APPM/MATH 4650 Project #1 Fall 2015

Non-adiabatic Explosion Due Wednesday, December 2, 2015

The non-adiabatic explosion problem describes a mixture of fuel and oxidizer, at temperature T, in a box. A chemical reaction converts the fuel and oxidizer into products and releases heat as a result. This heat raises the temperature of the material in the box which, in turn, causes the reaction to proceed at a faster rate. The rate of transformation of fuel is described by $\dfrac{dA}{dt} = -\bar{c}A\, e^{-E/RT}$ where R is the universal gas constant, E is the activation energy for the reaction and $\bar{c}$ is a constant of proportionality. Initially the thermal energy of the gas, RT, is small compared to E, so the exponential term is small, thus the reaction rate is very slow and the temperature rise is correspondingly small. As the gas temperature increases, the exponential term increases in magnitude.

Conservation of energy leads to

$$c_v \frac{dT}{dt} = -\bar{c}\frac{dA}{dt} - h(T - T_0) \tag{1}$$

where c_v is the heat capacity at constant volume, and h is a convective heat transfer coefficient associated with heat loss from the exterior of the container. The left–hand side of the equation represents the rate of change of internal energy, and the terms on the right–hand side represent heat release due to the chemical reaction and heat loss from the container, respectively.

We non–dimensionalize the problem with the following variables, δ which is proportional to $\dfrac{1}{h}$, $\epsilon = \dfrac{T_0 R}{E}$, $\sigma = \dfrac{t}{\delta t_{ref}}$ where t_{ref} is a reference time, and $\bar{T} = \dfrac{T}{T_0} = 1 + \epsilon\Theta$. Note that since we are dealing with a high activation energy problem, it follows that $\epsilon \ll 1$. Also note that the new temperature variable Θ is an order–one size variable. In other words, the dimensionless temperature $\bar{T}$ is 1 plus a small correction, $\epsilon\Theta$. After making the substitutions, and accounting for the fact that $\epsilon \ll 1$, one is left with

$$\frac{d\theta}{d\sigma} = \delta e^{\theta} - \theta \tag{2}$$

along with the initial condition $\theta(0) = 0$.

The problem has two outcomes of interest, explosions and fizzles, where the magnitude of δ determines which will occur. If $\delta < 1/e$ a fizzle occurs while $\delta > 1/e$ leads to an explosion. In each case, "short–time" and "long–time" solutions were derived in class.

1. Consider $\delta = 1/5$ corresponding to a fizzle, in which case we work in terms of $\Theta(\sigma)$.

   (a) Use an RK–4 scheme with appropriate uniform step sizes to numerically integrate the equation $\dfrac{d\theta}{d\sigma} = \delta e^{\theta} - \theta$ subject to the initial condition $\theta(0) = 0$.

(b) Use any root finding scheme to determine the asymptotic value of Θ_{fiz} from the "large–time" approximation to the solution, in particular, $\dfrac{e^{\Theta_{fiz}}}{\Theta_{fiz}} = \dfrac{1}{\delta}$. Also recall the "short–time" approximate solution $\Theta \approx \left(\dfrac{\delta}{\delta-1}\right)\left[e^{(\delta-1)\sigma} - 1\right]$.

(c) Plot the results of your numerical integration along with the "short–time" and the "long–time" approximations derived in class, and given above. Comment on the results and clearly indicate which curve corresponds to the numerical results, and which curves are the approximations.

2. Now consider the case of $\delta = 1$ which corresponds to an explosion. For this problem it is easier to work in terms of $\sigma(\Theta)$.

   (a) Using a fourth–order Runge-Kutta scheme, numerically integrate the equation $\dfrac{d\sigma}{d\theta} = \dfrac{1}{\delta e^{\theta} - \theta}$ subject to the initial condition $\sigma(0) = 0$.

   (b) Use an appropriate numerical integration scheme to determine the asymptotic value of σ_{exp} from the integral $\sigma_{exp} = \displaystyle\int_0^\infty \frac{dx}{\delta e^x - x}$.

   (c) Once σ_{exp} is known, one may now evaluate the "long–time" approximate approximate solution $\sigma \approx \sigma_{exp} - \dfrac{1}{\delta e^{\Theta}}$. Also note that the same "short–time" solution from the fizzle problem is valid for the explosion problem, however for the special case $\delta = 1$ you will need to determine $\sigma(\Theta)$ using L'Hopital's rule.

   (d) Plot your numerical results of $\sigma(\theta)$ along with the approximations that are valid for small and large values of θ. Comment on the comparison. Clearly indicate which curve corresponds to the numerical results, and which curves are the approximations.

Some comments to consider when preparing your written report.

- You must work in groups of two or three.

- Be sure to clearly explain what the problem is about in physical terms. Also clearly show what equations are involved, both in their original form as well at the dimensionless form. Be sure to explain what each term represents.

- After you present the numeric/graphic results, be sure to comment on what your solution tells you about the "physics" of the problem. In other words, what mechanisms are important as the solution evolves. Also clearly explain how a fizzle differs from an explosion.

- Do not plot your "short–time" and "long–time" approximations past their appropriate range. Once they have deviated significantly from the "real" solution, stop plotting the curves!