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Dynamics of Combustion Waves in Premixed Gases

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Theoretical analyses + laboratory experiments
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Combustion Waves and Fronts in Flows
P. Clavin and G. Searby
Cambridge University Press 2016
Lecture 1: **Orders of magnitude**

1-1: Overall combustion chemistry

1-2: Combustion waves in gaseous mixtures

1-3: Arrhenius law

1-4: Hydrocarbon/air flames

1-5: Instabilities of flames
1-1: Overall combustion chemistry

reactants $\rightarrow$ products + heat release

binding energy of small molecules $\approx$ a few eV

$1 eV$/molecule $\approx 23$ kcal/mole $\Rightarrow T_b - T_u \approx 2000$ K

$(C_p \approx 10$ cal/mole/K$)$

reaction time $\tau_r(T)$ extremely sensitive to temperature:

$T < 500K : \tau_r(T) \approx \infty$ (frozen mixture of reactants)

$T \approx 2500K : \tau_r(T) \approx 10^{-6}$ s.

thermal feedback $\Rightarrow$ combustion waves
1-2: Combustion waves in gaseous mixtures

Flames: $10 \text{ cm/s} - 10 \text{ m/s}$, $\Delta p/p \approx -10^{-5}$

Laminar propagation

Fast deflagrations: $\approx 100 \text{ m/s}$, $\Delta p/p \approx -10^{-1}$

Turbulent propagation

Detonations: $\approx 2000 \text{ m/s}$, $\Delta p/p \approx +30$

Cellular structure
Back to the kinetic theory of gases

Binary collisions of molecules

\[
<\text{distance}> = l \\
<\text{velocity}> = V \equiv \sqrt{3k_BT/m} \\
<\text{time}> = \tau_{\text{coll}} \equiv l/V
\]

Equilibrium state. The Maxwell-Boltzmann distribution

\[
f^{(eq)}(v, n, T) \, d^3v \, d^3r = n \frac{m^{3/2}}{(2\pi k_B T)^{3/2}} e^{-m|v|^2/(2k_BT)} \, d^3v \, d^3r
\]

\(m\) : mass of molecules, \(n\) : number density, \(T\) : temperature, \(k_B\) : Boltzmann cst.

Molecular diffusion \(\equiv\) Random Walk

\[
\text{spreading} : \frac{1}{(4\pi D t)^{3/2}} e^{-r^2/4Dt}
\]

\(D = lV = l^2/\tau_{\text{coll}} \approx a^2\tau_{\text{coll}}\)

Diffusion coefficient
Parameters

chemical energy/unit mass $q_m \Rightarrow T_b/T_u = 5 - 10$

sound speed, $a_b/a_u = \sqrt{T_b/T_u}$

reaction rate $1/\tau_r(T_b)$

molecular and thermal diffusion coefficients $D \approx D_T$  

$\text{(length)}^2 / \text{time}$

Detonation= shock driven reaction wave; Flame=reaction-diffusion wave

Dimensional analysis

[qm] = (velocity)$^2$

propagation velocity

[D] = (velocity)$^2 \times \text{time}$

$D \approx 10^{-3}\text{m}^2/\text{s}$

Detonation: $D \approx \sqrt{q_m} \approx a_b$

$\approx 1000 \text{ m/s}$

supersonic $D/a_u > 1$

laminar flames: $U_L \approx \sqrt{D/\tau_r(T_b)}$

$\approx 1 \text{ m/s}$

subsonic $U_L/a_u < 1$
1-3: Arrhenius law

Overall reaction rate: highly sensitive to temperature, Arrhenius law

large activation energy

\[ \frac{E}{k_B T_b} \approx 8 \]

\[ e^{-E/k_B T_b} \approx 3 \times 10^{-4} \]

\[ T_b/T_u = 8 \implies e^{-E/k_B T_u} \approx 1.6 \times 10^{-28} \]

high thermal sensitivity

Collision in gases

Maxwell-Boltzmann distribution

Kinetic theory of gases \(\implies\) Arrhenius law

\[ \text{MB distribution } \propto e^{-\frac{1}{2} \frac{m v^2}{k_B T}} \implies \frac{1}{\tau_r(T)} = \frac{1}{\tau_{\text{coll}}} e^{-E/k_B T} \]

Arrhenius factor

Kinetic theory of gases \(\implies\) Flame properties

\[ D \approx a^2 \tau_{\text{coll}} \approx l^2/\tau_{\text{coll}} \]

\[ a \approx l/\tau_{\text{coll}} \]

sound speed

men free path

laminar flame velocity

\[ U_L \approx \sqrt{D_T/\tau_r} \]

subsonic

\[ U_L/a \approx \sqrt{e^{-E/k_B T_b}} \ll 1 \]

sound speed

\[ d_L \approx D_T/U_L \]

macroscopic structure

flame thickness

\[ d_L \approx l \sqrt{e^{-E/k_B T_b}} \gg l \]

mean free path

elastic collision rate \(1/\tau_{\text{coll}} \approx 10^9 \text{s}^{-1}\)

\[ \implies 1/\tau_r(T_b) \approx 3 \times 10^5 \text{s}^{-1} \]

\[ T_b/T_u = 8 \implies \tau_r(T_u) \approx 10^{10} \text{ years} !! \]
Molecular diffusion $\equiv$ Random Walk

\[ <\text{distance}> = l \]
\[ <\text{velocity}> = V \equiv \sqrt{3k_B T/m} \]
\[ a \approx V \]
\[ <\text{time}> = \tau_{\text{coll}} \equiv l/V \]

spreading: \[ \frac{1}{(4\pi Dt)^{3/2}} e^{-r^2/4Dt} \]

mean free path

\[ D = lV = l^2/\tau_{\text{coll}} \approx a^2 \tau_{\text{coll}} \]

Flame structure

\[ U_L \approx \sqrt{D/\tau_r(T_b)} \]
\[ \frac{1}{\tau_r(T_b)} = \frac{1}{\tau_{\text{coll}}} e^{-E/k_BT_b} \]
\[ d_L/l \approx U_L \tau_r/l \approx \sqrt{D\tau_r/l} \approx \sqrt{e^{E/k_BT_b}} \geq 1 \]

Limitations of the dimensional analysis

\[ e^{-E/k_BT_b} \approx 3 \times 10^{-4} \]
\[ a \approx 500 \text{ m/s} \]
\[ l \approx 10^{-7} \text{ m} \]

\[ \Rightarrow \]
\[ U_L \approx 8.6 \text{ m/s} \]
\[ d_L \approx 0.6 \times 10^{-5} \text{ m} \]

too large hydrocarbon/air

too small 10 - 50 cm/s

1 - 10^{-1} \text{ mm}
Methane-air flame

\[
\vartheta_F^+ F + \vartheta_O^+ O_2 \rightleftharpoons P
\]

Equivalence ratio
\[
\phi = \frac{N_F}{N_{O_2}} / \vartheta_F^+ / \vartheta_O^+
\]

\( \phi = 1 \): stoichiometry
\( \phi > 1 \): fuel rich
\( \phi < 1 \): fuel lean

near to the flammability limit

\( \phi = 0.65 \)

"thicker flame"

\[
d_L \approx U_L \tau_r(T_b)
\approx \sqrt{D_T \tau_r(T_b)}
\approx D_T \sqrt{\tau_r(T_b)/D_T}
\approx D_T / U_L
\]

\( U_L \downarrow \quad d_L \uparrow \)
Intrinsic instabilities

Planar flames are linearly unstable:

- hydrodynamic instability of the flame front
  \[ \rho_u > \rho_b \]

induced flow  
Propane lean flame  
Cusp formation  
Huygens construction

- thermo-diffusive instability
  \[ D_T < D \]

Unstable inner structure  
Propane rich flame
System instability (combustion in a cavity)

The coupling of flames with acoustics can be unstable

Thermo-acoustic instabilities (Rayleigh criterion)

Combustion chambers
Rocket engine
Gas turbines
Vibratory instability of flames in tubes

Lean methane-air flame

\[ \phi = 0.73 \quad U_L = 23 \text{ cm/s} \]

\[ \phi = 0.8 \quad U_L = 30 \text{ cm/s} \]

Acoustic instability in Premixed Flames

G. Searby IRPHE 2006

Effect of geometrical parameters on thermo-acoustic instability of downward propagating flames in tubes

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**Effect of acceleration**

**Gravity**

Propane flame propagating upwards  \( \rightarrow \) Slow downwards propagating flame  \( \rightarrow \) slightly faster

**Effect of an acoustic field on a Bunsen flame**

Methane rich Bunsen flame \( \phi = 1.5 \)  \( \rightarrow \) in the presence of an axial acoustic field  \( \rightarrow \) equipotential surface in the absence of flame
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Lecture 11
 Governing equations of reacting flows
Gaseous mixtures in normal conditions $\approx$ continuum medium in local equilibrium

mean free path $\ll$ macroscopic length

many microscopic particles $\in$ a fluid ”particle”

relaxation time towards equilibrium of fluid particles $\ll$ macroscopic time scale

⚠️

internal structure of shock waves
Lecture 2: **Governing equations**

(simplified form, see de Groot et Mazur (1962) or Williams (1985) for more details)

2-1. Conserved extensive quantities
2-2. Continuity
2-3. Fick’s law. Diffusion equation
2-4. Conservation of momentum
2-5. Conservation of total energy
   
   *Thermal equation*
   
   *Inviscid flows in reactive gases*
   
   *Conservative forms*
   
   *One-dimensional inviscid and compressible flow*

2.6. Entropy production
2-1. Conserved extensive quantities

extensive quantities \[ A_V = \iiint_V \rho a \, d^3 r \] mass weighted distribution \( a(r, t) \)

mass density \( \rho(r, t) \)

conservation equation \( V \) fixed \[ \frac{dA}{dt} = \iiint_V [\partial(\rho a)/\partial t] \, d^3 r = (dA/dt)_1 + (dA/dt)_2 \]

\[ (dA/dt)_1 = - \iiint_{\Sigma} \mathbf{n} \cdot \mathbf{J}_a \, d^2 \sigma \]

\[ (dA/dt)_2 = \iiint_V \omega_a(r, t) \, d^3 r \]

vector field \( \mathbf{J}_a(r, t) \)

Gauss-Ostrogradsky theorem

\[ \partial(\rho a)/\partial t = - \nabla \cdot \mathbf{J}_a + \omega_a \]

conserved quantities: no production terms \( \omega_a = 0 \) No volumetric production

conserved scalar \( a(r, t) \)

conserved vector \( \mathbf{a}(r, t) \)

conserved tensor field \( \mathbf{J}_a(r, t) \)

\[ \partial(\rho \mathbf{a})/\partial t = - \nabla \cdot \mathbf{J}_a \]
2-2. Continuity

Mass is a conserved scalar (classical mechanics)

\[
\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}
\]
\[
\mathbf{J} \equiv \rho \mathbf{u}
\]
\[
\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u})
\]

\[
\nabla \cdot (\rho \mathbf{u}) = \mathbf{u} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{u}
\]

Material (convective) derivative

\[
\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla
\]

\[
\frac{1}{\rho} \frac{D\rho}{Dt} = -\nabla \cdot \mathbf{u}
\]

Continuity equation

\[
v \equiv 1/\rho
\]

Volume/unity of mass

\[
\frac{1}{v} \frac{Dv}{Dt} = \nabla \cdot \mathbf{u}
\]

Lagrangian form of conservation equation

\[
\frac{\partial (\rho \alpha)}{\partial t} = -\nabla \cdot \mathbf{J}_\alpha + \dot{\omega}_\alpha
\]

\[
\rho \frac{Da}{Dt} = -\nabla \cdot \mathbf{J}'_\alpha + \dot{\omega}_\alpha
\]

Conserved scalar:

\[
\frac{\partial (\rho \alpha)}{\partial t} = -\nabla \cdot \mathbf{J}_\alpha
\]

\[
\rho \frac{Da}{Dt} = -\nabla \cdot \mathbf{J}'_\alpha
\]

(definition of the diffusion flux in the equation for energy is slightly different)

