Ignition

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Ignition refers to the transition,

slow chemistry $\longrightarrow$ fast chemistry

Almost everything is reacting chemically:

- Detonation: reaction in $O(10^{-6})$ sec.
- Premixed flame: in $O(10^{-4})$ sec.
- Diesel & air (40 bar): $O(10^{-3})$ sec.
- Smoldering combustion: $O(1)$ minute.
- Wet oxidation: eg. lignite, hay, O(days)
- Degradation of foodstuff: O(days)–O(months)
- Environment: changes in O(years)
- Dry wood/hay/food/oil in air: O(decades)
- Geology: metamorphosis over $O(10^8)$ years

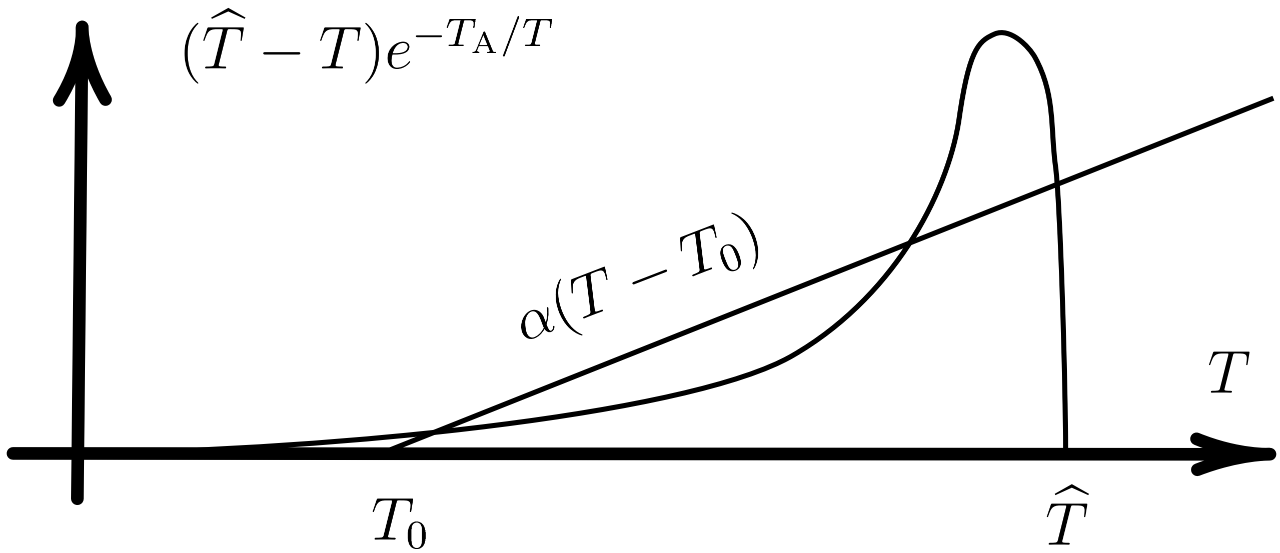
(That is why there is a cold boundary “difficulty” ...)

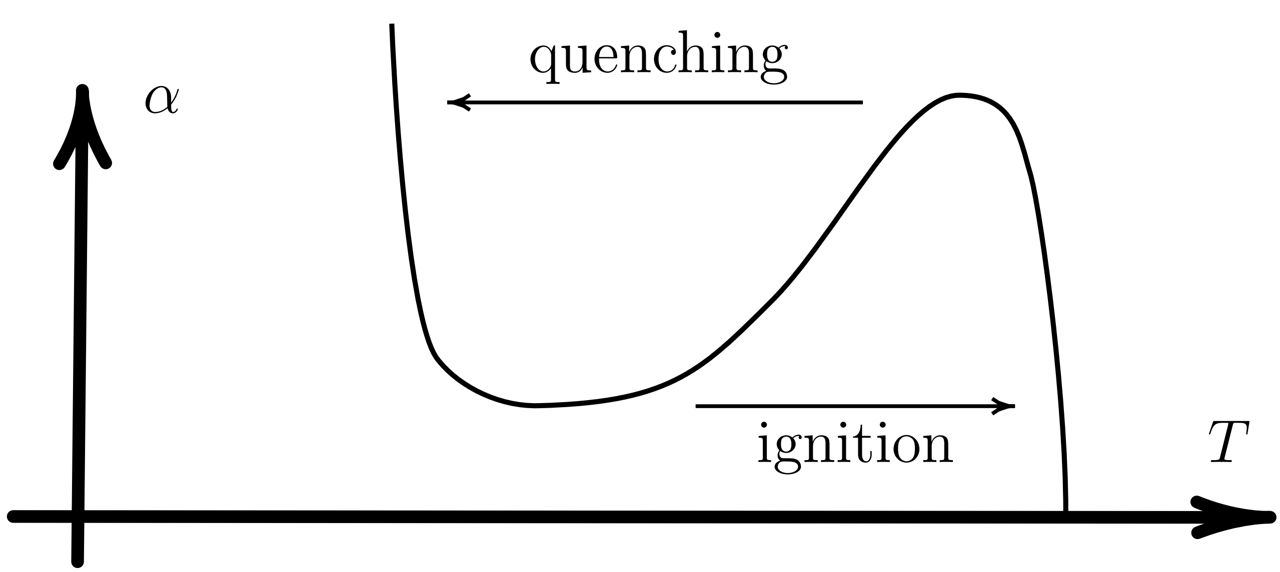
Multiple states:

