Could even have coupled higher order systems:

$$y'' = f(x, y, y', w, w')$$
$$w'' = g(x, y, y', w, w')$$

$$y = u_1$$
$$y' = u_1' = u_2$$
$$y'' = u_2' = f(x, y, y', w, w') = f(x, u_1, u_2, u_3, u_4)$$
$$w = u_3$$
$$w' = u_3' = u_4$$
$$w'' = u_4' = g(x, y, y', w, w') = g(x, u_1, u_2, u_3, u_4)$$

System is finally

$$\boxed{\begin{aligned} u_1' &= u_2 \\ u_2' &= f(x, u_1, u_2, u_3, u_4) \\ u_3' &= u_4 \\ u_4' &= g(x, u_1, u_2, u_3, u_4) \end{aligned}}$$

<u>Adiabatic</u> <u>Explosion</u> Fuel + Ox → Prod

<u>Reaction Kinetics</u>

$$k \approx B e^{-E/RT}$$

E ~ activation energy

$$\frac{dA_F}{dt} = -c A_F e^{-E/RT}$$

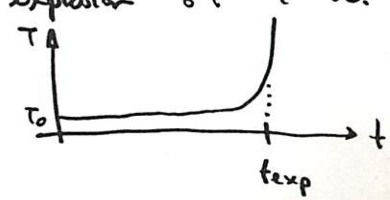
$T = T(t)$

<u>ENERGY BALANCE</u>

$$\left\{\begin{array}{l}\text{Rate of increase of} \\ \text{internal energy}\end{array}\right\} = \left\{\begin{array}{l}\text{Rate of} \\ \text{heat release}\end{array}\right\}$$

With all energy going to heat material, eventually you get an "explosion" where $T \uparrow$ "rapidly" with time t.

Will <u>always</u> get an explosion at $t = t_e$!



Non-adiabatic explosion

$$\frac{dE}{dt} = \frac{d\Theta}{dt} - S \qquad S = \text{Sink} = H(T-T_0)$$

$$C_v \frac{dT}{dt} = -q \frac{dA_F}{dt} - H(T-T_0) \qquad \boxed{T(0) = T_0}$$

↑ increase in internal energy — ↑ rate of heat release — ↑ rate of heat loss

where $\frac{dA_F}{dt} = -k A_F e^{-E/RT}$

Define $\hat{T} = \frac{T}{T_0}$ $\quad \tau = \frac{t}{t_r}$ $\quad \hat{T}(0) = 1$

$= 1 + \varepsilon\Theta$ $\quad \varepsilon = T_0 R / E$

⋮

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

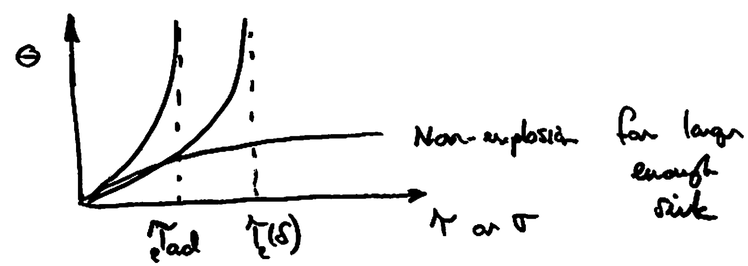
δ = Frank-Kamenetskii parameter

$\delta \propto 1/H$

Let $\tau = \delta\sigma$ then get

$$\boxed{\frac{d\Theta}{d\sigma} = \delta e^{\Theta} - \Theta \qquad \Theta(0) = 0}$$ ← Non-Ad. Exp. Prob.

In general will look like



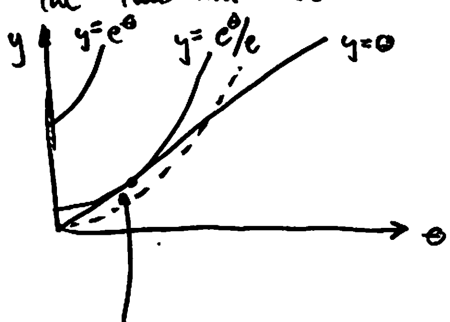
If $\delta e^{\Theta} > \Theta$ then Θ always grows exponentially with time

If $\delta e^{\Theta} < \Theta$ then Θ will decrease with time, for a while.

(but this can't always be true for $t \to \infty$)

Can get a hint about the "dividing line" for the value of δ.

