[2] = pw[0]*yw[0]*yw[1] - pw[1]*yw[2] - pw[2]*yw[2]
   dydt[3] = pw[2]*yw[2]

   return 0
End
```

We think that it is easiest to keep track of the results using a single multicolumn Y wave. These commands make a four-column Y wave and use dimension labels to keep track of which column corresponds to which substance:

```
Make/D/O/N=(100,4) ChemKin
SetScale/P x 0,10,ChemKin  // calculate concentrations every 10 s
SetDimLabel 1,0,A,ChemKin  // set dimension labels to substance names
SetDimLabel 1,1,B,ChemKin  // this can be done in a table if you make
SetDimLabel 1,2,C,ChemKin  // the table using edit ChemKin.ld
SetDimLabel 1,3,D,ChemKin
ChemKin[0][%A] = 1         // initial conditions: concentration of A
ChemKin[0][%B] = 1         // and B is 1, C and D is 0
ChemKin[0][%C] = 0         // note indexing using dimension labels
ChemKin[0][%D] = 0
Make/D/O KK={0.002,0.0001,0.004}    // rate constants
```