Homework Assignment Number Five

Problem (1) Single Non-Linear Parabolic PDE

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

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

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 $\sigma = 5.670373x10^{-8}$ [J/s/m^2/K^4]
gray body permittivity $\varepsilon = 0.15$ (for dull Cu)
surface area to volume ratio $S = 200$ [m^{-1}] (for a cylindrical rod of diameter 0.01 m)

A cylindrical Cu rod of diameter 0.01 m and length 0.1 m is initially at $T(z,t=0) = 1000$ K. One end of the rod is maintained at $T(z=0,t) = 1000$ K. The other end of the rod is insulated, $\left.\frac{dT}{dz}\right|_{z=0.1} = 0$ K/m.

(a) Plot the transient behavior.
(b) Find the approximate steady-state temperature in the material at z=0.1 m.

Problem (2) System of Non-Linear Parabolic PDEs

Consider a plug flow reactor. (This is a pipe with a reaction taking place in the fluid flowing inside it. Consider the irreversible reaction

A + 2B --> C + 2D

taking place in a non-reactive solvent.

The molar balance for each component is given by

$$\frac{\partial C_i}{\partial \mathrm{t}} = -v\frac{dC_i}{dz} + D_i\frac{d^2C_i}{dz^2} + \nu_i r$$

where *z* is the spatial dimension in the axial direction, *t* is time, C_i is the molar concentration of species *i*, *v* is the axial velocity, D_i is the diffusion coefficient of species *i*, ν_i is the stochiometric for species *i*, (namely -1, -2, +1, +2 and 0 for A, B, C, D, and S respectively) and r is the reaction rate. The reaction rate is given by

$$r = kC_A C_B^2$$

where k is the rate constant. Assume the reactor is operated isothermally so we have no need for an energy balance.

The pipe is 10 m long with a diameter of 0.1 m. The velocity is 0.1 m/s. The diffusivities are all $1.0\text{x}10^{-9}$ m^2/s. The rate constant is $k = 1x10^{-7}\,\frac{m^6}{mol^2 \cdot s}$. Initially, the pipe contains nothing but solvent. At the inlet, the reactants, A and B, are fed in at 1000.0 and 2000.0 mol/m^3 respectively. No C or D is present in the feed stream. At the outlet, assume the concentrations no longer change (i.e. a no flux boundary condition).

(a) Solve the problem. Estimate how long it takes this reactor to get to steady state.
(b) Show the steady state profile.
(c) What fraction of the reactants are used, i.e. what is the fractional yield?
(d) What can be done to the velocity to increase the fractional yield? How does this impact the amount of product made per hour, i.e. the through-put?

Problem (3) Hyperbolic PDE
Consider the wave equation

$$\frac{\partial^2 U}{\partial t^2} = c^2 \frac{\partial^2 U}{\partial x^2}$$

Consider a spatially one-dimensional problem where x ranges from 0 to 1. The hyperbolic problem generally requires two initial conditions (one for each order of the time derivative). Sample initial conditions are given below.

$$U(x,t=0) = \sin(2\pi x)$$
$$\frac{dU}{dt}(x,t=0) = 0.0$$

In the case of a string with each end fixed, the boundary conditions have the form:

$$U(x=0,t) = 0.0$$
$$U(x=1,t) = 0.0$$

(a) Show the profile of the wave at t = 5.0 for c = 1.5.
(b) What is the value of the wave at x = 0.75 and t = 5.0?

Problem (4) Elliptic PDE

Consider the two-dimensional Laplace equation:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

on the unit square subject to the following boundary conditions,

$$T(x=0,y) = 75y$$
$$T(x=1,y) = 50 + 50y$$
$$T(x,y=0) = 50x$$
$$T(x,y=1) = 75 + 25x + 50 * \sin(2\pi x)$$

(a) Show the steady state temperature distribution in the plate.
(b) What is the value of the wave at x = 0.5 and y = 0.5?

Problem (5) Numerical Integration
Consider the normal distribution

$$f(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

This function does not have an analytical integral.

For the standard normal distribution, where the mean is zero and the standard deviation is one, evaluate the integral from x = -2.0 to 1.0, i.e. $p(-2.0 \le x \le 1.0)$, using

(a) the trapezoidal method with 1 interval.
(b) the trapezoidal method with 10 intervals.
(c) the trapezoidal method with 100 intervals.
(d) the trapezoidal method with 1000 intervals.
(e) the Simpson's Second Order method with 100 intervals.
(f) the Simpson's Second Order method with 1000 intervals.
(g) the Simpson's Third Order method with 99 intervals.
(h) the Simpson's Fourth Order method with 100 intervals.
(i) Gaussian quadrature of sixth order.
(j) the cdf command in MatLab.
(k) Comment on the effect of number of intervals and order of the method.

Problem (6) Integral Equations

Classify and numerically solve the following integral equation.

$$\phi(x) = \frac{x^2}{100} + \frac{5}{2}\int_5^x e^{-\frac{(x+y)}{10}} \left[\sin(\phi(y))\right]^2 dy$$

Solve for x = 5 to 10.
Classify as linear/nonlinear, Volterra/Fredholm, first/second kind.
Provide a plot of the solution.
Demonstrate (1) the effect of changing the increment size (use say 5 and 20 intervals).
Demonstrate (2) the convergence of the method by looking at the solution at each iteration.