See slide 11
mass fraction \( Y_i = \frac{\rho_i}{\rho} \quad \sum_i Y_i = 1 \)

inert mixture mass fraction of species is a conserved scalar

\[ \rho \frac{D Y_i}{D t} = -\nabla . J'_i \quad \sum_i J'_i = 0 \]

Kinetic theory of gas (binary diffusion in an abundant species)

Fick’s law:

\[ J'_i = -\rho D_i \nabla Y_i \]

\( D_i > 0 \)

\[ \rho \frac{D Y_i}{D t} = \nabla . [\rho D_i \nabla Y_i] \]

diffusion equation

\[ \rho D_i \approx \text{cst.} \quad u = 0 \]

\[ \frac{\partial Y_i}{\partial t} = D_i \Delta Y_i \]

archetype of irreversible phenomenon

(random walk)
Diffusive damping. Dissipative phenomenon

\[ \frac{\partial Y}{\partial t} = D \Delta Y \quad D > 0 \quad [D] = (\text{length})^2/\text{time} \]

Fourier analysis

\[ Y(r, t) = \sum_k \tilde{Y}_k(t)e^{i\mathbf{k} \cdot \mathbf{r}} \quad k = |k| \]

\[ \frac{d\tilde{Y}_k(t)}{dt} = -(Dk^2)\tilde{Y}_k(t) \quad \tilde{Y}_k(t) = \tilde{Y}_k(0)e^{-Dk^2t} \]

Green function  Self-similar solution

\[ \frac{\partial G}{\partial t} = D \Delta G \]

\[ t = 0 : G(r, 0) = \delta(r) \quad G(r, t) = \frac{1}{(4\pi Dt)^{3/2}}e^{-r^2/4Dt} \quad r = |r| \quad \int \int \int G(r, t)d^3r = 1 \]

probability distribution of the test particle

number density

\[ \frac{\partial n}{\partial t} = D \Delta n \]

\[ n(r, t) = Ng(r, t) \]

\[ n(r, t) = \int \int \int n(r', 0)G(r - r', t)d^3r' \]
2-4. Conservation of momentum

Momentum is a conserved vector (isolated system)

\[ \rho \frac{Du}{Dt} = -\nabla \cdot \Pi - \rho g e_z, \]

surface force (stress tensor) \( \Pi = pI + \pi \) gravity (body force)
thermodynamic pressure (isotropic)

Viscous stress tensor

\[ \pi \equiv -2\eta(\nabla u)^{(s)} - I(\xi - 2\eta/3) \nabla \cdot u \]

Navier Stokes equations

\[ \rho \frac{Du}{Dt} = -\nabla (p + \rho g z) + \eta \Delta u + (\xi + \eta/3) \nabla (\nabla \cdot u) \]

Viscous shear diffusivity \( D_{vis} = \eta/\rho \)

Euler equations

\[ \rho \frac{Du}{Dt} = -\nabla p \]

non dissipative equations
2-5. Conservation of total energy

internal energy,  
(Additive in a gas when interactions are neglected)  
\[ e_{\text{int}} = e_T + e_{\text{chem}} \]

thermal energy, chemical energy (chemical bonds),  
(kinetic + rotational & vibrational energy)

total energy per unit mass  
\[ e_{\text{tot}} = |\mathbf{u}|^2/2 + e_T + e_{\text{chem}} + ... \]

\[ \delta e_T = c_V \delta T \]

Question: what is the expression of \( J_{e_{\text{tot}}} \)?

\[ \rho \mathbf{Du}/Dt = -\nabla p \]

\textbf{Inviscid flow}  
Euler equation  
\[ \Rightarrow \quad \frac{1}{2} \rho \frac{D}{Dt} |\mathbf{u}|^2 = -\mathbf{u}.\nabla p = -\nabla (p\mathbf{u}) + p\nabla.\mathbf{u} \]

\[ \rho \mathbf{De}_T/Dt = -\nabla \mathbf{J'}_q \]

\textbf{Inert flow}  
(1st law of thermodynamics)  
without internal viscous dissipation

\[ \rho \mathbf{De}_T/Dt = -\nabla \mathbf{J'}_q - p\nabla.\mathbf{u} \]

\[ p\nabla.\mathbf{u} = \rho p(D\rho^{-1}/Dt) \]

\textbf{Fourier law}  
(simplest form of heat flux)

\[ \mathbf{J'}_q = -\lambda \nabla T, \]

\[ \rho \mathbf{De}_T/Dt = -\nabla.\mathbf{J'}_q - p\nabla.\mathbf{u} \]

\textbf{Fourier equation}  
\( \partial T/\partial t = D_T \Delta T \)

inert material \( e_{\text{chem}} = \text{cst.} \)

no flow \( \mathbf{u} = 0 \)

\[ D_T \equiv \lambda/\rho c_V \]

\[ [D_T] = (\text{length})^2/\text{time} \]
Question: what is the expression of $J_{e_{\text{tot}}}$ for a single component inert and inviscid flow?

1st law

- **Internal energy**
  \[
  \rho D e_T /Dt = \nabla(\lambda \nabla T) - p \nabla \cdot u
  \]

- **Momentum**
  \[
  (1/2) \rho D |u|^2 /Dt = -\nabla.(p u) + p \nabla \cdot u
  \]

- **Compression**
  \[
  \rho D [e_T + |u|^2/2] /Dt = \nabla(\lambda \nabla T) - \nabla.(p u)
  \]

\[
\partial(\rho e_{\text{tot}})/\partial t = -\nabla \cdot J_{e_{\text{tot}}}
\]

\[
J_{e_{\text{tot}}} = J'_{e_{\text{tot}}} + \rho e_{\text{tot}} u
\]

\[
J'_{e_{\text{tot}}} = -\lambda \nabla T + p u
\]

Thermal balance of an inert and inviscid flow

\[
\delta e_T = c_v \delta T
\]

\[c_v \approx \text{cst.} \quad \text{(for simplicity, can be easily removed)}\]

\[
\rho c_v D T /Dt = \nabla(\lambda \nabla T) - p \nabla \cdot u
\]

continuity \quad \Rightarrow \quad -p \nabla \cdot u = \frac{p}{\rho D t} \rho = \frac{D}{D t} p - \frac{D}{D t} [(c_p - c_v) T]

ideal gas law \quad p = (c_p - c_v) \rho T.

\[
\rho c_p D T /Dt = D p /dt + \nabla(\lambda \nabla T)
\]

10
Reactive flows

elementary reaction

\[ \vartheta_1^+ A_1 + \ldots + \vartheta_n^+ A_n \Rightarrow \vartheta_1^- A_1 + \ldots + \vartheta_n^- A_n + Q. \]

reaction rate \( nb/(\text{volume } \times \text{time}) \)

\[ \dot{W}^{(j)} \equiv (J_+^{(j)} - J_-^{(j)}) \]

and \( \vartheta_i^{(j)} \equiv (\vartheta_i^-^{(j)} - \vartheta_i^+^{(j)}) \), stoichiometric coefficient

conservation equation for the species

\[ \rho \frac{\text{DY}_i}{\text{Dt}} = -\nabla \cdot \mathbf{J}'_i + \sum_j \vartheta_i^{(j)} m_i \dot{W}^{(j)}, \]

\[ \mathbf{J}'_i = -\rho D_i \nabla Y_i \]

\[ \rho \frac{\text{DY}_i}{\text{Dt}} = \nabla (\rho D_i \nabla Y_i) + \sum_j \vartheta_i^{(j)} m_i \dot{W}^{(j)}(T, p, \ldots Y_k \ldots) \]

sum over the reactions

equation for the chemical energy

\[ e_{\text{chem}} \equiv \sum_i h_i Y_i \]

\[ Q^{(j)} = \sum_{i=1}^{n} (\vartheta_i^{(j)+} - \vartheta_i^{(j)-}) m_i h_i(T_o), \]

enthalpy of formation per unit of mass of species \( i \)

\[ \rho \frac{\text{De}_{\text{chem}}}{\text{Dt}} = -\sum_i \nabla \cdot (h_i \mathbf{J}'_i) - \sum_j Q^{(j)} \dot{W}^{(j)} \]
\[ P.\text{Clavin II} \]
\[ e_{\text{chem}} \equiv \sum_{i} h_i Y_i \]
\[ \rho D e_{\text{chem}} / Dt = - \sum_{i} h_i \nabla J'_i - \sum_{j} Q^{(j)} \dot{W}^{(j)} \quad J'_i = -\rho D_i \nabla Y_i \]

heat released by the \( j^{th} \) reaction
rate of the \( j^{th} \) reaction
(number per unit time and unit volume)

1st law without internal viscous dissipation

\[ e_{\text{int}} = e_T + e_{\text{chem}} \quad \rho D e_{\text{int}} / Dt = -\nabla J'_q - p \nabla u \]
work done by volume change

\[-\nabla J'_q = \nabla(\lambda \nabla T) - \sum_{i} h_i \nabla J'_i \]
diffusive flux of internal energy

\[ \rho D (e_T + e_{\text{chem}}) / Dt = \nabla(\lambda \nabla T) - \sum_{i} h_i \nabla J'_i - p \nabla u \]

Thermal balance of inviscid flow of reactive gas

\[ \delta e_T = c_v \delta T \quad c_v \approx \text{cst.} \quad \text{(for simplicity, can be easily removed)} \]

\[ \rho D (e_T + e_{\text{chem}}) / Dt = \rho c_v D T / Dt - \sum_{i} h_i \nabla J'_i - \sum_{j} Q^{(j)} \dot{W}^{(j)} \]

\[ \rho c_v D T / Dt - \sum_{i} h_i \nabla J'_i - \sum_{j} Q^{(j)} \dot{W}^{(j)} = \nabla(\lambda \nabla T) - \sum_{i} h_i \nabla J'_i - p \nabla u \]

continuity \[ \Rightarrow -p \nabla u = \rho \frac{D}{Dt} \rho = \frac{D}{Dt} p - \rho \frac{D}{Dt} [(c_p - c_v) T] \quad \Leftarrow \rho / p = (c_p - c_v) T \]

\[ \rho c_p D T / Dt = D p / Dt + \nabla(\lambda \nabla T) + \sum_{j} Q^{(j)} \dot{W}^{(j)} \]

compression conduction chemistry
Governing equations for inviscid flows of reactive gas

\[ \frac{1}{\rho} \frac{D\rho}{Dt} = -\nabla \cdot \mathbf{u}, \quad \rho \frac{Du}{Dt} = -\nabla p, \quad p = (c_p - c_v) \rho T, \]

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

\[ \rho \frac{DY_i}{Dt} = \nabla \cdot (\rho D_i \nabla Y_i) + \sum_j \varphi_i^{(j)} m_i \dot{W}^{(j)}. \]

Conservative form of the energy equation (inviscid approximation)

\[ e_{tot} \equiv e_{int} + |\mathbf{u}|^2/2, \quad e_{int} = e_T + e_{chem} \]

\[ \rho D(e_T + e_{chem})/Dt = \nabla \cdot (\lambda \nabla T) - \sum_i h_i \nabla \cdot J'_i - p \nabla \cdot \mathbf{u} \]

\[ (1/2) \rho D |\mathbf{u}|^2 / Dt = -\nabla (p \mathbf{u}) + p \nabla \cdot \mathbf{u} \]

\[ \rho D e_{tot} / Dt = -\nabla \left[ J_q + \sum_i h_i J'_i + p \mathbf{u} \right] J_q = -\lambda \nabla T \]

\[ \prod (\rho e_{tot}) / \partial t = -\nabla \left[ \rho \mathbf{u} e_{tot} + p \mathbf{u} + J_q + \sum_i h_i J'_i \right] = -\nabla \left[ \rho \mathbf{u} (e_{tot} + p/\rho) + J_q + \sum_i h_i J'_i \right] \]