In combustion, reaction-rate (rate of heat release) depends strongly on temperature.

Basic idea: Dynamic (*fast*) changes occur until heat production balances heat loss.

***Illustration*:** $(\widehat{T} - T)e^{-T_{\mathrm{A}}/T} = \alpha(T - T_0), \ T_{\mathrm{A}} \gg \widehat{T}.$





The Frank-Kamenetskii Problem

In some domain Ω consider

$$\begin{aligned} T_t - \Delta T &= \tfrac{1}{L}\Delta F - F_t \\ &= D\beta^{-1} F e^{\beta(1-1/T)} \end{aligned} \qquad \begin{cases} T = 1,\ F = 1 \ \text{ at } t = 0 \\ T = 1,\ F_n = 0 \text{ on } \partial\Omega \end{cases}$$

Thermal sensitivity of chemistry $\implies \beta \gg 1$.

Asymptotic approach, as $\beta \to \infty$:

$$T \sim 1 + \beta^{-1}\theta(t, \mathbf{r}), \quad F \sim 1 - \beta^{-1}\phi(t, \mathbf{r})$$

leads to

$$\theta_t - \Delta\theta = D\, e^{\theta} \quad \text{and} \quad \phi_t - \tfrac{1}{L}\Delta\phi = D\, e^{\theta}.$$

D.A. Frank-Kamenetskii (1939) considered *steady solutions*, $\theta = \theta(\mathbf{r})$ in Ω, satisfying

$$\Delta\theta + D\, e^{\theta} = 0 \quad \text{with } \theta = 0 \text{ on } \partial\Omega$$

Solutions for 3 domains:

Interval, $x \in [-1, 1]$:

$$\theta = \theta_0 - 2\ln\cosh\left(x e^{\theta_0/2}\sqrt{D/2}\,\right)$$

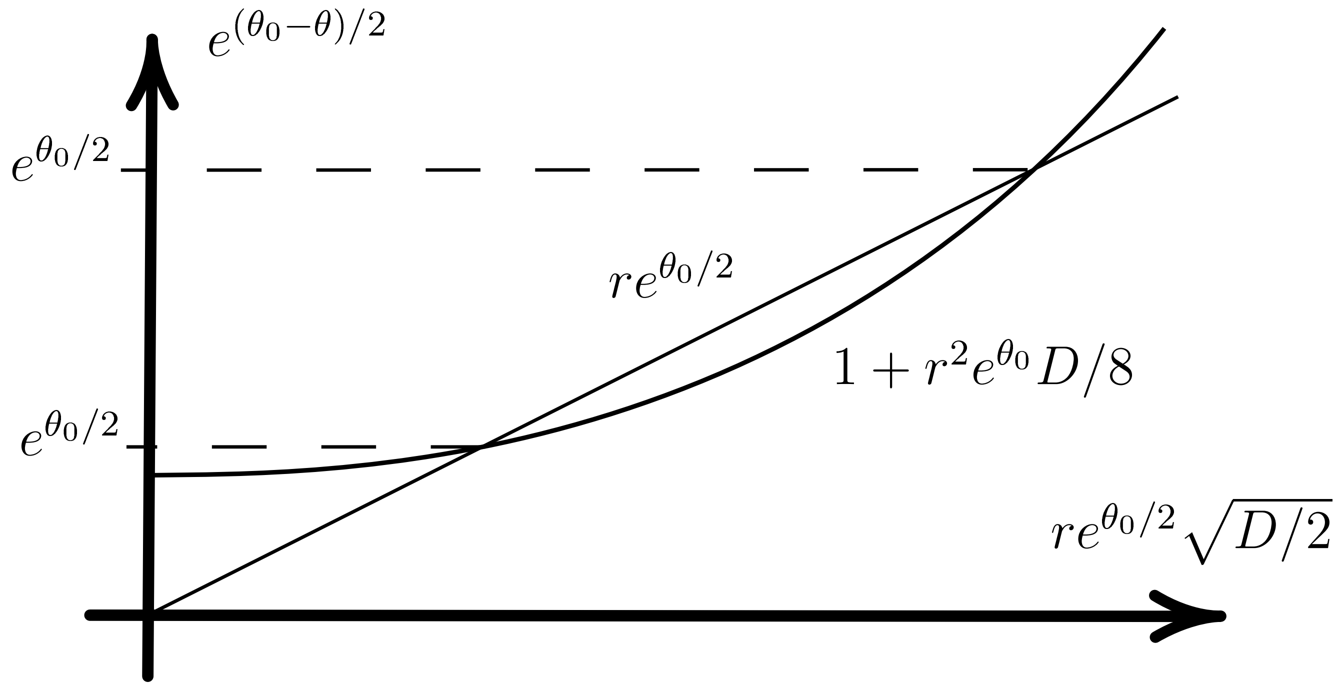
Cylinder, $r \leq 1$:

$$\theta = \theta_0 - 2\ln\left(1 + r^2 e^{\theta_0} D/8\right)$$

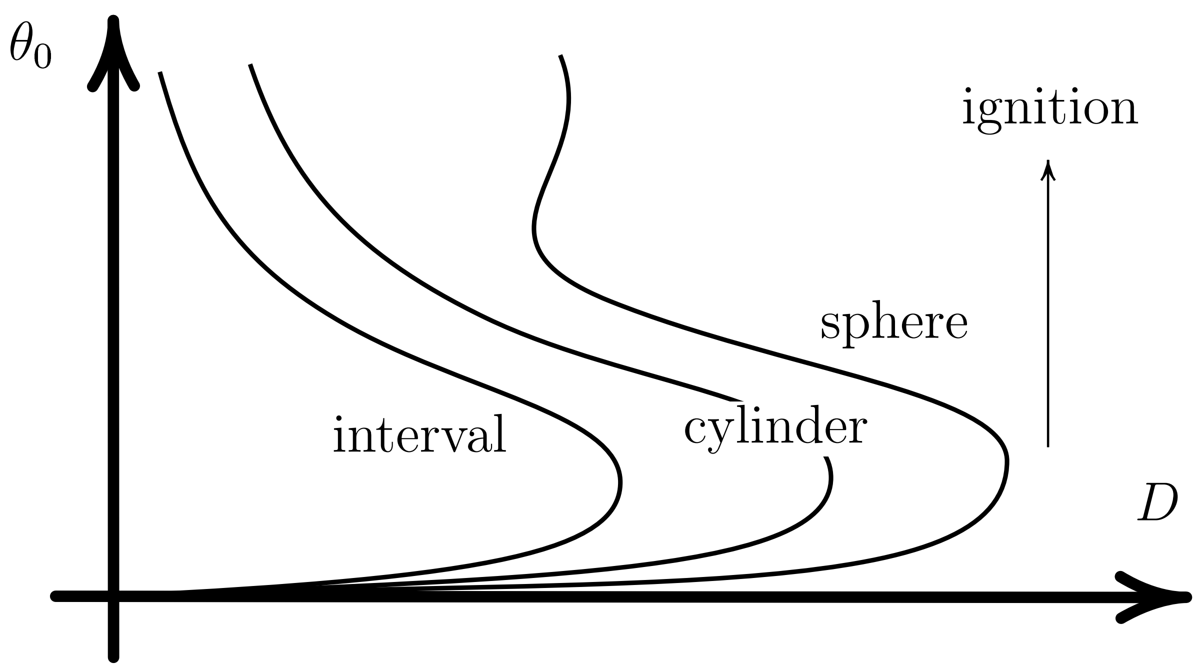
Sphere, $r \leq 1$: (numerical solution only)

Frank-Kamenetskii Solutions

For example, the cylinder:



In general:



Steady solutions exist only for $D \leq D_c(\Omega)$

Descriptions involving an invariant manifold

Example (from Goldshtein et al., 1997):

