

Thermal explosion by putting chemicals in a box

Let T_0 be the initial temp

T is a function of time, so $T(t) = T$
 $\Rightarrow T_0 = T(t_0)$

Note that T is in Kelvin.

Reaction Kinetics:

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

$$\text{and } \frac{dA_F}{dt} = -k A e^{-E/RT}$$

$$\text{and } \frac{dE}{dt} = \frac{d\theta}{dt} - S$$

Rate of change (in box):

$$C_N \frac{dT}{dt} = -k \frac{dA_F}{dt} - H(T - T_0)$$

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

Who wants
to write about
this part?

PHYSICS
— (4)

Scaling

Define $\hat{T} = \frac{T}{T_0}$

and $\tau = \frac{t}{t_r}$ where $t_r = t_{\text{relative}}$

Which makes our initial condition

$$\hat{T}(0) = 1$$

if $\hat{T} = 1 + \epsilon \Theta$ and $\epsilon = \frac{T_0 R}{E}$

and we get

$$\frac{d\Theta}{d\tau} = e^{\Theta} - \Theta \quad \text{where } \delta \text{ is proportional to } \frac{1}{H}$$

Now let $\tau = \delta \sigma$

$$\Rightarrow \boxed{\frac{d\Theta}{d\sigma} = \delta e^{\Theta} - \Theta} \quad \text{--- (1)}$$

for $\Theta(0) = 0$

Three cases

1) $\delta e^\Theta > \Theta \implies \Theta$ ALWAYS grows EXPONENTIALLY

2) $\delta e^\Theta < \Theta \implies \Theta$ will decrease for a while

3) $\delta e^\Theta = \Theta \implies$ (ie. TRANSITION
Math speculation)

Where all three happen over time.

So we are solving for δe^Θ and Θ

(2)

AND

The oscillation point; which happens when

$$\delta^* e^{\Theta^*} = \Theta^*$$

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

So we choose δ such that $\delta > \frac{1}{e}$ ——— (3)

to ensure $\delta e^\Theta > \Theta$

Which causes unbounded growth in Θ and
guarantees an explosion.

• We want to show...

- 1) Solve for (1) using R₁H.
- 2) show cases 1 and 2 in (2)
- 3) show case 3 in (2) by using (3)
- 4) Write about the physics in (4)
- 5) Write about the numerics between (1) and (3).