ChE/MSE 505
Fall, 2005
Final Examination

Consider a single component, inviscid fluid in a one dimensional system in the absence of any external fields (such as gravitational or electromagnetic). The material balance is given by

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho v}{\partial x} \tag{1}$$

where ρ is the fluid density (kg/m^3), v is the velocity (m/s), x is the spatial coordinate (m), and t is the temporal coordinate (s). The momentum balance is given by

$$\rho \frac{\partial v}{\partial t} = -\rho v \frac{\partial v}{\partial x} - \frac{\partial p}{\partial x} \quad , \tag{2}$$

where p is the pressure (Pa). The energy balance is given by

$$\frac{\partial \rho\left(\frac{1}{2}v^2 + \hat{U}\right)}{\partial t} = -\frac{\partial}{\partial x}\rho\left(\frac{1}{2}v^3 + \hat{U}v\right) - \frac{\partial q}{\partial x} - \frac{\partial p v}{\partial x} \tag{3}$$

where $\hat{U}$ is the internal energy per mass (J/kg) and q is the conductive heat flux (J/m^2/s). In order to solve this system of three coupled, nonlinear, parabolic partial differential equations, we have to introduce some constitutive equations for p, $\hat{U}$, and q. For example, we might use Fourier's law, in which

$$q = -k_c \frac{\partial T}{\partial x} \tag{4}$$

where k_c is the thermal conductivity. For the heat capacity, one may use an approximate thermal equation of state,

$$\hat{U} = C_V T \tag{5}$$

For the pressure, one can use a mechanical equation of state, such as the ideal gas law, in which

$$p = \frac{\rho}{M} RT \tag{6}$$

where M is the molecular weight and R is the gas constant, which works when the fluid is a compressible gas. Another common assumption, used when the fluid is a liquid, is the assumption of incompressibility, in which the density is constant.

Problem 1.

Assume the fluid is incompressible. Solve/simplify as far as possible, then, if necessary, indicate what sort of numerical method is necessary to solve the problem.

Solution:

If the fluid is incompressible, then the density, ρ, is constant and the mass balance, equation (1) becomes,

$$\frac{\partial \rho}{\partial t} = 0 = -\rho \frac{\partial v}{\partial x} \tag{7}$$

A consequence of this equation is that

$$\frac{\partial v}{\partial x} = 0 \tag{8}$$

This is typically called the "divergence free condition, i.e. in multiple dimensions, $\nabla \cdot \mathbf{v} = 0$. In other words the velocity is constant. If the velocity is constant, the momentum balance becomes

$$\rho \frac{\partial v}{\partial t} = -\frac{\partial p}{\partial x} \quad , \tag{9}$$

If the velocity is constant through equation (8), it may likely also be constant in time. In other words, the pressure gradient is zero and the pressure is constant at p_{in}. This absence of pressure drop is due to the fact that we have assumed that we are dealing with an inviscid fluid, so we don't have any source of friction in the model. However, we don't have to assume that the pressure gradient is zero. Combining equations (4), (5), and (9) and the assumptions of constant density and velocity into the energy balance (equation (3)) yields

$$\rho v \frac{\partial v}{\partial t} + C_V \rho \frac{\partial T}{\partial t} = -\rho v C_V \frac{\partial T}{\partial x} + k_c \frac{\partial^2 T}{\partial x^2} - v \frac{\partial p}{\partial x} \tag{10}$$

We can simplify this further, by realizing that the first on the LHS and the last term on the RHS cancel, due to the momentum balance in equation (9).

$$\frac{\partial T}{\partial t} = -v \frac{\partial T}{\partial x} + \frac{k_c}{C_V \rho} \frac{\partial^2 T}{\partial x^2} \tag{11}$$

This is a single, linear parabolic PDE. We can solve this easily using the Crank Nicholson method. We need an initial condition on the temperature and we need boundary conditions on the temperature. The only assumptions that we have made are that the thermal conductivity and the heat capacity are constants.

Problem 2.

Continue Problem 1, assuming we are only interested in the steady state solution. Again, simplify as far as possible, if possible solve analytically, otherwise indicate the necessary numerical method needed to solve this problem.

Solution:

At steady state, we have

$$0 = -v\frac{dT}{dx} + \frac{k_c}{C_V\rho}\frac{d^2T}{dx^2} \tag{13}$$

This is a single second-order linear ODE. Furthermore, the coefficients are constant and the problem is homogeneous due to the absence of any nonzero constant term. This problem has an analytical solution. In order to obtain this analytical solution, we first write the second-order ODE as two first-order ODEs. We define the transformation.

$$y_1 = T \tag{14.a}$$

$$y_2 = \frac{dT}{dx} \tag{14.b}$$

We write the ODEs

$$\frac{dy_1}{dx} = y_2 \tag{15.a}$$

$$\frac{dy_2}{dx} = \frac{C_V\rho v}{k_c} y_2 \tag{15.b}$$

In matrix notation, we write this as

$$\frac{d\mathbf{y}}{dx} = \mathbf{Ay} \tag{16}$$

where

$$\mathbf{A} = \begin{bmatrix} \mathbf{0} & 1 \\ \mathbf{0} & \frac{C_V\rho v}{k_c} \end{bmatrix} \tag{17}$$

This problem has an analytical solution. The equation for y_2 does not contain any reference to y_1, so we can solve the second equation individually. (In other words, the ODE for y_2 is not coupled to y_1.) Solving just the second ODE, we have

$$\frac{dy_2}{dx} - \frac{C_V \rho v}{k_c} y_2 = 0 \tag{18}$$

We can use the method of separation of variables to solve this problem.