Heat released per unit mass

\[ e_{tot} + p/\rho = c_p T + |\mathbf{u}|^2/2 - q_m \psi \]
Viscous flow:

shear viscosity
\[
\Pi = p \Pi + \pi
\]
bulk viscosity
\[
\pi \equiv -2\eta(\nabla \mathbf{u})^{(s)} - \mathbf{I}(\xi - 2\eta/3) \nabla \cdot \mathbf{u}
\]

\[
\partial(\rho e_{tot})/\partial t = -\nabla \cdot [\rho \mathbf{u} (c_p T + |\mathbf{u}|^2/2 - q_m \psi) + \mathbf{J}_q + \mathbf{u} \cdot \pi]
\]

Ideal gas:
\[
p = (c_p - c_v) \rho T
\]

Compressible reacting flow in planar geometry (conservative form)
\[
\frac{\partial \rho}{\partial t} = - \frac{\partial (\rho u)}{\partial x}
\]
\[
\frac{\partial (\rho u)}{\partial t} = - \frac{\partial}{\partial x} \left( p + \rho u^2 - \mu \frac{\partial u}{\partial x} \right)
\]
\[
\frac{\partial(\rho e_{tot})}{\partial t} = - \frac{\partial}{\partial x} \left[ \rho u (c_p T + u^2/2 - q_m \psi) - \lambda \frac{\partial T}{\partial x} - \mu u \frac{\partial u}{\partial x} \right]
\]

Jumps across a planar wave between 2 uniform flows \(\psi_b = 1, \psi_o = 0\)
(inner structure in steady state !!)

\[
[\rho u]_{\pm}^+ = 0 \quad [c_p T + u^2/2 - q_m \psi]_{\pm}^+ = 0 \quad [p + \rho u^2]_{\pm}^+ = 0
\]

\[
\mathbf{u} = (\rho_o/\rho) \mathcal{D} \quad T/T_o = (p/p_o)(\rho_o/\rho)
\]

Propagation velocity
\[
\left( \frac{p}{p_o}, \frac{\rho_o}{\rho} \right) = \left( \frac{p}{p_o} - 1 \right) = -\rho_o \mathcal{D} \left( \frac{\rho_o}{\rho} - 1 \right)
\]

Rankine (1870) Hugoniot (1889)
\(q_m = 0\)

Michelson (1893) Rayleigh (1910)
\(q_m > 0\)
Compressible and viscous flow in planar geometry

**Conservative form**

**Mass**  
\[
\frac{\partial \rho}{\partial t} = - \frac{\partial (\rho u)}{\partial x}
\]

**Momentum**  
\[
\frac{\partial (\rho u)}{\partial t} = - \frac{\partial}{\partial x} \left( p + \frac{\rho u^2}{2} - \mu \frac{\partial u}{\partial x} \right)
\]

**Energy**  
\[
\frac{\partial (\rho e_{tot})}{\partial t} = - \frac{\partial}{\partial x} \left[ \rho u (c_p T + \frac{u^2}{2} - q_m \psi) - \lambda \frac{\partial T}{\partial x} - \mu u \frac{\partial u}{\partial x} \right]
\]

**Lagrangian Form**

**Mass**  
\[
\frac{1}{\rho} \frac{D \rho}{D t} = - \frac{\partial u}{\partial x}
\]

**Momentum**  
\[
\rho \frac{D u}{D t} = - \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left[ \mu \frac{\partial u}{\partial x} \right]
\]

Inert flow:  
\[e_{tot} = c_v T + \frac{u^2}{2}\]

Energy: extended 1st law  
\[
\frac{D (c_v T)}{Dt} = -p \frac{D (1/\rho)}{D t} + \frac{1}{\rho} \frac{\partial}{\partial x} \left[ \lambda \frac{\partial T}{\partial x} \right] + \mu \frac{\lambda}{\rho} \left( \frac{\partial u}{\partial x} \right)^2
\]

- heating by compression
- heat flux
- internal viscous dissipation
2.6. Entropy production

entropy is a function of state that is not a conserved quantity
\[ \partial (\rho s) / \partial t = - \nabla \cdot \mathbf{J}_s + \dot{w}_s, \]

2\textsuperscript{nd} law of thermodynamics  
dissipative effects \( \Rightarrow \dot{w}_s \geq 0 \)

\[ T \delta s = \delta e_T + \rho \delta v - \sum_i \mu_i \delta Y_i \]

\[ T \frac{Ds}{Dt} = \frac{De_T}{Dt} + p \frac{D(1/\rho)}{Dt} - \sum_i \mu_i \frac{DY_i}{Dt} \]

inert mixture:
\[ \dot{w}_s = \mathbf{J}_q \cdot \nabla \left( \frac{1}{T} \right) - \sum_i \mathbf{J}_i' \cdot \nabla \left( \frac{\mu_i}{T} \right) - \frac{1}{T} \pi : (\nabla \mathbf{u})^{(s)} \]

simple fluid:  
(inert flow)
\[ \mathbf{J}_s = \rho u_s - \frac{\lambda}{T} \frac{\partial T}{\partial x}, \]

\[ \rho \frac{Ds}{Dt} = \frac{\partial}{\partial x} \left( \frac{\lambda}{T} \frac{\partial T}{\partial x} \right) + \dot{w}_s \]

\[ \rho T \frac{Ds}{Dt} = \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) + \mu \left( \frac{\partial u}{\partial x} \right)^2 \]

ideal gas
\[ \frac{(s - s_o)}{c_v} = \ln \left( \frac{p/\rho^\gamma}{p_o/\rho_o^\gamma} \right) \]

\[ T_D s \frac{Ds}{Dt} = T_D s \frac{De_T}{Dt} + \rho \frac{D(1/\rho)}{Dt} - \sum_i \mu_i \frac{DY_i}{Dt} \]

\[ \mu > 0, \quad \lambda > 0 \]
Dynamics of Combustion Waves in Premixed Gases

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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*
3-1. Quasi-isobaric approximation (Low Mach number)

order of magnitude

\[ \rho (\mathbf{u} \cdot \nabla) \mathbf{u} \approx -\nabla p \quad \Rightarrow \quad \delta p \approx \rho u \delta u \]
\[ p \approx \rho a^2 \quad \Rightarrow \quad \delta p/p \approx u^2/a^2 \equiv M^2 \quad \Leftrightarrow \delta u \approx u \]

slow evolution

\[ \frac{\partial}{\partial t} \approx \mathbf{u} \cdot \nabla \ll a|\nabla| \]

+ very subsonic flow

\[ M^2 \ll 1 \quad \Rightarrow \quad \delta p/p \ll \delta T/T = O(1) \]

\[ \frac{p}{\rho c_p T} = O(1) \]

\[ \left| \frac{1}{p} \frac{Dp}{Dt} \right| \ll \left| \frac{1}{T} \frac{DT}{Dt} \right| \quad \Rightarrow \quad \left| \frac{Dp}{Dt} \right| \ll \left| \rho c_p \frac{DT}{Dt} \right| \]

\[ \rho c_p DT/Dt = Dp/Dt + \nabla \cdot (\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)} \quad \text{quasi-isobaric flame structure} \]

(in open space)

\[ \rho T = \rho_0 T_0 \]
\[ \rho DY_i/Dt = \nabla \cdot (\rho D_i \nabla Y_i) + \sum_j \psi_i^{(j)} m_i \dot{W}^{(j)}(T, Y_k...) \]
1-D flame in a tube

one end is closed and the other open

Quasi-steady inner structure: Velocity of the front / Fresh mixture $U_L = \text{cst.}$

Propagation towards the closed end

- Burned gas: $u_b = U_b - U_L$
  - $u = 0$
  - $U = (T_b/T_u)U_L$

Reference frame of the lab
- Wall at rest

Propagation from the closed end

- Burned gas: $u = U_b - U_L$
  - $u = (T_b/T_u)U_L$

Reference frame of the lab
- Wall at rest

Conservation of mass: $\rho U = \text{cst.}$

Quasi-isobaric approximation: $\rho T \approx \text{cst.}$

$$\frac{\rho_u}{\rho_b} = \frac{T_b}{T_u} = \frac{U_b}{U_u} > 1$$
Problem set up of the steady inner structure of a planar flame

\[
\rho \frac{D}{Dt} = md/dx
\]

mass: \( \rho u = \text{constant} \)

mass flux across the flame

\[
m \equiv \rho_u U_L = \rho_b U_b, \quad \frac{U_b}{U_L} \approx \frac{T_b}{T_u}, \approx 4 - 8
\]

quasi-isobaric approximation: \( \rho T \approx \text{cst.} \)

energy:

\[
mc_p \frac{dT}{dx} - \frac{d}{dx} \left( \lambda \frac{dT}{dx} \right) = \sum_j Q^{(j)} \dot{W}^{(j)}(T, \ldots Y_i \ldots)
\]

species:

\[
m \frac{dY_i}{dx} - \frac{d}{dx} \left( \rho D_i \frac{dY_i}{dx} \right) = \sum_j \theta_i^{(j)} M_i \dot{W}^{(j)}(T, \ldots Y_i \ldots),
\]

closed system of equations for \( T \) and \( Y_i \)

boundary conditions:

\[
x = -\infty : \quad T = T_u, \quad Y_i = Y_{iu}, \quad \dot{W}^{(j)} = 0
\]

unburned gas

frozen state

\[
x = +\infty : \quad \frac{dT}{dx} = 0, \quad Y_i = Y_{ib}, \quad \dot{W}^{(j)} = 0
\]

burned gas

equilibrium state

axis oriented towards the burned gas

reference frame of the flame
3-2. One-step irreversible reaction

\[ R \rightarrow P + Q \]

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

Velocity and structure of the planar flame

(Reference frame of the flame) \( \rho u = \) constant

\[
m c_p \frac{dT}{dx} - \frac{d}{dx} \left( \lambda \frac{dT}{dx} \right) = \rho q_R \dot{W}
\]

\[
m \frac{dY}{dx} - \frac{d}{dx} \left( \rho D \frac{dY}{dx} \right) = -\rho \dot{W}
\]

\( x \to -\infty: \quad Y = Y_u, \quad T = T_u \quad \text{unburned} \)

\( m Y_u = \int_{-\infty}^{+\infty} \rho \dot{W} \, dx \)

\( x \to +\infty: \quad Y = 0, \quad \frac{\partial T}{\partial x} = 0 \quad \text{burned} \)

\[
c_p (T_b - T_u) = q_m \equiv q_R Y_u
\]

Arrhenius law

\[
\rho \dot{W} = \rho_b \frac{Y}{\tau_r(T)}
\]

\[
\frac{1}{\tau_r(T)} = \frac{1}{\tau_{rb}} e^{-\frac{E}{k_B T_b}} \beta (1 - \theta)
\]

\[
\beta = \frac{E}{k_B T_b} \left(1 - \frac{T_u}{T_b}\right)
\]

\[
\theta = \frac{T - T_u}{T_b - T_u} \in [0, 1]
\]
3-3. Unity Lewis number and large activation energy

\[ \text{Le} \equiv \frac{D_T}{D} \]

Reduced temperature and mass fraction

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

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

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

\[ \text{Le} = 1 \]

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

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

\[ \beta \gg 1 \]

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

\[ \frac{1}{\tau_{rb}} \equiv \frac{e^{-\frac{E}{k_B T_b}}}{\tau_{coll}} \]

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

(reaction rate is non negligible only when \( T \approx T_b \))
3.4. Zeldovich & Frank-Kamenetskii asymptotic analysis

\[ \beta \rightarrow \infty \]
\[ \beta \equiv \frac{E}{k_B T_b} \left( 1 - \frac{T_u}{T_b} \right) \]

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

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

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

\[ \frac{1}{\tau_{rb}} \equiv \frac{e^{-E/k_B T_b}}{\tau_{coll}} \]