Consider the functions δe^{θ} and θ



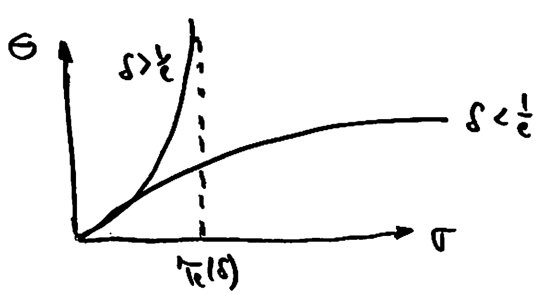
At <u>oscillation</u> <u>point</u> $\quad \delta^* e^{\theta^*} = \theta^*$ $\quad$ equal magnitude

$\delta^* e^{\theta^*} = 1$ $\quad$ equal slopes

Soln is $\delta^* = 1/e \quad \theta^* = 1$

If $\delta > \frac{1}{e}$ then $\delta e^{\theta} > \theta$ always explodes

$\delta < 1/e$ then intersection is possible and will not get unbounded growth in θ.



The problem must actually be calculated numerically.

H.W. $\quad$ solve (integrate) $\dfrac{d\theta}{d\tau} = \delta e^{\theta} - \theta \qquad \theta(0) = 0$

Integrate for $\delta = 1 > 1/e$ $\quad$ explosion

$\delta = 1/3 < 1/e$ $\quad$ fizzle

Use any scheme you want.

What is $\tau_{exp}(\delta = 1)$?

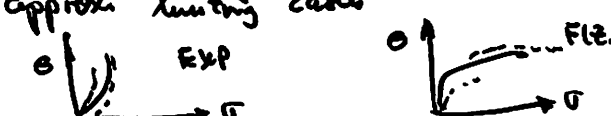
What is θ_{fiz} for $\delta = 1/3$?

Note that $\displaystyle d\tau = \frac{d\theta}{\delta e^{\theta} - \theta} \qquad \tau = \int_0^{\theta} \frac{dx}{\delta e^{x} - x}$

$$\tau_{exp} = \int_0^{\infty} \frac{dx}{\delta e^{x} - x}$$

Hint!

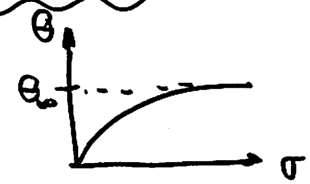
Plot each case along with the 4 approx limiting cases



Can actually extract a certain amount of info w/o numerically integrating.

- For $\delta = \frac{1}{3} < \frac{1}{e}$

FIZZLE



1) Small time limit $\theta \ll 1$ and $\sigma \ll 1$

$$\frac{d\theta}{d\sigma} = \delta e^{\theta} - \theta \approx \delta\left(1 + \theta + \frac{\theta^2}{2} + \dots\right) - \theta$$
$$\approx \delta + \theta(\delta - 1) + \cdots$$

so $\frac{d\theta}{d\sigma} = \delta + \theta(\delta-1) \qquad \theta(0) = 0$

$$\frac{d\theta}{\delta + \theta(\delta-1)} = d\sigma \quad \Rightarrow \quad \frac{d\theta}{\theta + \left(\frac{\delta}{\delta-1}\right)} = (\delta-1)d\sigma$$

$$\ln\left(\theta + \frac{\delta}{\delta-1}\right) = (\delta-1)\sigma + c$$

$$\theta(0) = 0 \quad \Rightarrow \quad c = \ln\left(\frac{\delta}{\delta-1}\right)$$

$$\ln \frac{\theta + \left(\frac{\delta}{\delta-1}\right)}{\left(\frac{\delta}{\delta-1}\right)} = (\delta-1)\sigma$$

or $$\theta + \frac{\delta}{\delta-1} = \left(\frac{\delta}{\delta-1}\right)e^{(\delta-1)\sigma}$$

$$\boxed{\theta = \left(\frac{\delta}{\delta-1}\right)\left[e^{(\delta-1)\sigma} - 1\right] \quad \text{for } \sigma, \theta \ll 1}$$

