10.34 – Fall 2006
Homework #3
Due Date: Wednesday, Sept. 27th, 2006 – 9 AM

Problem 1: Peak Temperature

For safety reasons, it is useful to be able to bound the peak temperature which could be realized in an exothermic reaction. An overestimate can be computed by assuming the limiting reactant is 100% converted to products, and the process is adiabatic (no heat losses). A more accurate bound can be computed by considering the fact that the reaction will reach equilibrium before the limiting reactants is 100% consumed.

In an adiabatic process, enthalpy is conserved, so for an ideal mixture

$$\sum_{in} m_i H_i\left(T_{in}\right) = \sum_{out} m_k H_k\left(T_{out}\right)$$

For many common molecules, expressions for H(T) are presented in the NIST Webbook http://webbook.nist.gov. Usually these are given as coefficients for a Shomate functional form. A program `Shomate.m` is provided on the 10.34 Web page which can read these coefficients and compute H(T) (and other thermodynamic properties) for these molecules. Note that `Shomate.m` only takes in coefficients A – G, T_{min}, and T_{max}; you will need to read the file to determine the format for the inputs.

In this problem, we will investigate the peak temperature which could be reached in an adiabatic reactor for the Water-Gas Shift reaction. In this case, the flow rates (in *millimoles/second*) into the reactor are:

$[H_2] = 2$, $[H_2O] = 5$, $[CO] = 1$, and $[CO_2] = 0.1$.

Part A:
Generate a plot showing the temperature dependence of the ΔHrxn, T*ΔSrxn, and ΔGrxn over the range of 500 – 1500 K.

Part B:
For the worst case scenario (100% conversion), generate a plot showing the peak temperatures as a function of the inlet temperature to the system over the range.

Part C:

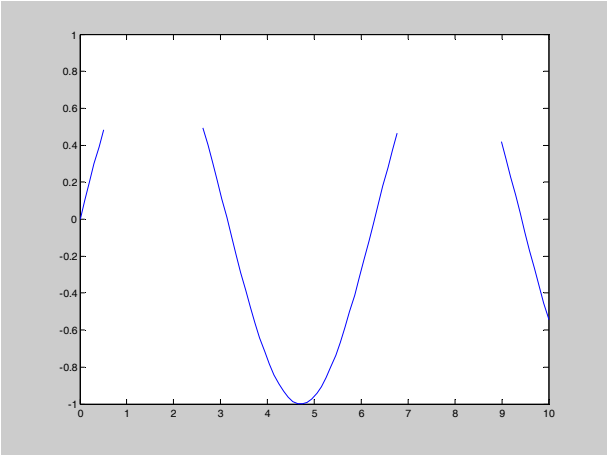
You know that the system cannot proceed beyond equilibrium under steady state conditions; therefore, solve for the realistic outlet temperature and CO conversion for the given range of inlet temperatures, and plot the results.

Part D:

You found the equilibrium boundary in the previous part, but this does not represent the entire range of accessible operating conditions. Generate a surface or mesh plot of the reactor temperature using Matlab that displays ONLY the valid parameter space which is accessible experimentally. (i.e. do not plot any points that are non-feasible based on equilibrium considerations). The figure should have x- and y-axes as the conversion and inlet temperature, and the z-axis should be the reactor temperature. You may find it useful that if a "NaN" appears in a vector or matrix being plotted, those points are ignored.

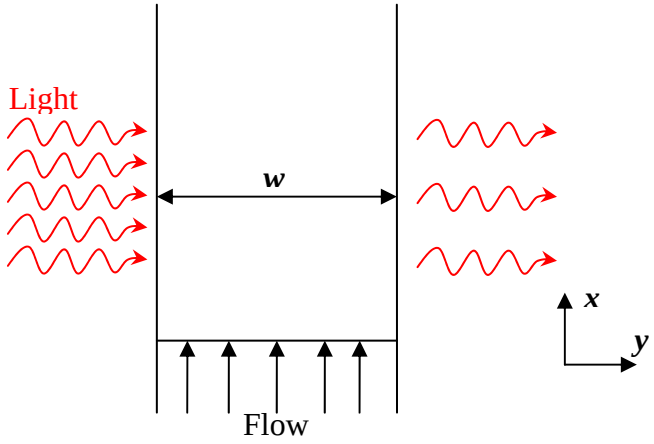
Inlet temperature should span 500 K – 1500 K and conversion should span 0 – 100 %. Use 25 K increments for inlet temperature and 5% increments for CO conversion.