Consider monodisperse inert, vapourising droplets, radius R with two time scales, $t \mapsto t + \beta\tau$:

$$\theta_t + \beta^{-1}\theta_\tau = F \exp\left(\frac{\theta}{1+\gamma\theta/\beta}\right) - 3\mu\omega R\theta$$

$$F = F_0 - \mu(1-R^3) - \beta^{-1}\theta$$

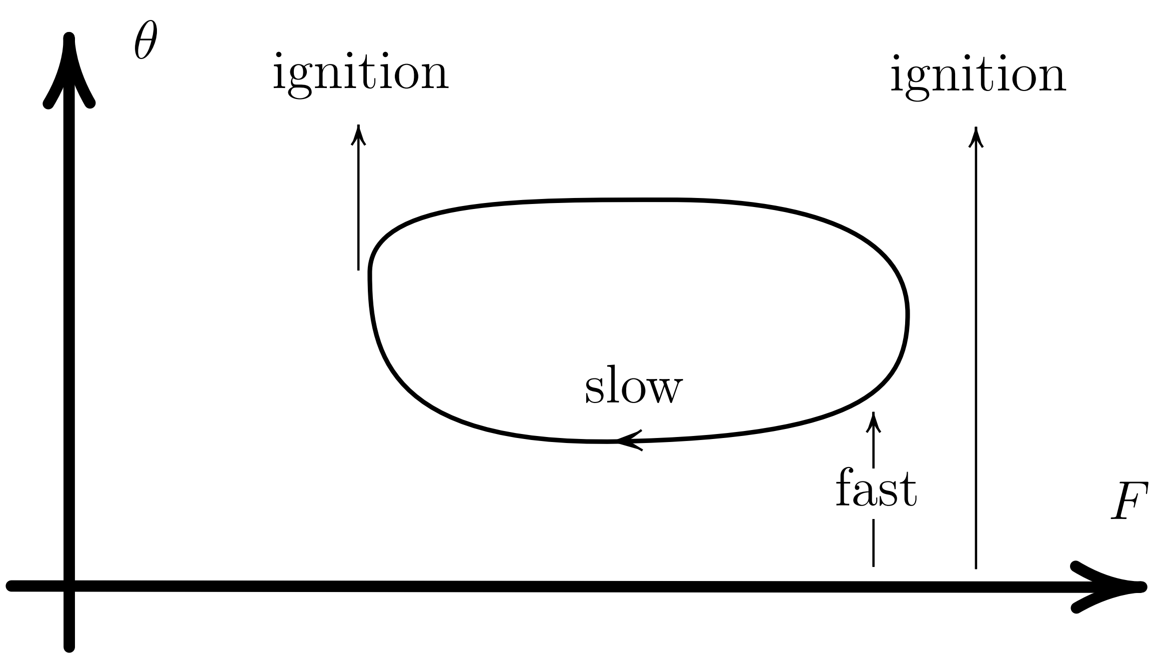
$$R(\beta R_t + R_\tau) = -\omega\theta.$$

There is an invariant manifold, approximated for $\beta \gg 1$ by

$$e^\theta = \frac{3\mu\omega R}{F}\theta$$

where slow evolutions satisfy, to leading order

$$RR_\tau = -\omega\theta.$$



Revised Frank-Kamenetskii Approach
(including an invariant manifold, *with Zinoviev & Sell*)

Using two time-scales again, $t \mapsto t + \beta\tau$, with:

$$T \sim 1 + \beta^{-1}\theta, \quad F \sim \frac{\psi(\tau)}{D} - \beta^{-1}\phi, \quad \langle\phi\rangle = 0.$$

gives

$$\theta_t - \Delta\theta = \psi\, e^{\theta}$$
$$\phi_t - \tfrac{1}{L}\Delta\phi = \psi\left(e^{\theta} - \langle e^{\theta}\rangle\right)$$

- If $\psi(0) > D_c$ there is a finite time "blowup" in θ :

$$\theta\big(\widetilde{t}, \widetilde{\mathbf{r}}\big) = \infty$$

- Otherwise, fast time evolution approaches the manifold for which

$$\Delta\theta + \psi e^{\theta} = 0, \quad \theta(\partial\Omega) = 0$$
$$\tfrac{1}{L}\Delta\phi + \psi\big(e^{\theta} - \langle e^{\theta}\rangle\big) = 0, \quad \psi_n(\partial\Omega) = 0.$$

- Slow evolution on the stable manifold satisfies

$$\frac{d\psi}{d\tau} = -D\psi\langle e^{\theta}\rangle$$

(describing slow consumption of reactant).