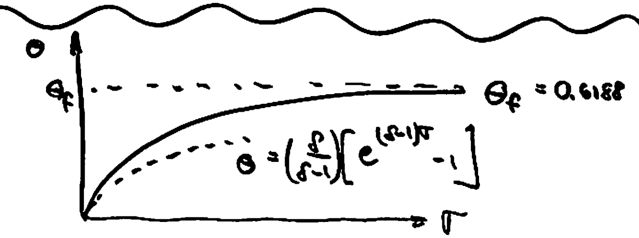
2) Large time limit $\sigma \to \infty \quad \theta \to \theta_\infty$

note that $\frac{d\theta}{d\sigma} \ll 1$ then

$$\frac{d\theta}{d\sigma} = \delta e^{\theta} - \theta \approx 0 \quad \Rightarrow \quad \delta e^{\theta} = \theta$$

or $\boxed{\frac{e^{\theta_f}}{\theta_f} = \frac{1}{\delta}}$ fizzle limit

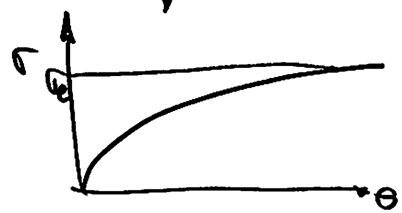
For $\delta = 1/3$ get $\boxed{\theta_f = 0.6188}$ 0.61906



EXPLOSION

For $\delta = 1 > \frac{1}{e}$

$\Downarrow$



3) For $\theta, \sigma \ll 1$ still have same results as before

$$\theta = \frac{\delta}{\delta - 1}\left[e^{(\delta-1)\sigma} - 1 \right]$$

$$\Rightarrow \quad \sigma = \left(\frac{1}{\delta-1}\right) \ln\left[\frac{\theta + \left(\frac{\delta}{\delta-1}\right)}{\left(\frac{\delta}{\delta-1}\right)} \right]$$

Take limit as $\delta \to 1$ + get $\boxed{\theta = \sigma}$

Early time soln $\delta = 1$

4) Large $\theta \to \infty$ and $\sigma \to \sigma_e$

$$\frac{d\theta}{d\sigma} = \delta e^{\theta} - \theta \approx \delta e^{\theta} \quad \text{subject to} \quad \lim_{\theta \to \infty} \sigma = \sigma_e$$

$$e^{-\theta} d\theta = \delta\, d\sigma$$

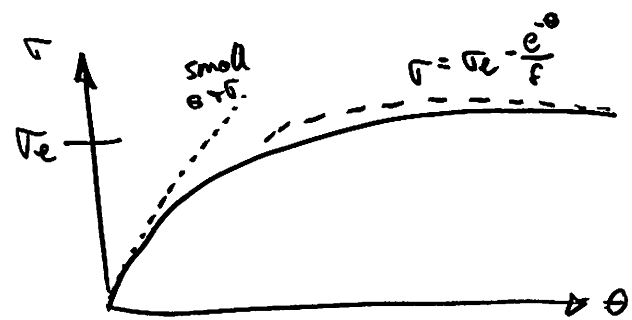
$$-e^{-\theta} = \delta \sigma + c$$

B.C. $\Rightarrow$ $c = -\delta \sigma_e$

so $e^{-\theta} = \delta(\sigma_e - \sigma)$

$$\theta = -\ln \delta(\sigma_e - \sigma)$$

or $\boxed{\sigma = \sigma_e - \frac{e^{-\theta}}{\delta} \quad \text{explosion limit solution}}$



Still need to numerically integrate

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

to find $\tau_{explosion}(\delta=1)$

Easiest to find $\tau(\theta)$ than $\theta(\tau)$.

So $\frac{d\tau}{d\theta} = \frac{1}{\delta e^{\theta}-\theta}$

$$\int \frac{d\tau}{d\theta} d\theta = \int_{\theta_0}^{\theta} \frac{d\theta}{\delta e^{\theta}-\theta} = \int_{0}^{\theta} \frac{dx}{\delta e^{x}-x}$$

$$\boxed{\tau - 0 = \int_{0}^{\theta} \frac{dx}{\delta e^{x}-x}}$$

As $\theta \to \infty$ $\tau \to \tau_e$

$$\tau_e = \int_0^{\infty} \frac{dx}{\delta e^{x}-x}$$

$\left(= 1.3591 \text{ for } \delta=1 \right)$

Must decide what $\theta = \infty$ means in a numerical sense.

Do this for θ getting larger & larger till $\tau(\theta)$ does not change any more.

 END