Lectures on
Dynamics of Gaseous Combustion Waves
(from flames to detonations)
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Lecture III
Thermal propagation of flames
Lecture 3: Thermal propagation

3-1. Quasi-isobaric approximation (Low Mach number)
3-2. One-step irreversible reaction
3-3. Unity Lewis number and large activation energy
3-4. Zeldovich & Frank-Kamenetskii asymptotic analysis
   Preheated zone
   Inner reaction layer
   Matched asymptotic solution
3-5. Reaction diffusion waves
   Phase space
   Selected solution in an unstable medium
Quasi-isobaric approximation. LowMach number

\[ \rho(u, \nabla) u \approx -\nabla p \Rightarrow \delta p \approx \rho u \delta u \]
\[ p \approx \rho a^2 \Rightarrow \delta p/p \approx u^2/a^2 \equiv M^2 \]

slow evolution \[ \frac{\partial}{\partial t} \approx u, \nabla \ll a |\nabla| \]

+ very subsonic flow \[ \left| \frac{1}{p} \frac{Dp}{Dt} \right| \ll \left| \frac{1}{T} \frac{DT}{Dt} \right| \Rightarrow \left| \frac{Dp}{Dt} \right| \ll \left| \rho c_p \frac{DT}{Dt} \right| \]

\[ \rho c_p \frac{DT}{Dt} = \frac{Dp}{Dt} + \nabla \cdot (\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)} \]

(in open space)

\[ \rho T = \rho_o T_o \]
\[ \rho c_p \frac{DT}{Dt} = \nabla \cdot (\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)}(T, ..Y_{k..}) \]
\[ \rho D_i \frac{DY_i}{Dt} = \nabla \cdot (\rho D_i \nabla Y_i) + \sum_j \varphi_i^{(j)} M_i \dot{W}^{(j)}(T, ..Y_{k..}), \]

Planar flame reference frame of flame

\[ \rho D / Dt = m d/dx \quad m \equiv \rho_a U_L = \rho_b U_b, \quad U_b / U_L \approx T_b / T_u, \approx 4 - 8 \]

equations \[ m c_p \frac{dT}{dx} - \frac{d}{dx} \left( \lambda \frac{dT}{dx} \right) = \sum_j Q^{(j)} \dot{W}^{(j)}(T, ..Y_{i..}) \]
\[ m \frac{dY_i}{dx} - \frac{d}{dx} \left( \rho D_i \frac{dY_i}{dx} \right) = \sum_j \varphi_i^{(j)} M_i \dot{W}^{(j)}(T, ..Y_{i..}), \]

boundary conditions \[ x = -\infty : T = T_u, \quad Y_i = Y_{iu}, \quad \dot{W}_j = 0 \quad \text{frozen state} \]
\[ x = +\infty : \frac{dT}{dx} = 0, \quad Y_i = Y_{ib}, \quad \dot{W}_j = 0 \quad \text{equilibrium state} \]
III - 2) **One-step irreversible reaction**

\[ R \rightarrow P + Q \]

\( R \) in an inert; \( Y = \) mass fraction of \( R \)

Velocity and structure of the planar flame

\[
mc_p \frac{dT}{dx} - \frac{d}{dx} \left( \lambda \frac{dT}{dx} \right) = \rho q_R \dot{W} \quad q_R = \text{energy released per unit of mass of } R
\]

\[
m \frac{dY}{dx} - \frac{d}{dx} \left( \rho D \frac{dY}{dx} \right) = -\rho \dot{W} \quad m \equiv \rho_u U_L \text{ unknown}
\]

\[ x \rightarrow -\infty : \quad Y = Y_u, \quad T = T_u \]

\[ x \rightarrow +\infty : \quad Y = 0 \]

\[ mY_u = \int_{-\infty}^{+\infty} \rho \dot{W} \, dx \]

**Arrhenius law**

\[
\rho \dot{W} = \rho_b \frac{Y}{\tau_r(T)} \quad \frac{1}{\tau_r(T)} \equiv \frac{e^{-E/k_B T}}{\tau_{coll}} \quad \frac{1}{\tau_{rb}} \equiv \frac{e^{-E/k_B T_b}}{\tau_{coll}}
\]

\[
\frac{1}{\tau_r(T)} = \frac{1}{\tau_{rb}} e^{-T_b/T \beta(1-\theta)} \quad \beta \equiv \frac{E}{k_B T_b} \left(1 - \frac{T_u}{T_b}\right) \quad \theta \equiv \frac{T - T_u}{T_b - T_u} \in [0, 1]
\]

\[ c_p(T_b - T_u) = q_m \equiv q_R Y_u \]
Unity Lewis number and large activation energy

Le \equiv D_T/D

Reduced temperature and mass fraction

\[ \theta \equiv \frac{T - T_u}{T_b - T_u} \in [0, 1] \]
\[ \psi \equiv \frac{Y}{Y_u} \in [0, 1] \]

\[ m \frac{d\theta}{dx} - \rho_D T \frac{d^2 \theta}{dx^2} = \rho \frac{\dot{W}}{Y_1u}, \]
\[ m \frac{d\psi}{dx} - \rho_D T \frac{d^2 \psi}{Le \, dx^2} = -\rho \frac{\dot{W}}{Y_1u}, \]

\[ x = -\infty : \theta = 0, \psi = 1, \quad x = +\infty : \theta = 1, \psi = 0 \]

\[ \beta \equiv \frac{E}{k_BT_b} \left(1 - \frac{T_u}{T_b}\right) \]
\[ \rho \frac{\dot{W}}{Y_u} = \rho_b \frac{\psi}{\tau_{rb}} e^{-\frac{T_b}{T} \beta (1-\theta)} \]

\[ \dot{W} \approx (1 - \theta) e^{-\beta (1-\theta)} \]

