ME 1020 Engineering Programming with MATLAB

Problem 6.17:

17. Chemists and engineers must be able to predict the changes in chemical concentration in a reaction. A model used for many single-reactant processes is

$$\text{Rate of change of concentration} = -kC^n$$

where C is the chemical concentration and k is the rate constant. The order of the reaction is the value of the exponent n. Solution methods for differential equations (which are discussed in Chapter 9) can show that the solution for a first-order reaction ($n = 1$) is

$$C(t) = C(0)e^{-kt}$$

The following data describe the reaction

$$(CH_3)_3CBr + H_2O \rightarrow (CH_3)_3COH + HBr$$

Use these data to obtain a least-squares fit to estimate the value of k.

Time t (h)	C (mol of $(CH3)_3$ CBr/L)
0	0.1039
3.15	0.0896
6.20	0.0776
10.0	0.0639
18.3	0.0353
30.8	0.0207
43.8	0.0101

```
% Problem 6.17
clear
clc
disp('Problem 6.17: Scott Thomas')

format shortEng

time = [0 3.15 6.2 10 18.3 30.8 43.8];
timeplot = 0:0.1:45;
C = [0.1039 0.0896 0.0776 0.0639 0.0353 0.0207 0.0101];% torr
p = polyfit(time, log10(C),1)
m = p(1)
b = 10^p(2)
Cplot = b*10.^(m*timeplot);
%semilogy(time,C, 'o', timeplot, Cplot)
plot(time,C, 'o', timeplot, Cplot)
xlabel('Time (hr)'),
ylabel('Concentration C [mol of (CH_3)_3COH + HBr/L]'),
title('Problem 6.17: Scott Thomas')
text(2,0.01,'C = 0.1051(10)^{0.02332*t}');
```

```
Problem 6.17: Scott Thomas

p =

   -23.3255e-003  -978.4792e-003


m =

   -23.3255e-003


b =

   105.0802e-003
```