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

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

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

Zeldovich 1938

- Zeldovich & Frank-Kamenetskii asymptotic analysis
- Reduced temperature graph
- Reduced reaction rate graph
- Preheat reaction zone
- Burnt gas
- Unburnt gas
- Reduced temperature axis
- Reduced reaction rate axis
- Reaction zone location
- Matching condition
Inner reaction layer

\[ \frac{m \, \delta \theta}{d_r} \approx \frac{\rho_b \, D_{Tb} / \tau_{rb}}{d_r \, d_L / \beta} \]

\[ \delta \theta = O(1/\beta) \quad \Rightarrow \quad m = \rho D_T / d_L \]

\[ d_r \ll d_L \]

\[ d_r \approx \sqrt{D_{Tb} \tau_{rb}} \]

\[ m \, \delta \theta / d_r - \rho D_T d^2 \theta / dx^2 = \frac{\rho_b}{\tau_{rb}} (1 - \theta)e^{-\beta(1-\theta)} \]

\[ - \frac{D_{Tb}}{2} \frac{d}{dx} \left( \frac{d \theta}{dx} \right)^2 \approx \frac{1}{\tau_{rb}} (1 - \theta)e^{-\beta(1-\theta)} \frac{d \theta}{dx} \]

\[ \Theta = \beta (1 - \theta) \quad \Rightarrow \quad \tau_{rb} \frac{D_{Tb}}{2} \left( \frac{d \theta}{dx} \right)^2 \approx \int_0^1 (1 - \theta)e^{-\beta(1-\theta)} d\theta = \frac{1}{\beta^2} \int_0^{\beta(1-\theta)} \Theta e^{-\Theta} d\Theta \]

Asymptotic solution \( \beta \rightarrow \infty \quad \int_0^\infty \Theta e^{-\Theta} d\Theta = 1 \)

upstream exit of the inner layer \( \beta (1 - \theta) \rightarrow \infty : \quad D_{Tb} d\theta / dx \rightarrow \sqrt{(2/\beta^2)D_{Tb} / \tau_{rb}} \)

downstream entrance of the external zone \( \theta \rightarrow 1 : \quad \rho_b D_{Tb} d\theta / dx|_{\theta=1} = m \)

matching \( \]

\[ m = \rho_b \sqrt{(2/\beta^2)D_{Tb} / \tau_{rb}}, \quad U_L = m / \rho_u, \quad d_r / d_L = O(1/\beta) \]

\[ U_L \approx \sqrt{D_{Tb} / \tau_{rb}} \quad \text{dimensional analysis} \]
SUMMARY

Flame=quasi-isobaric reaction-diffusion wave. The flame velocity is highly sensitive to temperature.

ZFK result for a one-step first order reaction in the limit \( \beta \equiv \frac{E}{k_B T_b} \left(1 - \frac{T_u}{T_b}\right) \gg 1 \)

\[
U_b = \sqrt{\frac{2 D_{Tb}}{\beta^2 \tau_{rb}}} \quad \quad \quad \frac{1}{\tau_{rb}} \equiv \frac{e^{-E/k_B T_b}}{\tau_{coll}}
\]

\[
D_{Tb} \approx a_b^2 \tau_{coll} \quad \quad \quad \frac{U_b}{a_b} = \frac{1}{\beta} \sqrt{2 e^{-E/k_B T_b}} \ll 1
\]

\[
\frac{E}{k_B T_b} \gg 1: \text{ markedly subsonic } \quad \quad \text{high thermal sensitivity } \frac{\delta U_b}{U_b} \approx \frac{\beta \delta T_b}{2 T_b}, \quad \beta \gg 1
\]

Laminar flame velocity/unburned gas \( U_L = (T_u/T_b) U_b \in [15 \text{ cm/s} - 9 \text{ m/s}] \)

Transit time \( \tau_L = (d_L/U_L) \in [10^{-4} \text{s} - 10^{-3} \text{s}] \)
non-dimensional form
\[ \frac{\partial \theta}{\partial t} - \frac{\partial^2 \theta}{\partial x^2} = w(\theta) \quad \theta \geq 0 \quad \theta \in [0, 1] \]

propagation of steady state \( \theta = 1 \) into steady state \( \theta = 0 \)

steady state: \( \omega = 0 \)

stability of steady states

stability of steady states

(\text{equilibrium state}) \quad \theta = 1, \quad w = 0 \quad \text{stable steady state}

two different cases depending on the property of the initial state \( \theta = 0 \)

initial state:

(I) \quad \theta = 0, \quad w = 0 \quad \text{metastable steady state (less stable)}

(II) \quad \theta = 0, \quad w = 0 \quad \text{unstable steady state (out of equilibrium)}

\[ \frac{d\Phi}{d\theta} = -w(\theta) \]
propagating planar wave at constant velocity

\[ \frac{\partial \theta}{\partial t} - \frac{\partial^2 \theta}{\partial x^2} = w(\theta) \]  traveling wave solution (from right to left)

\[ \theta \in [0, 1] \]

\[ \xi = x + \mu t \]

\[ \partial / \partial t = \mu \frac{d}{d\xi} \]

\[ \partial / \partial x = d / d\xi \]

\[ \mu \text{ is an eigenvalue of the problem} \]

\( \xi = -\infty : \theta = 0, \ w = 0 \)

initial state

\( \xi = +\infty : \theta = 1, \ w = 0 \)

final (equilibrium) state

\[ \mu \text{ unknown, number of solutions?} \]

ZFK flame model: \( \omega > 0 \), case (II)
P. Clavin III

Number of solutions? phase space, phase portrait

\[ \theta \geq 0 \]

\[ X \equiv \theta, \quad Y \equiv \mu d\theta/d\xi \]

\[ \frac{dX}{d\xi} = \frac{Y}{\mu} \quad \frac{dY}{d\xi} = \mu [Y - \omega(X)] \]

\[ \mu \frac{dX}{d\xi} - \frac{d^2 X}{d\xi^2} = \omega(X) \quad \mu \]

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

second order system

Linearisation about \( X = 0, Y = 0 \)

One solution

Two eigenvalues \( r_+ \) and \( r_-\) and two eigenvectors \( k_+ \) and \( k_- \)

\[ \begin{align*}
\delta X &= A_+ e^{r_+ \xi} + A_- e^{r_- \xi}, \\
\delta Y &= k_+ A_+ e^{r_+ \xi} + k_- A_- e^{r_- \xi}
\end{align*} \]

\[ \begin{align*}
\mu \frac{d\delta X}{d\xi} - \frac{d^2 \delta X}{d\xi^2} &= \omega' \delta X \\
\mu r - r^2 - \omega' &= 0 \\
2r_\pm &= \mu \pm \sqrt{\mu^2 - 4\omega'} \\
k_\pm &= \mu r_\pm
\end{align*} \]

Case (I)

\[ \begin{align*}
& r_- < 0, \ r_+ > 0 \\
& \text{One solution}
\end{align*} \]

Case (II)

Infinite numbers of solutions

One particular solution

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

wave velocity

continuous spectrum with a lower bound

$$2r_{\pm} = \mu \pm \sqrt{\mu^2 - 4\omega_0'}$$

$$\mu_{\text{mini}} \equiv 2\sqrt{\frac{d}{d\theta}|_{\theta=0}}$$

lower bound: \( r_+ = r_- = \mu/2 \) \( k_+ = k_- \)

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

the lower bound solution is selected \( \mu_{\text{mini}} \equiv 2\sqrt{\frac{d}{d\theta}|_{\theta=0}} \)

\[ \frac{\partial \theta}{\partial t} - \frac{\partial^2 \theta}{\partial \xi^2} = \omega'_0 \theta, \text{ where } \omega'_0 \equiv \frac{\partial w}{\partial \theta}|_{\theta=0} > 0 \]

\[ \theta(\xi, t) \equiv Z(\xi, t)e^{+\omega'_0 t} \quad \frac{\partial Z}{\partial t} - \frac{\partial^2 Z}{\partial \xi^2} = 0 \]

\[ Z = e^{-\xi^2/4t}/\sqrt{t} \quad \theta \propto \exp[-\xi^2/4t + \omega'_0 t - \ln(t)/2] \]

\[ \xi^2 \approx 4\omega'_0 t^2 \]  

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 \( w(\theta, \beta) = (\beta^2/2)\theta(1-\theta)e^{-\beta(1-\theta)}, \beta \gg 1 \)
Dynamics of Combustion Waves in Premixed Gases

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Lecture IV
Hydrodynamic instability of flames
Lecture 4: *Hydrodynamic instability of flames*

4-1. Jump across an hydrodynamic discontinuity
4-2. Linearized Euler equations of an incompressible fluid
4-3. Conditions at the front
4-4. Dynamics of passive interfaces
4-5. Darrieus-Landau instability
4-6. Curvature effect: a simplified approach
IV - 1) Jump across an hydrodynamic discontinuity

flame considered as a discontinuity
flame thickness and curvature neglected

\( \Lambda \gg d_L \)

flame \( \approx \) surface of zero thickness separating two incompressible flows

Low Mach nb approx + inviscid approx: Euler eqs

\[
\begin{align*}
\frac{\partial \rho}{\partial t} &= -\nabla \cdot (\rho \mathbf{u}) \\
\rho \frac{D \mathbf{u}}{Dt} &= -\nabla p \quad \Leftrightarrow \quad \partial(\rho \mathbf{u})/\partial t = -\nabla \cdot (p \mathbf{i} + \rho \mathbf{uu}) \\
\end{align*}
\]

tilted planar front

reference frame of the flame \( \mathbf{r} = (x, z), \quad \mathbf{u} = (u, w) \)

\[
\begin{align*}
\frac{\partial \rho}{\partial t} &= -\frac{\partial (\rho u)}{\partial x} - \frac{\partial (\rho w)}{\partial z}, \\
\frac{\partial (\rho u)}{\partial t} &= -\frac{\partial (p + \rho u^2)}{\partial x} - \frac{\partial (\rho uw)}{\partial z}, \\
\frac{\partial (\rho w)}{\partial t} &= -\frac{\partial (\rho uw)}{\partial x} - \frac{\partial (p + \rho w^2)}{\partial z}
\end{align*}
\]

jumps in the normal direction (reference frame of the flame)

\[
\begin{align*}
[\rho u]^+_L &= 0 \\
[p + \rho u^2]^+_L &= 0 \\
\rho u \neq 0 \quad \Rightarrow \quad [w]^+_L &= 0
\end{align*}
\]

\[ \lim_{d_L \to 0} \int_{d_L} a(x, y, t) \, dx = 0 \]

if \( a(r, t) \) is regular

\[ \lim_{d_L \to 0} \int_{d_L} \frac{\partial a}{\partial x} \, dx = [a]_L^+ \]
$\rho_u > \rho_b$

reference frame of the flame front

\[
\frac{U_b}{U_L} = \frac{\rho_u}{\rho_b} = \frac{T_b}{T_u}
\]

conservation of mass + isobaric approx

"instantaneous" modification of the flow field, both upstream and downstream

(low Mach nb approx: the speed of sound is infinite, $a \approx \infty$)

Piston effect

$tilded front$

deviation of the stream lines

instability mechanism

\[
\Lambda \gg d_L, \quad d_L/\Lambda \rightarrow 0
\]
equation of the perturbed front \[ x = \alpha(y, t) \]
flow velocity at the front \[ \mathbf{u}_f = (u_f, w_f) \]

\[ \mathbf{n}_f = \left( \frac{1}{\sqrt{1 + \alpha_y'^2}}, -\frac{\alpha_y'}{\sqrt{1 + \alpha_y'^2}} \right), \quad \mathbf{u}_n \equiv \mathbf{u}_f \cdot \mathbf{n}_f = \frac{(u_f - \alpha_y' w_f)}{\sqrt{1 + \alpha_y'^2}} \]

\[ w_{tg} = \frac{(w_f + \alpha_y' u_f)}{\sqrt{1 + \alpha_y'^2}} \]

normal velocity of the front \[ \tilde{D}_f = \frac{\dot{\alpha}_t}{\sqrt{1 + \alpha_y'^2}} \]

flow velocity relative to the perturbed front

\[ \mathbf{U}_n \equiv \mathbf{u}_n - \tilde{D}_f = \frac{(u_f - \dot{\alpha}_t - \alpha_y' w_f)}{\sqrt{1 + \alpha_y'^2}} \]

normal component

\[ W_{tg} = w_{tg} \]
tangential component

conservation of mass

\[ \bar{\rho}^- U_n^- = \bar{\rho}^+ U_n^+ \]

\[ \bar{\rho}^- \left( u_f^+ - \dot{\alpha}_t - \alpha_y^' w_f^+ \right) = \bar{\rho}^+ \left( u_f^- - \dot{\alpha}_t - \alpha_y^' w_f^- \right) \]

conservation of momentum

\[ [p + \bar{\rho} U_n^2]^-_+ = 0 \quad [W_{tg}]^+_- = 0 \]

\[ p_f^- + \bar{\rho}^- \left( u_f^- - \dot{\alpha}_t - \alpha_y^' w_f^- \right)^2 \frac{1}{1 + \alpha_y^2} = p_f^+ + \bar{\rho}^+ \left( u_f^+ - \dot{\alpha}_t - \alpha_y^' w_f^+ \right)^2 \frac{1}{1 + \alpha_y^2} \]

\[ (w_f^- + \alpha_y^' u_f^-) = (w_f^+ + \alpha_y^' u_f^+) \]
Lecture 4: Hydrodynamic instability of flames