Homogeneous (Semenov) explosion

Dynamics of ignition, taking $T = T(t)$, $F = F(t)$ and

$$T_t = -F_t = \beta^{-1} F e^{\beta(1-1/T)}$$

with

$$T(0) = 1, \quad F(0) = F_0$$

so that

$$T + F \equiv \widehat{T} = 1 + F_0,$$

and, taking

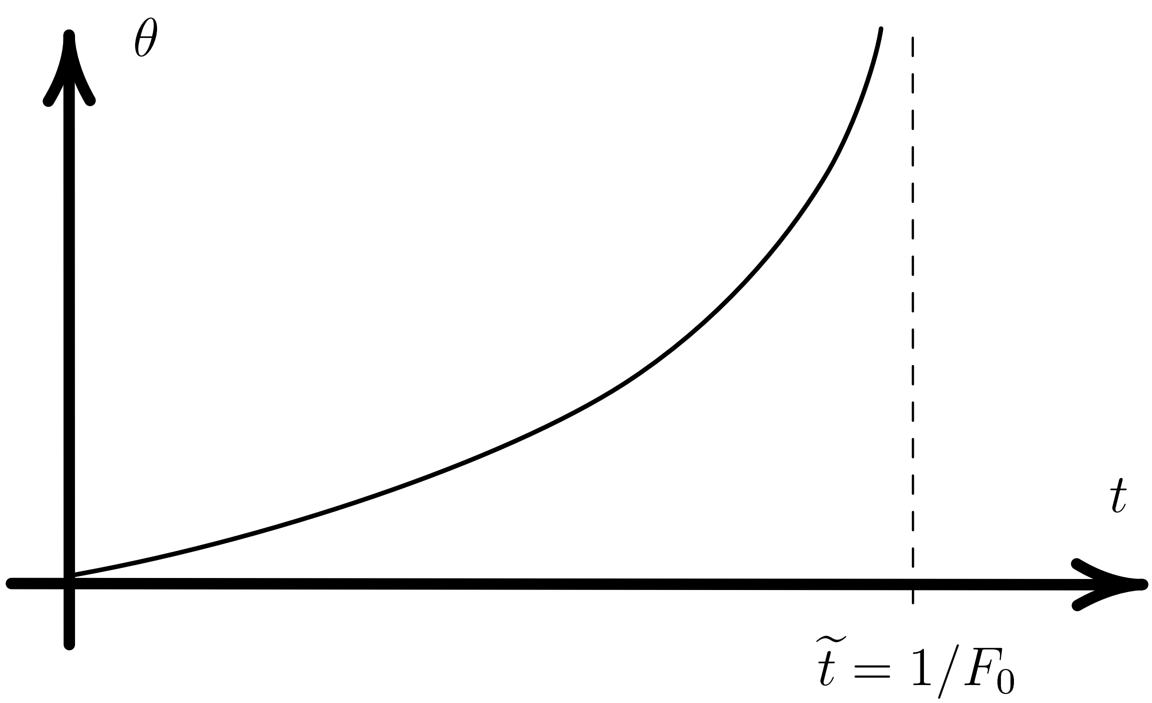
$$T \sim 1 + \beta^{-1}\theta(t)$$

leads to

$$\theta_t = F_0 e^{\theta} \quad \text{so that} \quad \theta = -\ln(1 - F_0 t).$$

The time to self ignition is estimated as

$$\widetilde{t} = 1/F_0.$$



Homogeneous explosion (fuller description)

Using **Kassoy**'s stretched coordinate for any $g(\,\cdot\,)$:

$$\widehat{t}(\beta) - t = e^{-\beta s + g(s)}$$

$$T_s = (\widehat{T} - T)(1 - \tfrac{dg}{ds}/\beta)e^{g+\beta(1-1/T-s)}$$

and fixing $g(\,\cdot\,)$ by defining $1 - 1/T - s = 0$, gives

$$\bigl(1 - \beta^{-1}T^2\tfrac{dg}{dT}\bigr)e^g = \tfrac{T^2}{\widehat{T}-T}$$

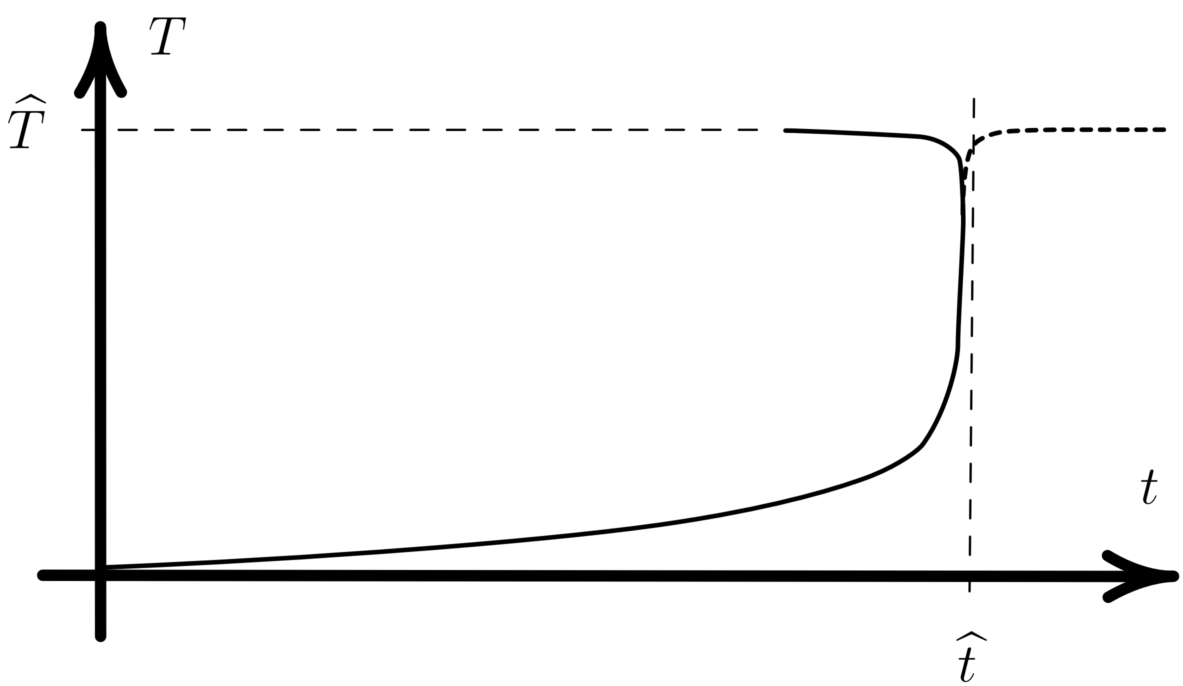
For $\beta \gg 1$: $\quad g = \ln\tfrac{T^2}{\widehat{T}-T} + \beta^{-1}T\tfrac{2\widehat{T}-T}{\widehat{T}-T} + \cdots$ and so

$$\widehat{t} - t = e^{-\beta(1-1/T)}\tfrac{T^2}{\widehat{T}-T}(1 + \beta^{-1}T\tfrac{2\widehat{T}-T}{\widehat{T}-T} + \cdots).$$

At $t = 0$, when $T = 1$, the "self-ignition time" is found

$$\widehat{t} = \tfrac{1}{\widehat{T}-1} + \beta^{-1}\tfrac{2\widehat{T}-1}{(\widehat{T}-1)^2} + \cdots$$

$$= \tfrac{1}{F_0} + \beta^{-1}\tfrac{1+2F_0}{F_0^2} + \cdots .$$



The Kassoy problem (for the shape of blowup)

With spatial variation, the ignition equation

$$\theta_t = \Delta\theta + e^{\theta}$$

has the invariant scaling (for any c)

$$t - \widetilde{t} \mapsto c^2 t, \quad \mathbf{r} - \widetilde{\mathbf{r}} \mapsto c\mathbf{r}, \quad \theta \mapsto \theta - \ln c^2$$

suggesting the exact self-similar reduction

$$\theta = -\ln\left(\widetilde{t} - t\right) + g\left(\frac{\mathbf{r} - \widetilde{\mathbf{r}}}{\sqrt{\widetilde{t} - t}}\right).$$

However, $g(\,\cdot\,)$ has no suitable solutions . . . .
(Kassoy, Kapila, Bressan, Dold)

Instead, asymptotically

$$\theta \sim -\ln\left(\widetilde{t} - t\right) - \ln\left(1 + \frac{\frac{1}{4}(\mathbf{r} - \widetilde{\mathbf{r}})^2/(\widetilde{t} - t)}{\alpha - \ln(\widetilde{t} - t)}\right)$$

as $t \to \widetilde{t}$ for $O(1)$ values of

$$\frac{(\mathbf{r} - \widetilde{\mathbf{r}})^2/(\widetilde{t} - t)}{|\ln(\widetilde{t} - t)|}.$$

The shape of blowup:

Partial explanation:

$$w = e^{-\theta} \qquad \Longrightarrow \qquad w_t = \Delta w - (\nabla w)^2/w - 1.$$

