Final Exam
Administered: Thursday, December 12, 2013
24 points

Problem 1. (8 points)

Consider the isomerization reaction:

$$A \rightarrow B$$

The reaction rate is given by

$$rate = C_A k_o e^{-\frac{E_a}{RT}} \qquad [\text{moles/m}^3\text{/sec}]$$

where

concentration of A: C_A [moles/m^3]
prefactor: k_o [1/sec]
activation energy for reaction: E_a [Joules/mole]
constant: $R = 8.314$ [Joules/mole/K]
temperature: T [K]

Determine the rate constants, k_o and E_a, from experimental data. The reaction is measured at a constant concentration of A, C_A = 2000 mol/m^3, over a range of temperatures. The rate is recorded. The rate as a function of temperature is given in tabular form in the file "xm4p01_f13.txt" on the exam portion of the course website.

Solution:

Convert the data into a linear form necessary for a linear regression.

$$\ln(rate) - \ln(C_A) = -\frac{E_a}{RT} + \ln(k_o)$$

This equation is of the form: $y = b_1 x + b_0$ where

$$y = \ln(rate) - \ln(C_A),\ b_1 = E_a,\ x = -\frac{1}{RT},\ \text{and}\ b_0 = \ln(k_o).$$

I used the code linreg1.m for linear regression with one independent variable.

I wrote the small script xm4p01_f13.m

```
clear all;

%Temperature    rate of A loss
%K              mole/m^3/s
```

```
M = [500    0.000402223
525 0.001902014
550 0.005855487
575 0.020039784
600 0.053936753];

R = 8.314; % J/mol/K
CA = 2000; % mol/m^3
n = max(size(M));
for i = 1:1:n
    x(i) = -1.0/(R*M(i,1));
    y(i) = log(M(i,2)) - log(CA);
end
[b,bsd,MOF] = linreg1(x, y)
Ea = b(2)
ko = exp(b(1))
```

At the command line prompt, I executed the script

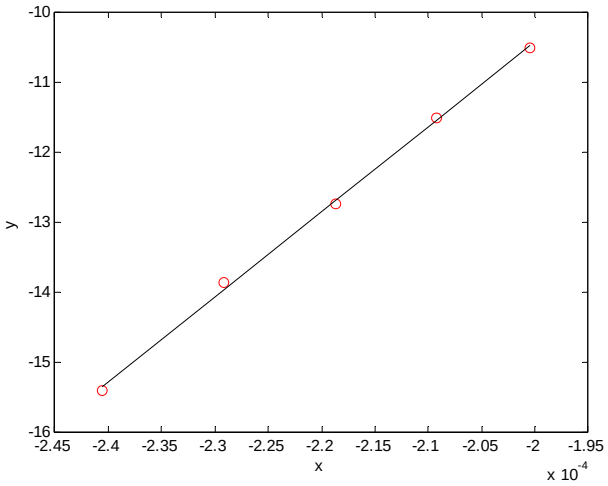
```
>> xm4p01_f13
```

This generated the following output for the means, standard deviations and Measure of Fit.

```
b =   1.0e+05 *
    0.0001
    1.2150

bsd =   1.0e+03 *
    0.0005
    2.4340
MOF =    0.9988
Ea =   1.2150e+05

ko =   1.0566e+06
```



The activation energy was 121,500 J/mol.
The rate constant was 1.0566×10^6 1/sec.

The code also generated a plot.

Problem 2. (8 points)

The complementary error function is defined as

$$erfc(x) = 1 - \frac{2}{\sqrt{\pi}} \int_0^x \exp\left(-t^2\right) dt$$

(a) Evaluate the complementary error function for $x = 2$ using the intrinsic erfc function. You likely will need to use the `format long` statement in MatLab to get enough digits to display.
(b) How many intervals so you need in the second-order Simpson's method to obtain this result to four significant digits?

Solution:

(a) Evaluate the complementary error function for $x = 2$ using the intrinsic erfc function.

```
>> format long
>> y = erfc(2)

y =   0.004677734981047
```

(b) How many intervals so you need in the second-order Simpson's method to obtain this result to four significant digits?