4-1. Jump across an hydrodynamic discontinuity
4-2. Linearized Euler equations of an incompressible fluid
4-3. Conditions at the front
4-4. Dynamics of passive interfaces
4-5. Darrieus-Landau instability
4-6. Curvature effect: a simplified approach
Linearized Euler equations of an incompressible fluid

\[ \frac{\partial}{\partial x} \delta u^\pm + \frac{\partial}{\partial y} \delta w^\pm = 0, \]
\[ \left( \bar{\rho}^\pm \frac{\partial}{\partial t} + \bar{m}_f^\pm \frac{\partial}{\partial x} \right) \delta u^\pm = -\frac{\partial}{\partial x} \delta \pi^\pm, \]
\[ \left( \bar{\rho}^\pm \frac{\partial}{\partial t} + \bar{m}_f^\pm \frac{\partial}{\partial x} \right) \delta w^\pm = -\frac{\partial}{\partial y} \delta \pi^\pm, \]

\( x \to +\infty : \) disturbances remain finite,
\( x \to -\infty : \) no disturbances, \( \delta u^- = 0 \)

Laplace equation for the pressure

\[ \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \delta \pi^\pm = 0 \]

Fourier decomposition of the flame surface \( x = \alpha(y, t) \)

\[ \alpha(y, t) = \tilde{\alpha}(t) e^{i k \cdot y} \]

wave vector \( k = (2\pi/\Lambda) n_k \)

\( k = |k| = 2\pi/\Lambda \)

wave length

\[ \delta a(x, y, t) = \tilde{\alpha}(x, t) e^{ik \cdot y} \]

\[ \alpha(y, t) = \tilde{\alpha}(t) e^{ik \cdot y} \]
\[
\pi^\pm \equiv p^\pm - \bar{\rho}^\pm g(t)x,
\]

\[
\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \delta \pi^\pm = 0
\]

\( x \to +\infty \) : disturbances remain finite,

\( x \to -\infty \) : no disturbances, \( \delta u^- = 0 \)

\[
\alpha(y, t) = \tilde{\alpha}(t) e^{i k.y}
\]

wave vector \( k = (2\pi/\Lambda)n_k \), \( k = |k| = 2\pi/\Lambda \) given!

\[
\delta \pi^\pm(x, y, t) = \tilde{\pi}^\pm(x, t) e^{i k.y}
\]

pressure

\[
\frac{\partial^2 \tilde{\pi}^\pm}{\partial x^2} - |k|^2 \tilde{\pi}^\pm = 0
\]

flow velocity

\[
\delta u^\pm(x, y, t) = \tilde{u}^\pm(x, t) e^{i k.y}
\]

\[
\delta w^\pm(x, y, t) = \tilde{w}^\pm(x, t) e^{i k.y}
\]

\[
\frac{\partial \tilde{u}^\pm}{\partial x} + i k \tilde{w}^\pm = 0
\]

\[
\bar{\rho}^\pm \left( \frac{\partial}{\partial t} + \tilde{u}^\pm \frac{\partial}{\partial x} \right) \tilde{u}^\pm(x, t) = \pm |k| \tilde{\pi}^\pm(t) e^{\mp |k|x}
\]
\[
\tilde{\pi}^\pm (x, t) = \tilde{\pi}^\pm (t) e^{\mp |k|x}
\]

\[
\frac{\partial \tilde{u}^\pm}{\partial x} + i k \tilde{w}^\pm = 0 \quad \quad \rho^\pm \left( \frac{\partial}{\partial t} + \tilde{u}^\pm \frac{\partial}{\partial x} \right) \tilde{u}^\pm (x, t) = \pm |k| \tilde{\pi}^\pm (t) e^{\mp |k|x}
\]

general solution to the homogeneous equation + particular solution of the full equation

\[
\tilde{u}^\pm (x, t) = \tilde{u}^\pm_R (x, t) + \tilde{u}^\pm_P (x, t)
\]

general solution to the homogeneous equation

\[
\frac{\partial \tilde{u}^\pm_R}{\partial t} + \tilde{u}^\pm \frac{\partial \tilde{u}^\pm_R}{\partial x} = 0, \quad \tilde{u}^\pm_R = \tilde{u}^\pm_r (t - x/\tilde{u}^\pm),
\]

\[
\tilde{u}^-_R = 0, \quad \tilde{u}^+_R = \tilde{u}^+_r (t - x/\tilde{u}^\pm)
\]

vorticity of the burnt gas flow

\[
u^- (x, t) = u^-_P (x, t)
\]

potential flow in unburned gas

particular solution

look for a particular solution of the form

\[
\tilde{u}^\pm_P (x, t) = \tilde{u}^\pm_p (t) e^{\mp kx}, \quad \Rightarrow \quad \rho^\pm \left( \frac{d}{dt} \mp \tilde{u}^\pm k \right) \tilde{u}^\pm_p (t) = \pm k \tilde{\pi}^\pm (t)
\]

\[
x \to -\infty : \tilde{u}^- = 0; \quad \tilde{u}^- (x, t) = \tilde{u}^-_f (t) e^{kx}
\]

3 unknown functions: \[
\tilde{u}^-_f (t), \tilde{u}^+_p (t), \tilde{u}^+_r (t) \quad \tilde{u}^-_f (t) \equiv \tilde{u}^-_p (t)
\]

corresponding to the flow at the front \( x = 0 \)
Linear solution of the Euler equations

3 unknown functions: $\tilde{u}_f^-(t)$, $\tilde{u}_p^+(t)$, $\tilde{u}_r^+(t)$

flow on the front

$x < 0$:

Unburned gas flow

\[
\begin{align*}
\tilde{u}^-(x, t) &= \tilde{u}_f^-(t)e^{+kx}, \\
k\tilde{\pi}^-(x, t) &= -\rho^-(\frac{d}{dt} + \bar{u}^- k)\tilde{u}_f^-(t)e^{+kx},
\end{align*}
\]

$x > 0$:

Burned gas flow

\[
\begin{align*}
\tilde{u}^+(x, t) &= \tilde{u}_p^+(t)e^{-kx} + \tilde{u}_r^+(t - x/\bar{u}^+), \\
k\tilde{\pi}^+(x, t) &= \rho^+(\frac{d}{dt} - \bar{u}^+ k)\tilde{u}_p^+(t)e^{-kx},
\end{align*}
\]

Boundary conditions on the front

4 boundary conditions at the flame front involving the additional unknown $\tilde{\alpha}(t)$

2 for the conservation of mass (inner flame structure not modified)

\[
\delta m_f^- = \delta m_f^+ = 0 \\
\delta m_p^+ = 0
\]

$m \equiv \rho(u - \partial \alpha/\partial t)$

2 for the conservation of normal and tangential momentum
Lecture 4: **Hydrodynamic instability of flames**

4-1. Jump across an hydrodynamic discontinuity
4-2. Linearized Euler equations of an incompressible fluid

4-3. **Conditions at the front**

4-4. Dynamics of passive interfaces
4-5. Darrieus-Landau instability
4-6. Curvature effect: a simplified approach
IV-3) Conditions at the front

Mass  \( \tilde{\rho}^- (u_f^- - \dot{\alpha}_t - \alpha'_f w_f^-) = \tilde{\rho}^+ (u_f^+ - \dot{\alpha}_t - \alpha'_f w_f^+) = 0 \)

\[
\begin{align*}
\tilde{\rho}^- (\delta u^-_f - \dot{\alpha}_t) &= \tilde{\rho}^+ (\delta u^+_f - \dot{\alpha}_t) \\
\Rightarrow \quad \delta u^-_f &= \delta u^+_f = \dot{\alpha}_t 
\end{align*}
\]

Tangential momentum

\[
\frac{\partial}{\partial y} (w^-_f + \alpha'_y u^-) = \frac{\partial}{\partial y} (w^+_f + \alpha'_y u^+) \\
\Rightarrow \quad k \tilde{u}^+_p (t) + \frac{1}{u^+} \frac{d\tilde{u}^+_r(t)}{dt} + k\tilde{u}^-_f (t) = m_f \left( \frac{1}{\rho^+} - \frac{1}{\rho^-} \right) k^2 \ddot{\alpha}(t)
\]

\[
\begin{align*}
&\frac{1}{u^+} \frac{d\tilde{u}^+_r}{dt} = - \frac{d\tilde{u}^+_p}{dt} + \frac{d^2 \ddot{\alpha}}{dt^2} \\
\end{align*}
\]

Normal momentum

\[
\dot{\delta}p^-_f + 2\tilde{\rho}^- u^-_f (\delta u^-_f - \dot{\alpha}_t) = \delta p^+_f + 2\tilde{\rho}^+ u^+_f (\delta u^+_f - \dot{\alpha}_t) \\
\begin{align*}
&\begin{cases}
\tilde{u}^- (x, t) = \tilde{u}^- (t)e^{ikx}, \\
k\tilde{u}^- (x, t) = -\tilde{\rho}^- \left( \frac{d\tilde{u}^-}{dt} + u^-k \right) \tilde{u}^- (t)e^{ikx}, \\
\tilde{u}^+ (x, t) = \tilde{u}^+_p (t)e^{-kx} + \tilde{u}^+_r (t-x/u^+), \\
k\tilde{u}^+ (x, t) = \tilde{\rho}^+ \left( \frac{d\tilde{u}^+_p}{dt} - u^+k \right) \tilde{u}^+_p (t)e^{-kx},
\end{cases}
\end{align*}
\]

\[
\begin{align*}
&\begin{cases}
x < 0: \\
x > 0: 
\end{cases}
\end{align*}
\]

Linear dynamical Equation for the front

\[
\tilde{u}^-_f = \frac{d\ddot{\alpha}}{dt} \\
\Rightarrow \quad (\tilde{\rho}^- + \tilde{\rho}^+) \frac{d^2 \ddot{\alpha}}{dt^2} + 2m_f k \frac{d\ddot{\alpha}}{dt} - [\tilde{\rho}^- - \tilde{\rho}^+]g(t)k + (\tilde{u}^+ - \tilde{u}^-)m_f k^2] \ddot{\alpha} = 0
\]

\[
\begin{align*}
&\begin{cases}
\delta a(x, y, t) = \ddot{\alpha}(t)e^{ik\cdot y} \\
\alpha(y, t) = \ddot{\alpha}(t)e^{ik\cdot y}
\end{cases}
\end{align*}
\]
SUMMARY

Equation for the Fourier components of the front

Fourier decomposition of the flame surface $x = \alpha(y, t)$

$$\alpha(y, t) = \tilde{\alpha}(t) e^{i k \cdot y}$$

wave vector $k = (2\pi/\Lambda) n_k$

$$k = |k| = 2\pi/\Lambda$$

wave length

$$\left( \bar{\rho}^- + \bar{\rho}^+ \right) \frac{d^2 \tilde{\alpha}}{dt^2} + 2m_f k \frac{d\tilde{\alpha}}{dt} - \left[ (\bar{\rho}^- - \bar{\rho}^+) g(t) k + (\bar{u}^+ - \bar{u}^-) m_f k^2 \right] \tilde{\alpha} = 0$$

$$\bar{m}_f = \bar{\rho}_- U_L$$
Lecture 4: **Hydrodynamic instability of flames**