Try $w \sim \widetilde{t} - t + a(t)x^2$:

$$-1 + a'x^2 \sim 2a - \frac{4a^2x^2}{\widetilde{t} - t + a(t)x^2} - 1$$

$$\frac{a'}{a^2} \sim -\frac{4}{\widetilde{t} - t}$$

$$4a \sim \frac{1}{\alpha - \ln(\widetilde{t} - t)}.$$

So

$$e^{-\theta} \sim \widetilde{t} - t + \frac{x^2/4}{\alpha - \ln(\widetilde{t} - t)}$$

$$\theta \sim -\ln\left(\widetilde{t} - t + \frac{x^2/4}{\alpha - \ln(\widetilde{t} - t)}\right).$$

- In fact there are only three free parameters in the asymptotic structure of the blowup, taken to any order:

$$\widetilde{t}, \quad \widetilde{\mathbf{r}} \quad \text{and} \quad \alpha.$$

The shape of flame initiation

$$\theta \sim -\ln\left(\widetilde{t}-t\right) - \ln\left(1 + \frac{\frac{1}{4}(\mathbf{r}-\widetilde{\mathbf{r}})^2/(\widetilde{t}-t)}{\alpha - \ln(\widetilde{t}-t)}\right)$$

implies

$$\Delta\theta/e^{\theta} \sim \tfrac{1}{2}/\theta.$$

- Apart from details, the same solution continues until

$$\beta(1-1/T) \to \beta(1-1/\widehat{T}) - O(1).$$

- Diffusion is demoted at the end of thermal runaway until

$$\Delta T/e^{\beta(1-1/T)} = O(\beta^{-1})$$

- Model for $T = \widehat{T} - \beta^{-1}\eta$:

$$\eta_t = \beta^{-1}\Delta\eta - \eta e^{-\eta}$$

$$\int_1^{\eta} \frac{e^{\nu}}{\nu}\mathrm{d}\nu \sim \widehat{t} - t + x^2 \quad \text{for} \quad \eta \gg 1.$$

- Initial flames are diffusionless with speed

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \tfrac{1}{2}/x.$$

- Self-propagation (via diffusion) takes over as flames slow down.

Critical flame boundaries (flame balls, *with Joulin*)

Sources of heat do not always ignite.

Consider a flame-ball around a point source of heat, with a reaction-sheet at $\mathbf{r} \in \Gamma$

$$\beta^{-1} u T_x = \Delta T, \quad \beta^{-1} u F_x = \tfrac{1}{\mathrm{L}} \Delta F$$

$$\text{on } \Gamma : \quad -\mathrm{L}[T_n] = [F_n] = \exp\left(\tfrac{1}{2}\beta(T - \tfrac{1}{\mathrm{L}})\right)$$

$$\lim_{r\to 0} r^2 T_r = -\beta^{-1} q, \quad \lim_{r\to\infty} (T, F) = (0, 1).$$

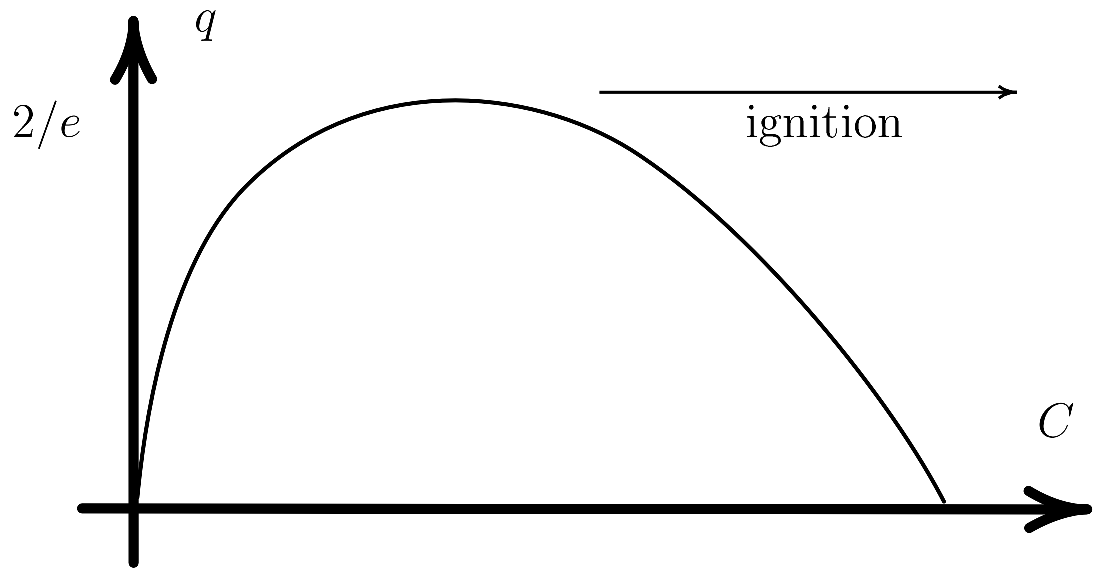
The case, $q = V = 0$, makes Γ the unit ball in $\mathbb{R}^3$.