I used the simpson2.m code and changed the integrand function to

```
function f = funkeval(x)
f = 2.0/sqrt(pi)*exp(-x^2);
```

From the command line prompt.

```
>> erfc_2 = 1.0 - simpson2(0,2,100)
Using the Simpsons Second Order method
to integrate from 0.000000 to 2.000000 with 100 nintervals,
the integral is 9.953223e-01
erfc_2 =   0.004677735715887
```

So 100 intervals gives about 7 good significant digits.

```
>> erfc_2 = 1.0 - simpson2(0,2,10)
Using the Simpsons Second Order method
to integrate from 0.000000 to 2.000000 with 10 nintervals,
the integral is 9.953149e-01
erfc_2 =   0.004685085139049
```

So 10 intervals gives about 3 good significant digits.

```
>> erfc_2 = 1.0 - simpson2(0,2,20)
Using the Simpsons Second Order method
to integrate from 0.000000 to 2.000000 with 20 nintervals,
```

```
the integral is 9.953218e-01
erfc_2 =   0.004678194420860
```

So 20 intervals gives about 4 good significant digits.

Problem 3. (8 points)

The one-dimensional heat equation at steady state can describe heat transfer in a material with both heat conduction and radiative heat loss.

$$0 = \frac{k}{\rho C_p}\frac{d^2T}{dz^2} - \frac{\varepsilon\sigma S}{\rho C_p}\left(T^4 - T_s^4\right)$$

where the following variables [with units] are given as

temperature in the material T [K]
surrounding temperature $T_s = 300$ [K]
axial position along material z [m]
thermal conductivity $k = 401$ [J/K/m/s] (for Cu)
mass density $\rho =$ 8960 [kg/m^3] (for Cu)
heat capacity $C_p = 384.6$ [J/kg/K] (for Cu)
Stefan–Boltzmann constant $\sigma = 6.6404x10^{-8}$ [J/s/m^2/K^4]
gray body permittivity $\varepsilon = 0.05$
surface area to volume ratio $S = 200$ [1/m] (for a cylindrical rod of diameter 0.01 m)

If the temperature of the material at z=0 is $T(z=0) = 1000\,\text{K}$ and the flux at z=0 is $\left.\frac{dT}{dz}\right|_{z=0} = -2000$ K/m, find the temperature in the material at z=0.1 m.

Solution:

Let us begin by rearranging this ODE.

$$\frac{d^2T}{dz^2} = \frac{\varepsilon\sigma S}{k}\left(T^4 - T_s^4\right)$$

This is a single second-order nonlinear ODE, subject to initial conditions. We must convert this single second-order ODE to a system of two first-order ODEs. The conversion is a three step process. The first step is defining *2* new variables, which always have the following form:

$$y_1(z) = T(z)$$
$$y_2(z) = \frac{dT(z)}{dz}$$

The second step is writing one first-order ODE for each of these *2* variables.

$$\frac{dy_1(z)}{dz} = y_2(z)$$
$$\frac{dy_2(z)}{dz} = \frac{\varepsilon\sigma S}{k}\left(y_1(z)^4 - T_s^4\right)$$

The third and final step of the conversion process is to rewrite the initial conditions, equation (7.15), in terms of the new variables,

$$y_1(z_0) = T_0 = 300 \ \ K,$$
$$y_2(z_0) = -2000 \ K/m$$

This set of two ODEs is an IVP we can solve using the Runge-Kutta method.

We set the input function as

```
function dydx = funkeval(x,y);
sigma = 6.6404e-8; % J/s/m^2/K^4
S = 200; % 1/m
k = 401; % J/K/m/s
Ts = 300; % K
eps = 0.05;
factor = eps*sigma*S/k;
dydx(1) = y(2);
dydx(2) = factor*(y(1)^4-Ts^4);
```

Let's solve these ODEs from z = 0 to 0.1 with 100 intervals.
At the command line prompt, we write:

```
>> [x,y]=rk4n(100,0,0.1,[1000,-2000]);
```

This yields the following plot.
The temperature at z = 0.1 m can be determined from

```
>> y(101,1)

ans = 8.063372642787826e+02
```

So the temperature is 806 K.

If we repeat this with 1000 intervals, we find that the temperature is the same to six digits, so we have a reliable answer.