Decomposition of H2O2

Kurt Bryan and SIMIODE

Worksheet for examining first order chemical reaction data for decomposition of H2O2.

```
> restart;
  with(plots) : #Load in plots package
  with(CurveFitting) : #Maple's curve fitting package
```

Times at which data was taken (seconds)

```
> times := [0, 120, 300, 600, 1200, 1800, 2400, 3000, 3600]; #Times, in seconds
```

H2O2 concentration, moles per liter at each time above

```
> data := [1.00, 0.91, 0.78, 0.59, 0.37, 0.22, 0.13, 0.08, 0.05];
      #H2O2 concentrations, moles per liter
```

Number of data points

```
> N := nops(data)
```

Logarithmic transformation of data

```
> log_of_data := [seq(ln(data[j]), j = 1 ..N) ]
```

Plot the log data versus time. Call the plot "plot1".

```
> plot1 := pointplot([seq([times[j], log_of_data[j]], j = 1 ..N) ], symbol = solidcircle, symbolsize
      = 20)
```

Fit a line y = -k*t to this data. We'll use Maple's built-in curve fitting (and examine how it works in Chapter 3).

```
> bestline := LeastSquares(times, log_of_data, t, curve = -k·t);
      #Alternatively, use "curve = -k·t+b" to include y-intercept
```

Plot this line and display with plot of data

```
> plot2 := plot(bestline, t = 0 ..3600, color = blue) :
  display(plot1, plot2)
>
```