1 Project 2

$$k = Be^{-\frac{E}{RT}}$$
$$\frac{dA_f}{dt} = -kA_f e^{-\frac{E}{RT}} \qquad T = T(t)$$

1.1 Non-adiabotic explosion

$$\frac{dE}{dt} = \frac{dQ}{dt} - S \qquad S = H(T - T_0)$$
$$C_N \frac{dT}{dt} = -k\frac{dA_f}{dt} - H(T - T_0) \qquad T(0) = T_0$$

where the LHS is the increase in internal energy, first term of RHS is the rate of heat release, and the last term is the rate of heat loss. Define $\hat{T} = \frac{T}{T_0} = 1 + \epsilon\theta$, $\tau = \frac{t}{t_r}$, so that $\hat{T}(0) = 1$. $\epsilon = \frac{T_0 R}{E}$.

$$\frac{d\theta}{d\tau} = e^{\theta} - \frac{\theta}{\delta}.$$

where $\delta \propto \frac{1}{H}$.

Let $\tau = \delta\sigma$ and we obtain

$$\frac{d\theta}{d\sigma} = \delta e^{\theta} - \theta \qquad \theta(0) = 0.$$

The more heat is lost to the environment, the more delay there is for the explosion time. We can do this to prevent explosion for forever. It's called a fizzle.

If $\delta e^{\theta} > \theta$, then θ always grows exponentially with time. If $\delta e^{\theta} < \theta$, then θ converges. At osculation point, both the magnitude and slope are equal:

$$\delta^* e^{\theta^*} = \theta^*$$
$$\delta^* e^{\theta^*} = 1$$

If $\delta > \frac{1}{e}$, explosion; If $\delta < \frac{1}{e}$, fizzle.

- $\theta << 1$ and $\sigma << 1$: we can use taylor expansion on e^θ,giving

$$\begin{aligned}\frac{d\theta}{d\sigma} &= \delta(1+\theta+\frac{\theta^2}{2}+\ldots)-\theta \\ &\approx \delta+(\theta-1)\delta \\ \theta &= \frac{\delta}{\delta-1}(e^{(\delta-1)\sigma}-1)\end{aligned}$$

- $\sigma \to \infty$ and $\theta \to \theta_\infty$, so $\frac{d\theta}{d\sigma} << 1$

$$\begin{aligned}\frac{d\theta}{d\sigma} &\approx \theta \\ \frac{e^{\theta_f}}{\theta_f} &= \end{aligned}$$

- we can swap independent and dependent variables to avoid a stiff problem using RK4, solve for σ

$$\sigma = \frac{1}{\delta-1}\ln\left[\frac{\theta+\frac{\delta}{\delta-1}}{\frac{\delta}{\delta-1}}\right].$$

  This is zero divide by zero, so we need to use L'Hopital's Rule with respect to δ and get

$$\theta = \sigma \text{ early solution.}$$

- $\theta \to \infty$ and $\sigma \to \sigma_t$:

$$\begin{aligned}\frac{d\theta}{d\sigma} &\approx \delta e^\theta \\ -e^{-\theta} &= \delta\sigma + C, \text{let } C = -\delta\sigma_e \\ \sigma &= \sigma_e - \frac{e^{-\theta}}{\delta} \text{ explosion limit solution}\end{aligned}$$

We still need to find σ_e

$$\begin{aligned}
\frac{d\sigma}{d\theta} &= \frac{1}{\delta e^{\sigma} - \theta} \\
\int \frac{d\sigma}{d\theta} &= \int_{\theta_0}^{\theta} \\
&= \int_0^{\eta} \frac{dx}{\delta e^{x} - x} \\
\sigma - 0 &= \int_0^{\eta} \frac{dx}{\delta e^{x} - x}
\end{aligned}$$