(reaction rate is non negligible only when \( T \approx T_b \))
III - 4) Zeldovich, Frank-Kamenetskii asymptotic analysis

\[ \beta \to \infty \]

\[
m \frac{d \theta}{dx} - \rho D_T \frac{d^2 \theta}{dx^2} = \rho \dot{W} / Y_{1u},
\]

\[
x = -\infty : \theta = 0, \quad x = +\infty : \theta = 1,
\]

\[
w'(\theta) \approx (1 - \theta)e^{-\beta(1-\theta)}
\]

\[
\rho \dot{W} / Y_u = \rho_b w'(\theta) / \tau_{rb}
\]

preheated zone \(\dot{W} \approx 0\)

\[
md\theta/dx - \rho D_T d^2\theta/dx^2 = 0 \quad \rho D_T = \text{cst.}
\]

origin \(x = 0\) : location of the reaction zone \(\theta = 1\)

\[
d_L \equiv \rho D_T / m = D_{T_u} / U_L
\]

matching condition

heat flux into the preheated zone

\[
\rho D_T d\theta/dx|_{\theta=1} = m
\]

should be equal to the heat flux from the thin reaction layer
Inner reaction layer

\[ 1 - \theta = O(1/\beta) \]

\[ w'(\theta) \approx (1 - \theta)e^{-\beta(1-\theta)} = O(1/\beta) \]

\[ \frac{d\theta}{dx} \approx \frac{\delta\theta}{d_r} \frac{\rho_b D_T b}{d_r d_L \beta} \]

\[ \delta\theta = O(1/\beta) \]

\[ d_r \ll d_L \]

\[ d_r \approx \sqrt{D_T b \tau_{rb}} \]

\[ m = \rho D_T / d_L \]

Matching. Solution

upstream exit of the inner layer \( \beta(1 - \theta) \to \infty \): \( D_T b d\theta / dx \to \sqrt{(2/\beta^2) D_T b / \tau_{rb}} \)

downstream entrance of the external zone \( \theta \to 1 \): \( \rho_b D_T b d\theta / dx \big|_{\theta=1} = m \)

\[ m = \rho_b \sqrt{(2/\beta^2) D_T b / \tau_{rb}} \]

\[ U_L = m / \rho_u \Rightarrow d_r / d_L = O(1/\beta) \]

\[ U_L \approx \sqrt{D_T b / \tau_{rb}} \]

dimensional analysis
non-dimensional form
\[ \frac{\partial \theta}{\partial t} - \frac{\partial^2 \theta}{\partial x^2} = w(\theta), \quad \theta \geq 0, \quad x = \pm \infty : \theta = 0, w = 0 \]
unstable or metastable
\[ \frac{d\Phi}{d\theta} = -w(\theta) \]
\[ \theta = 1, w = 0 \]
stable state

propagating wave at constant velocity
\[ \xi = x + \mu t \]
\[ \xi = -\infty : \quad \theta = 0, \quad w = 0, \quad \xi = +\infty : \quad \theta = 1, \quad w = 0 \]
limited \( \theta > 0 \)
\[ \mu \frac{d\theta}{d\xi} - \frac{d^2 \theta}{d\xi^2} = w(\theta) \]

\( \mu \) unknown, number of solutions?
Number of solutions? Phase space

\[ \theta \geq 0 \]

\[ X \equiv \theta, \quad Y \equiv \mu \theta / \xi \]
\[ dX/d\xi = Y/\mu \quad dY/d\xi = \mu [Y - \omega(X)] \]
\[ \mu \frac{dX}{d\xi} - \frac{d^2X}{d\xi^2} = \omega(X) \]

\[ dY/dX = \mu^2 [Y - w(X)]/Y \]

Linearisation about \( X = 0, Y = 0 \) and \( X = 1, Y = 0 \) \( \omega'_0 < 0 \)
\[ \xi \to -\infty \quad \xi \to \infty \) (equilibrium state)

Two eigenvalues \( r_+ \) and \( r_- \) and two eigenvectors \( k_+ \) and \( k_- \)
\[ \delta X = A_+ e^{\xi r_+} + A_- e^{\xi r_-}, \quad \delta Y = k_+ A_+ e^{\xi r_+} + k_- A_- e^{\xi r_-} \]
\[ \mu \frac{d\delta X}{d\xi} - \frac{d^2\delta X}{d\xi^2} = \omega'_0 \delta X \quad \mu r^2 - \omega'_0 = 0 \]
\[ 2r_\pm = \mu \pm \sqrt{\mu^2 - 4\omega'_0} \]
\[ k_\pm = \mu r_\pm \]

One solution

Infinite numbers of solutions

One particular solution

No solution \((\theta \geq 0)\)
Unstable medium

wave velocity

continuous spectrum with a lower bound

$$2r_\pm = \mu \pm \sqrt{\mu^2 - 4\omega' \theta}$$

lower bound : $$r_+ = r_- = \mu/2 \quad k_+ = k_-$$

soft case \(\Rightarrow\) collapse of the 2 eigenvalues

the lower bound solution is selected

$$\mu_{\text{mini}} \equiv 2d\mu/d\theta|_{\theta=0}$$

soft nonlinear term \(\omega(\theta)\)

OK for a soft term \(\omega(\theta)\)

Wrong for a stiff term \(\omega(\theta)\)

The lower bound solution changes of nature when \(\omega(\theta)\) get stiffer

Soft \(\omega(\theta) = \theta(1-\theta)\)

Stiff \(w(\theta, \beta) = (\beta^2/2)\theta(1-\theta)e^{-\beta(1-\theta)}, \beta \gg 1\)