As a 2-D example of what we are looking for in this problem, assume you we asked to plot the $y(x) = \sin(x)$, but do not show the points where $y > 0.5$ for $x = 0 – 10$. The result would be this:



Problem 2: Finite Differences (Many variable problem)

Consider the plug flow of water in a thin channel with optically clear walls. A laser beam is expanded and used to heat the water as shown in the figure below. The light is uniform on the left wall, and may or may not exit the channel depending on the absorbance.



If the region that is being heated by the laser is long enough we can assume that the temperature is independent of *x* and it is only a function of y. If heat provided by the laser is uniform across all *y* in the channel, then equation for variation of temperature with *y* becomes.

$$k\frac{d^2T}{dy^2}+H=0$$

Here *H* is the heat delivered to the water by the laser. If the walls of the channel are perfectly conducting, then the temperature of the water at the channel wall is equal to the ambient temperature. Thus the boundary conditions for this problem can be written as

$$T\Big|_{y=0}=T_a \quad \text{and} \quad T\Big|_{y=w}=T_a \qquad \text{where } T_a \text{ is the ambient temperature}$$

This problem is a second-order differential equation in temperature and has two boundary conditions, and can be solved to calculate the temperature profile along the *y* axis.

To do this, we discretize the problem using the formula:

$$\left.\frac{d^2T}{dy^2}\right|_{y_i}=\frac{T_{i-1}-2T_i+T_{i+1}}{(\Delta y)^2}$$

If we divide the y axis into *n* intervals then we have *n+1* points on the y axis, namely, $y_1, y_2, y_3, \ldots\ldots, y_{n+1}$ having temperatures $T_1, T_2, T_3, \ldots\ldots, T_{n+1}$ respectively, we will get *n-1* equations with *n+1* variables.

In addition to the equations we obtain by discretization, we also have the two boundary equations, which can be written as

$$T_1 = T_a \quad and \quad T_{n+1} = T_a$$

Putting all the equations together we get the system of equations described below.

$$T_1 = T_a$$

$$T_1 - 2T_2 + T_3 = \frac{-H(\Delta y)^2}{k}$$

$$\vdots$$

$$T_{i-1} - 2T_i + T_{i+1} = \frac{-H(\Delta y)^2}{k}$$

$$\vdots$$

$$T_{n-1} - 2T_n + T_{n+1} = \frac{-H(\Delta y)^2}{k}$$

$$T_{n+1} = T_a$$

These equations constitute *n+1* equations with *n+1* temperature variables, and in this case, the system of equations are linear and so we can just use a linear solver to solve the system of equations.

a) Formulate the problem to form a system of 101 equations (n=100) and solve the 101 values of temperature. It is given that the width of the channel is 1 cm, the intensity of light is 0.3 MW/m^2, the ambient temperature is 300 K. Assume 10% of photons are absorbed uniformly over the width of the channel. Plot the resulting temperature profile and state the maximum temperature and the y-value at which it occurs.

b) In reality, the intensity of light absorbed is proportional to the intensity of light, the concentration of the solution, and the absorption cross-section of the absorbing molecule. This causes the intensity of the light to decrease as it passes through the channel, also varying the heating rate across the channel. The appropriate differential equation for intensity is:

$$\frac{dI}{dy} = \varepsilon(T)\, I$$

In the above equation *c* is the concentration of the absorbing species. In our problem the concentration is constant and is absorbed in the temperature-dependent absorption cross-section, $\varepsilon(T)$.

The intensity absorbed is converted into heat in the system, and the rate of change of temperature along the y direction is given as:

$$k\frac{d^2T}{dy^2}-\frac{dI}{dy}=0$$

Using the following expressions for $\varepsilon(T)$, solve for the temperature profile. Plot the results and specify the maximum temperature and y-value where it occurs for each case.

1) $\varepsilon(T)=-10-1\times10^{-7}\cdot T^2$ (number of grid points = 101).
2) $\varepsilon(T)=-1000-1\times10^{-7}\cdot T^2$ (number of grid points = 101).
3) $\varepsilon(T)=-1000-1\times10^{-7}\cdot T^2$ (number of grid points = 501).

Is there a difference between the answer of 2) and 3), if so why?

[Hint: Perform the discretization of I as:

$$\left.\frac{dI}{dy}\right|_{y_i}=\frac{I_i-I_{i-1}}{\Delta y}=\varepsilon(T_i)\times I_i$$

Notice that equations for I and T are couple with each other and they have to be solved simultaneously. Use `fsolve` to solve the system of non-linear equations.]

c) Solve the problem once again with the following expression for the absorption cross-section:

$$\varepsilon(T)=-10-3\times10^{-4}\cdot T^2$$

Plot the resulting temperature profile and state the maximum temperature and the y-value at which it occurs.