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Dynamics of a passive interface \( \bar{m}_f = 0 \)

\[
(\bar{\rho}^- + \bar{\rho}^+) \frac{d^2 \tilde{\alpha}}{dt^2} + 2 \bar{m}_f k \frac{d\tilde{\alpha}}{dt} - k [ (\bar{\rho}^- - \bar{\rho}^+) g(t) + (\bar{\rho}^+ - \bar{\rho}^-) \bar{m}_f k ] \tilde{\alpha} = 0
\]

Normal mode analysis \( \tilde{\alpha}(t) = \hat{\alpha} e^{\sigma t} \)

\[
\alpha(y, t) = \tilde{\alpha}(t) e^{ik\cdot y}
\]

\[\text{Rayleigh-Taylor instability} \]

\[
g = \text{cst.} \quad (\bar{\rho}^- - \bar{\rho}^+) g > 0
\]

\[\text{Rayleigh-Taylor bubble (upwards propagation)}\]

\[g > 0, \quad A_t \equiv \frac{\rho_- - \rho_+}{\rho_- + \rho_+} > 0 \quad \sigma = \sqrt{A_t g k} \quad U_{\text{bubble}} = 0.361 \sqrt{2gR} \]

\[\text{Gravity waves} \]

\[
g = \text{cst.} \quad (\bar{\rho}^- - \bar{\rho}^+) g < 0
\]

\[\tilde{\alpha}(t) = \hat{\alpha} e^{i\varpi t} \quad \varpi = B \sqrt{gk} \quad B \equiv \sqrt{\frac{(\rho_+ - \rho_-)}{(\rho_+ + \rho_-)}}
\]

\[\text{Faraday (parametric) instability. Mathieu's equation} \]

\[
g(t) \text{ oscillating} \quad \frac{d^2 \tilde{\alpha}}{dt^2} + \varpi_o^2 [ 1 + \epsilon \cos(\varpi \tau) ] \tilde{\alpha} = 0
\]

\[\varpi \equiv \text{Im} \sigma \neq 0 \]

\[\text{Nonlinear analysis} \]
Lecture 4: **Hydrodynamic instability of flames**

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IV-5) Darrieus-Landau instability of flames

\[ g = 0 \quad \bar{m}_f = \bar{\rho} - \bar{u} = \bar{\rho}^+ \bar{u}^+ \]

\[ (\bar{\rho}^- + \bar{\rho}^+) \frac{d^2 \tilde{\alpha}}{dt^2} + 2\bar{m}_f k \frac{d\tilde{\alpha}}{dt} - (\bar{u}^+ - \bar{u}^-)\bar{m}_f k^2 \tilde{\alpha} = 0 \]

\[ \tilde{\alpha}(t) = \hat{\alpha} e^{\sigma t} \]

\[ \sigma = A U_L k, \quad A > 0 \]

\[ \bar{u}_- \equiv U_L \]

\[ \frac{\sigma}{U_L k} = \frac{1}{1 + v_b^{-1}} \left[ -1 \pm \sqrt{1 + v_b - v_b^{-1}} \right] \]

\[ d_L / \Lambda \to 0: \text{no length scale in the problem; dimensional analysis } \Rightarrow \sigma \propto U_L k \]

\[ \rho_u \gg \rho_b: \sigma = \sqrt{U_b U_L k} \quad (\rho_u - \rho_b) / \rho_u \ll 1: \sigma = (U_b - U_L)k / 2 \]

\[ k = 2\pi / \Lambda \quad \text{shorter is the wavelength stronger is the instability !?} \]

however the analysis is valid only in the limit \( d_L / \Lambda \to 0 \)

\[ \frac{\partial \alpha}{\partial t} = B D_T \frac{\partial^2 \alpha}{\partial y^2}. \quad \sigma_{\text{diff}} \equiv 1 / \tau_{\text{diff}} = -B D_T k^2 = -B U_L k (d_L k) \]

first order correction \( B > 0 ? \)

\[ kd_L < 1: \quad \sigma / U_L = Ak - B k^2 d_L + \ldots \]

Stabilisation at small wavelength, \( \Lambda \approx d_L \)
Lecture 4: **Hydrodynamic instability of flames**

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Curvature effect: a simplified approach


G.H. Markestein (1964) Nonsteady flame propagation New York: Pergamon

Modification to the inner flame structure
\[ \delta m_f(t) \approx \delta m_f(t) \neq 0 \]

First order in perturbation analysis \( d_L/\Lambda \ll 1 \)
\[ \frac{\delta m_f}{\bar{\rho}^+} \equiv (\delta u_f^- - \dot{\alpha}_t) = -BD_T \partial^2 \alpha/\partial y^2 \]
\[ \frac{\bar{m}_f(t)}{\bar{m}_f} \approx Bd_L k^2 \ddot{\alpha}(t) \quad D_T = U_L d_L \]

Normal momentum
\[ \delta p_f^- + 2\bar{\rho}^- \bar{u}_f^- (\delta u_f^- - \dot{\alpha}_t) = \delta p_f^+ + 2\bar{\rho}^+ \bar{u}_f^+ (\delta u_f^+ - \dot{\alpha}_t) \]

(flame notations: \( \bar{\rho}^+ \rightarrow \rho_b, \bar{\rho}^- \rightarrow \rho_u, \rho_u > \rho_b \))
\[ \pi_f^+ - \pi_f^- = -2\bar{m}_f \left( \frac{1}{\rho_b} - \frac{1}{\rho_u} \right) \bar{\dot{m}}_f(t) + (\rho_u - \rho_b) g(t) \ddot{\alpha}(t) \]

Equation for the flame front (correction due to curvature, finite thickness effect \( kd_L \neq 0 \))
\[ (\rho_u + \rho_b) \frac{d^2 \ddot{\alpha}}{dt^2} + 2\bar{m}_f k \frac{d \ddot{\alpha}}{dt} (1 + Bd_k d_L) = k\ddot{\alpha}(\rho_u - \rho_b) [g(t) + U_b U_L k (1 - 2Bk d_L)] \]

Flame propagating downwards \( g < 0 \)
\[ \frac{1}{k_m} = 2Bd_L \]
\[ \left( 1 + \frac{\rho_b}{\rho_u} \right) \frac{d^2 \ddot{\alpha}}{dt^2} + 2U_L k \frac{d \ddot{\alpha}}{dt} = \left( \frac{\rho_u}{\rho_b} - 1 \right) k \left[ -\frac{\rho_b}{\rho_u} |g| + U_L^2 k \left( 1 - \frac{k}{k_m} \right) \right] \ddot{\alpha} \]

Non-dimensional parameters
\[ s = \sigma \tau_L \quad \kappa \equiv kd_L \]
\[ u_b \equiv \bar{\rho}^- / \bar{\rho}^+ = \bar{u}^+ / \bar{u}^- > 1 \]
\[ \kappa_m \equiv 1/(2B) \quad G_0 \equiv (\rho_b / \rho_u) Fr^{-1} \quad Fr^{-1} \equiv |g| d_L / U_L^2 \]
\[ (1 + u_b^{-1}) s^2 + 2\kappa s - (u_b - 1) \kappa \left[ -G_0 + \kappa \left( 1 - \frac{\kappa}{\kappa_m} \right) \right] = 0 \]

Stability limits of flames propagating downwards \( \sigma = 0 \)

Marginal wavenumber
\[ \left[ -G_0 + \kappa \left( 1 - \frac{\kappa}{\kappa_m} \right) \right] = 0, \]
Stability limits of flames propagating downwards

non-dimensional parameters \( \kappa \equiv k d_L \quad \kappa_m \equiv 1/(2B) \quad G_0 \equiv (\rho_b/\rho_u)Fr^{-1} \quad Fr^{-1} \equiv |g|d_L/U_L^2 \)

\[
s = \sigma \tau_L \quad (1 + v_b^{-1})s^2 + 2\kappa s - (v_b - 1)\kappa \left[-G_0 + \kappa \left(1 - \frac{\kappa}{\kappa_m}\right)\right] = 0
\]

marginal wavenumber \( \sigma = 0 \)

gravity stabilizes the large wavelengths of slow propagating flame
curvature stabilizes the small wavelengths
the planar flame is stable (at all wavelength) beyond a stability threshold, namely for slow flames \( U_L < 10 \text{cm/s} \)

Marginal wave number \( k_c \) at the instability threshold \( U_L \approx 10 \text{cm/s} \)

\[
G_{oc} = \frac{k_c d_L}{2}, \quad k_c = \frac{k_m}{2}, \quad U_{Lc} = \sqrt{\frac{2\rho_b |g|}{\rho_u k_c}}
\]

OK with experiments

G. Searby and J. Quinard (1990) Combust. Flame, 83 (3-4) 298-311

Flames propagating upwards: bubble flames
Princeton Summer School on Combustion
June 17- June 22, 2024

Dynamics of Combustion Waves in Premixed Gases

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Lecture V
Thermo-diffusive phenomena
Lecture 5: Thermodynamic phenomena

5-1. Flame stretch and Markstein numbers

*Passive interfaces*

*One-step flame model*

*The second Markstein number*

5-2. Thermo-diffusive instabilities

\[ \text{Le} \equiv \frac{D_T}{D} \quad \text{Planar flames for Le} \neq 1 \]

*Jump conditions across the reaction layer*

*Linear equations and linear analysis*

*Cellular instability (Le < 1)*

*Oscillatory instability (Le > 1)*
5-1. Flame stretch and Markstein numbers

Two mechanisms modify the inner flame structure

- transverse diffusion
- transverse convection

**One-step model** \[ R \rightarrow P + Q \quad \beta \gg 1 \]

A single scalar: the Markstein number \( \mathcal{M} \)

\[
(U_n^- - U_L)/U_L = -\mathcal{M}(\tau_L/\tau_s)
\]

\( U_n^- \) normal flame velocity in the fresh mixture

\[
U_n^- = u_n^- - D_f, \quad u_n^- \equiv n_f \cdot u_f^- 
\]

1/\( \tau_s \) rate of stretch of flame surface
Stretch rate, strain and curvature of a flame

Passive interface

Element of surface area:
\[
\delta^2 s = \frac{1}{\tau_s} = \frac{1}{\delta^2 s} \frac{d\delta^2 s}{dt}
\]

Element of volume:
\[
\delta^3 r = \delta^2 s \delta \zeta
\]

Coordinate normal to the front:
\[
\frac{1}{\delta^3 r} \frac{d}{dt} \delta^3 r = \frac{1}{\delta^2 s} \frac{d}{dt} \delta^2 s + \frac{1}{\delta \zeta} \frac{d}{dt} \delta \zeta
\]

\[
d\delta \zeta / dt = n_f \cdot \left[ u^e(r_f + \delta \zeta n_f) - u^e(r_f) \right]
\]

\[
\delta \zeta \ll 1 : u^e(r_f + \delta \zeta n_f) \approx u^e(r_f) + \delta \zeta n_f \cdot \nabla u^e
\]

\[
\frac{1}{\delta \zeta} \frac{d}{dt} \delta \zeta = n_f \cdot \nabla u^e \cdot n_f
\]

\[
\frac{1}{\tau_s} \equiv \frac{1}{\delta^2 s} \frac{d}{dt} \delta^2 s = \nabla u^e|_f - n_f \cdot \nabla u^e|_f \cdot n_f.
\]

Flame (first order correction):
\[
d_L / \Lambda \ll 1
\]

\[
u^e(r_f) = u_f^- - U_L n_f
\]

\[
n_f \cdot n_f = 1
\]

\[
n_f \cdot \nabla n|_f \cdot n_f = 0
\]

\[
1/\tau_s = -U_L \nabla n_f + \nabla u^-|_f - n_f \cdot \nabla u^-|_f \cdot n_f
\]
\[ 1/\tau_s = -U_L \nabla \cdot n_f + \nabla \cdot u^- |_f - n_f \cdot \nabla u^- |_f \cdot n_f \]

incompressibility

\[ -\nabla \cdot n_f = 1/R \equiv (1/R_1 + 1/R_2) \]

differential geometry

\[
1/\tau_s = U_L/R - n_f \cdot \nabla u^- |_f \cdot n_f
\]

front curvature

strain rate

First order correction to the laminar flame velocity \( R \to P + Q \)

\[ \tau_L/\tau_s \ll 1, \quad \tau_L \equiv d_L/U_L, \quad (U_n^- - U_L)/U_L \propto \tau_L/\tau_s \]