If $4\pi C$ is the total flux of reactant F into Γ, for small u :

$$C = C\left(\frac{q}{C}, \frac{1-\mathrm{L}}{\mathrm{L}} C u\right)$$

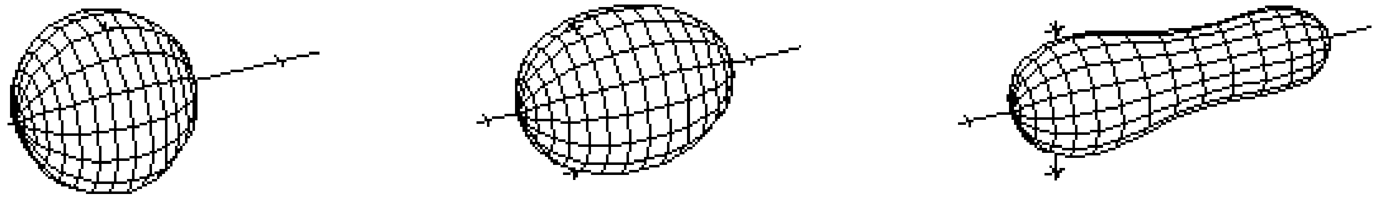
$$\sim \exp\left(\frac{1-\mathrm{L}}{4\mathrm{L}} C u - \frac{q}{2C}\right).$$

Sketch for $u = 0$:



Critical flame boundaries

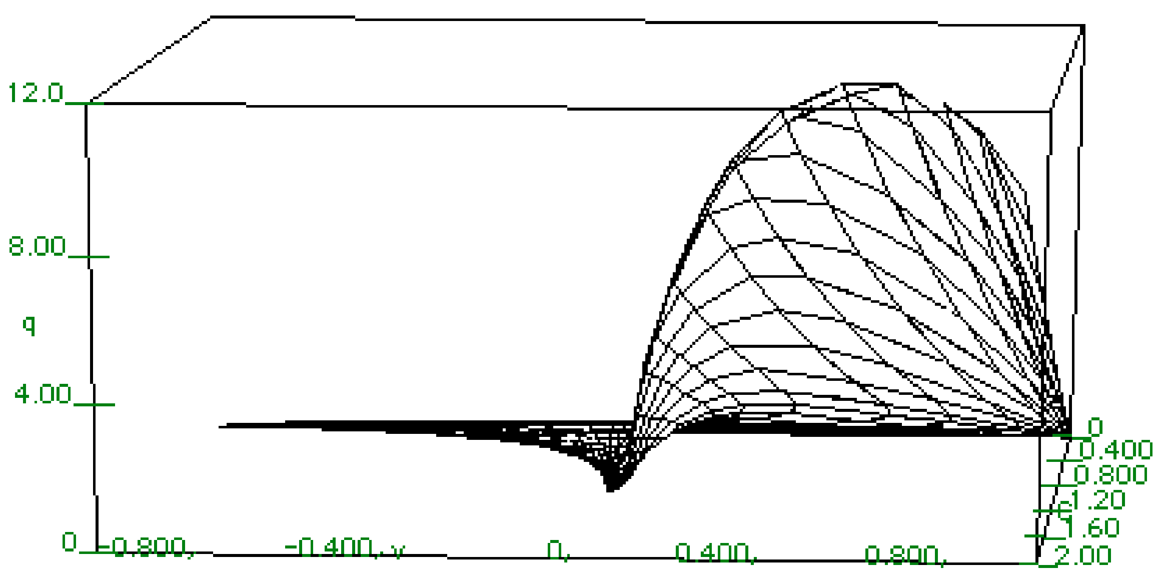
Solutions for $(1-\mathrm{L})Cu = O(1)$:



(increasing u)

in the space of solutions:

q



C

$$\tanh\left(\frac{(1-\mathrm{L})Cu}{4\mathrm{L}}\right)$$

Summary

Main characteristics of ignition

- Balances between heat production and heat loss provide:
  - critical conditions for imbalance
  - manifolds of "steady" equilibria
  - slow evolution on stable manifolds
- Fast dynamical changes involve:
  - ignition (induction) delay times
  - spatial blowup structure
  - transition from initially diffusionless "fast flames" to self-propagating flames