Problem 3: Options for Broyden's method

In Broyden's method, the procedure is similar to Newton's method, but an approximate Jacobian, $\mathbf{B}(x_{n+1})$, is used instead of the true Jacobian, $\mathbf{J}(x_{n+1})$. It is obtained by the update formula

$$\underline{\underline{B}}\left(\underline{x}_{n+1}\right) = \underline{\underline{B}}\left(\underline{x}_{n}\right) + \chi \underline{F}\left(\underline{x}_{n+1}\right) \cdot \left(\underline{x}_{n+1} - \underline{x}_{n}\right)^{T} \quad \text{Eq.(1)}$$

Note F and x are vectors and **B** is a matrix. $F(x_{n+1})*(x_{n+1} - x_n)^T$ is a matrix (this is the outer product). χ is a scalar:

$$\chi = \frac{1}{\left\|\underline{x}_{n+1} - \underline{x}_{n}\right\|^{2}} \quad \text{Eq.(2)}$$

Once one has $\mathbf{B}(x_{n+1})$, one then has to solve:

$$\underline{\underline{B}}\left(\underline{x}_{n+1}\right) \cdot \left(\underline{x}_{n+2} - \underline{x}_{n+1}\right) = -\underline{F}\left(\underline{x}_{n+1}\right) \quad \text{Eq.(3)}$$

In some implementations of Broyden's method, it is desired to update $\mathbf{B}^{-1}$ instead of updating **B**, this avoids the need to solve Eq.(3) – instead you would just use

$$\left(\underline{x}_{n+2} - \underline{x}_{n+1}\right) = -\underline{\underline{B}}^{-1}\left(\underline{x}_{n+1}\right) \cdot \underline{F}\left(\underline{x}_{n+1}\right) \quad \text{Eq.(4)}$$

One possibility is to use the Sherman-Morrison formula:

$$\left(\underline{\underline{A}} + \underline{u}\underline{v}^{T}\right)^{-1} = \underline{\underline{A}}^{-1} - \gamma\left(\underline{\underline{A}}^{-1}\underline{u}\underline{v}^{T}\underline{\underline{A}}^{-1}\right) \quad \text{Eq.(5)}$$

where $u*v^T$ is a matrix (the outer product of the two vectors) and γ is a scalar:

$$\gamma = \frac{1}{1 + \underline{v}^{T}\underline{\underline{A}}^{-1}\underline{u}} \quad \text{Eq.(6)}$$

Someone else suggests that if you had already **LU** factorized $\mathbf{B}(x_n)$, then you could update this factorized form instead of **LU** factorizing $\mathbf{B}(x_{n+1})$, this way:

Given: $\mathbf{L}(x_n)\ \mathbf{U}(x_n) = \mathbf{B}(x_n)$

Solve: $\mathbf{L}(x_n)\ \mathbf{U}(x_n)\ w = -F(x_{n+1})$ for w Eq.(7)
(of course you would solve this in two steps: solve $\mathbf{L}\ p = -F$ for p, then solve $\mathbf{U}\ w = p$ to get w)

set: $\mathbf{L}(x_{n+1}) = \lambda \mathbf{L}(x_n)$ Eq.(8)

where λ is a scalar.

Solve $\mathbf{L}(x_{n+1})*b = -F(x_{n+1})$ for b Eq.(9)

Solve $\mathbf{U}^*(x_{n+2} - x_{n+1}) = b$ for newest Δx Eq.(10)

Your friend says only **L** needs to be updated by multiplication by a scalar, and **U** can remain the same throughout.

(a) Show that Equation (5) is correct.

(b) If you already had computed the inverse $\mathbf{B}^{-1}(x_n)$, how would you update it to get $\mathbf{B}^{-1}(x_{n+1})$ given by Eq. (1)?

(c) Give the algebraic expression for the value of λ would make the procedure recommended in Eqs. (7) - (10) work, so that the Δx obtained in Eq.(10) would solve Eq.(3)?
[Hint: write $(x_{n+2} - x_{n+1}) = -\mathbf{B}^{-1}(x_{n+1})*F(x_{n+1})$ and expand out the inverse using Eq. 5, then multiply both sides by $\mathbf{B}(x_n)$]

N.B. There are very frequently numerous methods for computing the same thing, but often some approaches are a lot better than others. Which of these three methods for computing Δx take $O(N^2)$ operations, and which take $O(N^3)$ operations?