$$\frac{dy_2}{y_2} = \frac{C_V \rho v}{k_c} dx \tag{19}$$

Integrate

$$\ln[y_2(x)] = \frac{C_V \rho v}{k_c} x + c_1' \tag{20}$$

Take the exponential

$$y_2(x) = \exp(c_1')\exp\left(\frac{C_V \rho v}{k_c} x\right) = c_1 \exp\left(\frac{C_V \rho v}{k_c} x\right) \tag{21}$$

where c_1 is a constant of integration to be determined from the boundary conditions. We now can substitute equation (21) into equation (15.a), the ODE y_1.

$$\frac{dy_1}{dx} = y_2(x) = c_1 \exp\left(\frac{C_V \rho v}{k_c} x\right) \tag{22}$$

We integrate equation (22).

$$\int_{y_{1,o}}^{y_1(x)} dy_1 = \int_{x_o}^{x} \left[c_1 \exp\left(\frac{C_V \rho v}{k_c} x\right)\right] dx \tag{23}$$

$$y_1(x) - y_{1,o} = c_1 \frac{k_c}{C_V \rho v}\left[\exp\left(\frac{C_V \rho v}{k_c} x\right) - \exp\left(\frac{C_V \rho v}{k_c} x_o\right)\right] \tag{24}$$

where $y_{1,o}$ is the temperature at the inlet. We also have a temperature at the outlet, $y_1(x_f) = y_{1,f}$. We can solve c_1 to match this boundary condition.

$$y_{1,f} - y_{1,o} = c_1 \frac{k_c}{C_V \rho v}\left[\exp\left(\frac{C_V \rho v}{k_c} x_f\right) - \exp\left(\frac{C_V \rho v}{k_c} x_o\right)\right] \tag{25}$$

$$c_1 = \frac{\left(y_{1,f} - y_{1,o}\right)}{\frac{k_c}{C_V \rho v}\left[\exp\left(\frac{C_V \rho v}{k_c} x_f\right) - \exp\left(\frac{C_V \rho v}{k_c} x_o\right)\right]} \tag{26}$$

Thus the analytical solution is given by

$$y_1(x) = y_{1,o} + \left(y_{1,f} - y_{1,o}\right)\frac{\left[\exp\left(\frac{C_V \rho v}{k_c} x\right) - \exp\left(\frac{C_V \rho v}{k_c} x_o\right)\right]}{\left[\exp\left(\frac{C_V \rho v}{k_c} x_f\right) - \exp\left(\frac{C_V \rho v}{k_c} x_o\right)\right]} \tag{27}$$

This can also be written as

$$y_1(x) = y_{1,o} + \left(y_{1,f} - y_{1,o}\right)\frac{\exp\left(\frac{C_V \rho v}{k_c}\left(x - x_o\right)\right) - 1}{\exp\left(\frac{C_V \rho v}{k_c}\left(x_f - x_o\right)\right) - 1} \tag{28}$$

Problem 3.

Comment on the stability of the steady state solution in Problem 2.

Solution:

$$\mathbf{A} = \begin{bmatrix} \mathbf{0} & 1 \\ \mathbf{0} & \frac{C_V \rho v}{k_c} \end{bmatrix}$$

The characteristic equation is

$$-\lambda\left(\frac{C_V \rho v}{k_c} - \lambda\right) = 0 \tag{29}$$

The eigenvalues are 0 and $\frac{C_V \rho v}{k_c}$. The heat capacity, density, and thermal conductivity are always positive. If the velocity is positive, then the second eigenvalue is positive and the system is unstable. If the velocity is negative, then the second eigenvalue is negative and the system is stable. There is no imaginary component in the eigenvalues. Therefore, the solution is a node. (It has no spiralling or oscillatory behavior.)

Typically, when we talk about stability we are talking about the independent variable as time and we are dealing with an initial value problem. In this case, we had a boundary value problem, and our independent variable was space and was bounded. As a result, even if the velocity is positive and the system is unstable from the point of view of a stability analysis, we can still solve for a steady state over the range of spatial variable bounded by the two boundary conditions.

Problem 4.

Assume the fluid is an ideal gas. Solve/simplify as far as possible, then, if necessary, indicate what sort of numerical method is necessary to solve the problem.

Solution:

If the fluid is an ideal gas, then the density, velocity and temperature are all variables. The mass, momentum, and energy balances (equations (1), (2) and (3), become with (4), (5), and (6):

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho v}{\partial x} \tag{30}$$

$$\frac{\partial v}{\partial t} = -v\frac{\partial v}{\partial x} - \frac{1}{\rho}\left[\frac{RT}{M}\frac{\partial \rho}{\partial x} + \frac{\rho R}{M}\frac{\partial T}{\partial x}\right] \ , \tag{31}$$

$$\frac{\partial \rho\left(\frac{1}{2}v^2 + C_V T\right)}{\partial t} = -\frac{\partial}{\partial x}\rho\left(\frac{1}{2}v^3 + C_V T v\right) - k_c\frac{\partial^2 T}{\partial x^2} - \frac{R}{M}\frac{\partial \rho T v}{\partial x} \tag{32}$$

This is a system of three coupled nonlinear parabolic PDEs with independent variables x and t, and dependent variables, ρ, v, and T. We can solve it using an algorithm like the second-order Runge-Kutta method with the centered-finite-difference formula for the spatial first and second derivatives. (This is what is used in syspde_para.m). We need initial conditions and boundary conditions for each of the three dependent variables.

It turns out that the timescale for the evolution of the momentum balance is much shorter than the time scale for the mass or energy balances, but that is a practical issue that is not necessary to discuss in this final exam.