Clavin, Williams, JFM (1982) 116 p. 252-282,


Lewis number \( \text{Le} \equiv D_T/D \)  

Asymptotic analysis: \( \beta \gg 1 \quad \beta(\text{Le} - 1) = O(1) \)

\[
(U_n^- - U_L)/U_L = -\mathcal{M}(\tau_L/\tau_s)
\]

\[ \mathcal{M} = \frac{v_b}{v_b - 1} \mathcal{J} + \frac{l}{2(2v_b - 1)} \mathcal{D} \]

\[ \mathcal{J} = \int_0^1 \frac{(v_b - 1)\lambda(\theta)}{1 + (v_b - 1)\theta} d\theta, \quad \mathcal{D} = -\int_0^1 \frac{(v_b - 1)\lambda(\theta)\ln \theta}{1 + (v_b - 1)\theta} d\theta, \]

\[ \lambda(\theta) = \frac{v_b}{v_b - 1}(1 - \frac{v_b}{v_b - 1}) \theta - 1 \]

\[ v_b \equiv \rho_u/\rho_b > 1 \quad \theta \equiv (T - T_u)/(T_b - T_u) \quad l \equiv \beta(\text{Le} - 1) \quad \text{heat conductivity} \ 
\lambda(\theta) \quad \text{kinetics + diffusion} \]
The second Markstein number

**multiple-step flame model**

Clavin, Graña-Otero, *JFM* (2011) 689 p. 187-217,

\[
(U_n^- - U_L)/U_L = -\mathcal{M}_{fc}(d_L/R) + \mathcal{M}_{sr}(\tau_{Lf} \mathbf{n}_f \cdot \nabla \mathbf{u}^- |_{f} \mathbf{n}_f)
\]

front curvature  
flow strain rate

\[
\mathcal{M}_{fc} \neq \mathcal{M}_{sr}
\]

difficulty with the finite thickness:

\[
\mathcal{M}_{sr} \text{ varies with the position inside the flame structure}
\]

\[
\mathcal{M}_{sr}(\tau_{Lf} \mathbf{n}_f \cdot \nabla \mathbf{u}^- |_{f} \mathbf{n}_f) = \text{cst.}
\]

Markstein numbers in the burned gas

\[
U_n^+ \equiv u_n^+ - D_f \\
u_n^+ \equiv \mathbf{n}_f \cdot \mathbf{u}^+(r_f)
\]

\[
\frac{(U_n^+ - U_b)}{U_b} = -\mathcal{M}_{fc}^+ \frac{d_L}{R} + \mathcal{M}_{sr}^+ \tau_{Lf} \mathbf{n}_f \cdot \nabla \mathbf{u}^+ |_{f} \mathbf{n}_f
\]

\[
\mathcal{M}_{fc}^+ \neq \mathcal{M}_{fc}^- \quad \mathcal{M}_{sr}^+ \neq \mathcal{M}_{sr}^-
\]

numerical and experimental data

\[
\begin{align*}
D_f &= 0, \quad U_n^- = u_n^- \\
\frac{U_n^- - U_L}{U_L} &= -2(\mathcal{M}_{fc}^- - \mathcal{M}_{sr}^-) \frac{d_L}{R_f}
\end{align*}
\]

\[
\begin{align*}
u_n^+ &= 0, \quad U_n^+ = -D_f \\
\frac{U_n^+ - U_b}{U_b} &= -2\mathcal{M}_{fc}^+ \frac{d_L}{R_f}
\end{align*}
\]
5-2. Thermo-diffusive instabilities

Instability mechanism ≠ hydrodynamic instability

\[
\rho T = \rho_o T_o \quad \rho c_p DT/DT = \nabla.(\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)}(T, Y_{k..})
\]

\[
\rho DY_i/DT = \nabla.(\rho D_i \nabla Y_i) + \sum_j \theta_i^{(j)} m_i \dot{W}^{(j)}(T, Y_{k..}),
\]

**Thermo-diffusive flame model** for a one-step kinetics

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

\[
\frac{\partial \theta}{\partial t} - D_T \Delta \theta = \frac{\psi}{\tau_{rb}} e^{-\beta(1-\theta)} \quad \frac{\partial \psi}{\partial t} - D \Delta \psi = -\frac{\psi}{\tau_{rb}} e^{-\beta(1-\theta)}
\]

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

Unperturbed (steady state) planar flame Le≠ 1

(frame attached to the flame front)

\[
\mu \frac{d\theta}{d\xi} - \frac{d^2\theta}{d\xi^2} = \frac{\beta^2}{2} \psi e^{-\beta(1-\theta)} \quad \mu \frac{d\psi}{d\xi} - \frac{1}{Le} \frac{d^2\psi}{d\xi^2} = -\frac{\beta^2}{2} \psi e^{-\beta(1-\theta)}
\]

reaction layer

\[
-\frac{d^2\theta}{d\xi^2} \approx \frac{\beta^2}{2} \psi e^{-\beta(1-\theta)} \quad \frac{d^2\theta}{d\xi^2} + \frac{1}{Le} \frac{d^2\psi}{d\xi^2} = 0
\]

Matching

\[
\mu = \sqrt{Le}
\]

(first order reaction rate)
Mathematical model for analyzing the thermo-diffusive instability $\text{Le} \neq 1$:

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

$$\frac{\partial \theta}{\partial t} - D_T \Delta \theta = \frac{\psi}{\tau_{rb}} e^{-\beta(1-\theta)} \quad \frac{\partial \psi}{\partial t} - D \Delta \psi = -\frac{\psi}{\tau_{rb}} e^{-\beta(1-\theta)}$$

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

Lewis number $\text{Le} \equiv D_T/D$  

**Asymptotic analysis:** $\beta \gg 1 \quad \beta(\text{Le} - 1) = O(1)$


*Joulin, Clavin, Combust. Flame (1979) 35 p. 139-153*
Flame temperature of curved flame for \( \text{Le} \neq 1 \)

\[ \beta \gg 1 \quad \text{Le} - 1 = O(1/\beta) \quad \Rightarrow \quad (\theta_f - 1) = O(1/\beta) \]

\[ \theta_f \equiv \frac{T_f - T_u}{T_b - T_u} \]

the thin reaction layer of curved flame is quasi-planar

\[
- \frac{d^2\theta}{d\xi^2} \approx \frac{\beta^2}{2} \psi e^{-\beta(1-\theta)}
\]

\[ \psi = -\psi_1/\beta + .. \]

\[ \Theta_1 = \Psi_1/\text{Le} \]

\[ \frac{1}{\beta^2} \frac{d^2\Theta_1}{d\xi^2} = \frac{1}{2} e^{-\beta(1-\theta_f)} \psi_1 e^{-\Theta_1} \]

\[ \beta(\theta_f - 1) = O(1) 
\]

\[ \frac{d\theta}{d\xi}|_{\xi=0+} = O(1/\beta) \]

integration and matching

\[ \frac{d\theta}{d\xi}|_{\xi=0-} \approx \text{Le}^{1/2} e^{-\beta(1-\theta_f)/2} \]

jump conditions across the reaction layer

\[ \frac{d\theta}{d\xi}|_{\xi=0-} = e^{-\beta(1-\theta_f)/2} \]

valid at the leading order

\[ \left[ \frac{d\theta}{d\xi} + \frac{1}{\text{Le} \frac{d\psi}{d\xi}} \right]_{0-}^{0+} = 0 \]

valid up to 1\(^{st}\) order

\[ \text{valid up to 1}^{st} \text{ order} \]

Joulin, Clavin; Combust. Flame (1979) 35 p. 139-153

Clavin, Searby; Cambridge University Press (2014) p. 390-393

Preheated zone

non-dimensional equations in the reference frame attached to the unperturbed flame

\[ \xi \equiv x/d_L, \quad \eta = y/d_L, \quad \tau \equiv t/\tau_L \]

\[ \frac{\partial \theta}{\partial \tau} + \frac{\partial \theta}{\partial \xi} - \Delta \theta = 0, \quad \frac{\partial \psi}{\partial \tau} + \frac{\partial \psi}{\partial \xi} - \frac{1}{\text{Le}} \Delta \psi = 0 \]

boundary conditions: jump conditions and

\[ \xi = -\infty : \theta = 0, \psi = 1, \quad \xi = \infty : \theta = 1, \psi = 0. \]
Linear equations

frame of reference attached to the reaction sheet \((\zeta, \eta, \tau)\)

\[
\xi = \xi - \alpha(\eta, \tau), \quad \zeta = 0 : \text{reaction sheet}
\]

\[
\frac{\partial}{\partial \xi} = \frac{\partial}{\partial \xi'}, \quad \frac{\partial}{\partial \eta} \rightarrow \frac{\partial}{\partial \eta} - \frac{\partial \alpha}{\partial \eta} \frac{\partial}{\partial \xi'}, \quad \frac{\partial}{\partial \tau} \rightarrow \frac{\partial}{\partial \tau} - \frac{\partial \alpha}{\partial \tau} \frac{\partial}{\partial \xi'}
\]

linearization

\[
\theta = \bar{\theta}(\zeta) + \delta \theta, \quad \theta_f = 1 + \delta \theta_f, \quad \psi = \bar{\psi}(\zeta) + \delta \psi
\]

\[
\left[ \frac{\partial}{\partial \tau} + \frac{\partial}{\partial \zeta} - \left( \frac{\partial^2}{\partial \zeta^2} + \frac{\partial^2}{\partial \eta^2} \right) \right] \delta \theta = \left( \frac{\partial \alpha}{\partial \tau} - \frac{\partial^2 \alpha}{\partial \eta^2} \right) \frac{d \bar{\theta}}{d \zeta}
\]

external equations

\[
\left[ \frac{\partial}{\partial \tau} + \frac{\partial}{\partial \zeta} - \frac{1}{\text{Le}} \left( \frac{\partial^2}{\partial \zeta^2} + \frac{\partial^2}{\partial \eta^2} \right) \right] \delta \psi = \left( \frac{\partial \alpha}{\partial \tau} - \frac{1}{\text{Le}} \frac{\partial^2 \alpha}{\partial \eta^2} \right) \frac{d \bar{\psi}}{d \zeta}
\]

harmonic analysis
(normal modes)

\[
a(\eta, \tau) = \hat{\alpha} e^{(i \kappa \eta + \zeta \tau)}, \quad \delta \theta_f(\eta, \tau) = \tilde{\theta}_f \hat{\alpha} e^{(i \kappa \eta + \zeta \tau)}
\]

\[
\delta \psi = \tilde{\psi}(\zeta) \hat{\alpha} e^{(i \kappa \eta + \zeta \tau)}, \quad \delta \theta = \tilde{\theta}(\zeta) \hat{\alpha} e^{(i \kappa \eta + \zeta \tau)}
\]

\[
\frac{d}{d \zeta} \left[ - \frac{d^2}{d \zeta^2} \right] \tilde{\theta}(\zeta) + (\zeta + \kappa^2) \tilde{\theta}(\zeta) = (\zeta + \kappa^2) \frac{d \tilde{\theta}}{d \zeta}
\]

\[
\frac{d}{d \zeta} \left[ - \frac{1}{\text{Le}} \frac{d^2}{d \zeta^2} \right] \tilde{\psi}(\zeta) + (\zeta + \frac{\kappa^2}{\text{Le}}) \tilde{\psi}(\zeta) = \left( \zeta + \frac{\kappa^2}{\text{Le}} \right) \frac{d \tilde{\psi}}{d \zeta}
\]

boundary conditions: jump conditions and \(\zeta = -\infty : \tilde{\theta} = 0, \tilde{\psi} = 0, \quad \zeta = +\infty : \tilde{\theta} = 0, \tilde{\psi} = 0\)
\[
\begin{align*}
\left[ \frac{d}{d\zeta} - \frac{d^2}{d\zeta^2} \right] \tilde{\theta}(\zeta) + (\zeta + \kappa^2) \tilde{\theta}(\zeta) &= (\zeta + \kappa^2) \frac{d\tilde{\theta}}{d\zeta} \\
\left[ \frac{d}{d\zeta} - \frac{1}{\text{Le} d\zeta^2} \right] \tilde{\psi}(\zeta) + \left( \zeta + \frac{\kappa^2}{\text{Le}} \right) \tilde{\psi}(\zeta) &= \left( \zeta + \frac{\kappa^2}{\text{Le}} \right) \frac{d\tilde{\psi}}{d\zeta}
\end{align*}
\]

Linear solutions in the external zones (preheated and burned gas)

particular solutions
\[
\tilde{\theta} = \frac{d\bar{\theta}}{d\zeta} \quad \tilde{\psi} = \frac{d\bar{\psi}}{d\zeta}
\]
\[
\begin{align*}
\bar{\theta}^- &= e^\zeta \quad \bar{\theta}^+ = 1 \\
\bar{\psi}^- &= 1 - e^{\text{Le}\zeta} \quad \bar{\psi}^+ = 0
\end{align*}
\]

boundary conditions
\[
\begin{align*}
\zeta \to \pm \infty : \quad \bar{\theta} &= 0 \\
\theta(\zeta = 0) &= \theta_f \\
\tilde{\theta}^\pm &= \frac{d\bar{\theta}^\pm}{d\zeta} + \left( \tilde{\theta}_f - \frac{d\bar{\theta}^\pm}{d\zeta} \bigg|_{\zeta=0} \right) e^{r^\pm \zeta}
\end{align*}
\]
\[
\begin{align*}
\zeta \to -\infty : \quad \tilde{\psi} &= 0 \\
\psi(\zeta = 0) &= 0 \\
\tilde{\psi}^\pm &= \frac{d\bar{\psi}^\pm}{d\zeta} - \left( \frac{d\bar{\psi}^-}{d\zeta} \bigg|_{\zeta=0} \right) e^{s^- \zeta}
\end{align*}
\]
\[
\begin{align*}
\frac{1}{\text{Le}} s^2 - s - \left( \zeta + \frac{\kappa^2}{\text{Le}} \right) &= 0 \\
s^- &= \frac{\text{Le}}{2} \left[ 1 + \sqrt{1 + \frac{4}{\text{Le}} \left( \zeta + \frac{\kappa^2}{\text{Le}} \right)} \right]
\end{align*}
\]
jump conditions
\[ \frac{d\theta}{d\xi}|_{\xi=0^-} = e^{-\beta(1-\theta_f)/2} \]
valid at the leading order

\[ \left[ \frac{d\theta}{d\xi} + \frac{1}{Le} \frac{d\psi}{d\xi} \right]_{0^-} = 0 \]
valid up to 1\(^{st}\) order

asymptotic analysis \( \beta \gg 1 : \) \( Le = 1 + l/\beta, \quad l \equiv \beta(Le - 1) = O(1) \)
\[ \beta(1 - \theta_f) = O(1) \]
\[ \beta \tilde{\theta}_f = O(1) \]

2\(^{nd}\) condition \( \tilde{\theta}_f(r^+ - r^-) = (s^- - r^-) + (1 - Le) \)
\( Le \to 1 : \quad s^- - r^- \to 0 \)
to leading order in small values of \( (Le-1) = O(1/\beta) \)

\[ \tilde{\theta}_f \approx \frac{(Le - 1)}{2} \left[ \frac{1}{\sqrt{1 + 4(\zeta + \kappa^2)}} - 1 + \frac{2\zeta + 4\kappa^2}{1 + 4(\zeta + \kappa^2)} \right] \]

linearized 1\(^{st}\) condition \( \frac{d\tilde{\theta}^-}{d\zeta}|_{\zeta=0} = \beta \tilde{\theta}_f / 2 \)
\( 1 - r^- = r^+ = \beta \tilde{\theta}_f / 2 \)
valid to leading order using \( \tilde{\theta}_f = O(1/\beta) \)

\[ \beta \tilde{\theta}_f = 1 - \sqrt{1 + 4(\zeta + \kappa^2)} \]

dispersion relation \( \zeta(\kappa) \)

root of \( -\frac{l}{2} \left[ 1 - \sqrt{1 + 4(\zeta + \kappa^2)} + 2\zeta \right] = \left[ 1 - \sqrt{1 + 4(\zeta + \kappa^2)} \right] \left[ 1 + 4(\zeta + \kappa^2) \right] \)
\[ -\frac{l}{2} \left[ 1 - \sqrt{1 + 4(\zeta + \kappa^2)} + 2\zeta \right] = \left[ 1 - \sqrt{1 + 4(\zeta + \kappa^2)} \right] \left[ 1 + 4(\zeta + \kappa^2) \right] \]

\[ e^{\sigma t} = e^{\zeta \tau} \text{ linear instability: } \Re \zeta > 0 \ (\Re \sigma > 0) \]

Cellular instability for \( \Leq \equiv D_T/D < 1 \)

Weakly curved limit. Small wavenumber expansion \( \kappa \equiv kd_L \ll 1 \)

\[ \kappa = 0 : \zeta(\kappa) = 0 \quad |\zeta| \equiv |\sigma|\tau_L \ll 1 \]

\[ \bar{\theta}_f = (\Leq - 1)\kappa^2 \quad \zeta = -(l + 2)\kappa^2/2 \quad \sigma \equiv \zeta/\tau_L \text{ is real} \]

\[ l \equiv \beta(\Leq - 1) > -2 : \quad \sigma < 0 \quad \text{stable} \quad l \equiv \beta(\Leq - 1) < -2 : \quad \sigma > 0 \quad \text{unstable} \]

\[ \frac{\partial \alpha}{\partial t} = \left[ \frac{\beta(\Leq - 1) + 2}{2} \right] D_T \left( \frac{\partial^2 \alpha}{\partial y^2} + \frac{\partial^2 \alpha}{\partial z^2} \right) = \left[ \beta(\Leq - 1) + 2 \right] \frac{D_T}{R}, \quad 2/R = 1/R_1 + 1/R_2 \]

\[ \mathcal{M} = \beta(\Leq - 1) + 2 \quad \mathcal{M} = \frac{v_b}{v_b - 1} \mathcal{J} + \frac{l}{2} \frac{\mathcal{D}}{v_b - 1} \]

\[ \mathcal{J} = \int_0^1 (v_b - 1)\lambda(\theta) d\theta, \quad \mathcal{D} = -\int_0^1 (v_b - 1)\lambda(\theta) \ln \theta d\theta, \]

\[ \zeta = -(l + 2)\kappa^2/2 - 8\kappa^4 \]

Turing type of instability

\[ \Re \zeta > 0 \quad \Im \zeta = 0 \]

Unstable disturbances
heavy hydrocarbons: \( D_F < D_{O_2} \)

lean mixtures of an heavy hydrocarbon \( \Rightarrow \) limiting species = \( F \)

\( D = D_F \)

\( D_T = D_{O_2} > D_F \)

\[ \text{Le} \equiv \frac{D_T}{D} = \frac{D_{O_2}}{D_F} > 1 \Rightarrow \beta (\text{Le} - 1) > -2 \Rightarrow \text{thermo-diffusive stable} \]

rich mixtures of heavy hydrocarbons are thermo-diffusive \textbf{unstable}

eexample: propane-air

rich mixtures of light fuels are thermo-diffusive \textbf{stable}

eexample: hydrogen-air
Poincaré-Andronov bifurcation $l^* \approx 10$

Propane lean flame $\mathcal{M} > 0$
hydrodynamic instability only

Sivashinsky eq. 1977
\[ \frac{\partial \phi}{\partial \tau} - \mathcal{H}(\phi) - \Delta \phi + \frac{1}{2} |\nabla \phi|^2 = 0 \]
nonlinear equation (weak gas expansion)


Propane rich flame $\mathcal{M} < 0$
hydrodynamic + cellular instabilities
shorter wavelengths are unstable

Oscillatory instability $\text{Le} \equiv D_T / D > 1$

\[ \text{Im}(\zeta) \neq 0 \]

\[ l \equiv \beta(\text{Le} - 1) = l^* : \text{Re}(\zeta) = 0, \ \kappa^* \neq 0 \]
Poincaré-Andronov bifurcation $l^* \approx 10$

\[ l^{**} \approx 11 : \text{planar pulsation. OK for solid combustion} \]

Joulin, Clavin, Combust. Flame (1979) 35 p. 139-153

\[ \beta(\text{Le} - 1) \]
\[ l \approx 10.67 \]

Effect of heat losses

Adiabatic

18/5

Stable

Extinction

Cellular instability

Heat loss

Thermal quenching
Dynamics of Combustion Waves in Premixed Gases

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Lecture VI
Thermal quenching of flames and flammability limits
Lecture 6: **Thermal quenching and flammability limits**

6-1. Extinction through thermal loss

6-2. Basic concepts in chemical kinetics

*Combustion of hydrogen*

*Two-step model. Crossover temperature*

*One-step model with temperature cutoff*

6-3. Flame speed near flammability limits
6-1. Extinction through thermal loss

A small heat loss can quench the flame

Formulation (volumetric heat loss in a planar flame)

\[
\begin{align*}
\frac{d\theta}{d\xi} - \frac{d^2\theta}{d\xi^2} &= w - \frac{\tau_L}{\tau_{cool}} \theta, \\
\frac{d\psi}{d\xi} - \frac{1}{Le} \frac{d^2\psi}{d\xi^2} &= -w
\end{align*}
\]

\[
\xi \equiv x/d_L, \quad \mu = U_L/U_{Lad}, \quad 1/\tau_{cool} \approx D_T/R^2
\]

\[
\tau_L \approx D_T/U_L^2 \Rightarrow \frac{\tau_L}{\tau_{cool}} \approx \left( \frac{D_T}{RU_L} \right)^2 R = \text{tube radius}
\]

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

Asymptotic analysis for small heat loss and a one-step reaction

\[
\beta \to \infty \quad \frac{\tau_L}{\tau_{cool}} = h/\beta \\
h = \mathcal{O}(1) \quad \beta(1 - \theta_f) = \mathcal{O}(1) \quad w(\theta, \psi) = (\beta^2/2)\psi \exp[-\beta(1 - \theta)]
\]

unknown flame temperature < adiabatic flame temperature : \( \theta_f < 1 \)

external solutions : \( w = 0 \)

\[
\begin{align*}
\xi < 0 : \begin{cases} 
\theta_-(\xi) &= \theta_f e^{[\mu + h/((\beta \mu))\xi]} , \\
\psi_-(\xi) &= 1 - e^{Le \mu \xi}
\end{cases}, \\
\xi > 0 : \begin{cases} 
\theta_+(\xi) &= \theta_f e^{-[h/((\beta \mu))]\xi}, \\
\psi_+(\xi) &= 0,
\end{cases}
\end{align*}
\]

jumps across the thin reaction zone :

\[
\frac{d\theta}{d\xi} \bigg|_{\xi=0^-} = e^{-\beta(1-\theta_f)/2} \quad \left[ \frac{d\theta}{d\xi} + \frac{1}{Le} \frac{d\psi}{d\xi} \right]_{0^+} = 0
\]
\[ \xi < 0: \begin{cases} 
\theta_-(\xi) = \theta_f e^{[\mu + h/(\beta \mu)]\xi}, \\
\psi_-(\xi) = 1 - e^{Le \mu \xi}, 
\end{cases} \quad \xi > 0: \begin{cases} 
\theta_+(\xi) = \theta_f e^{-[h/(\beta \mu)]\xi}, \\
\psi_+(\xi) = 0, 
\end{cases} \]

\[
\left[ \frac{d\theta}{d\xi} + \frac{1}{Le} \frac{d\psi}{d\xi} \right]^{0+}_{0-} = 0 \quad \Rightarrow \quad -(h/\beta \mu)\theta_f - (\mu + h/\beta \mu)\theta_f + \mu = 0
\]

\[
\theta_f - 1 = O(1/\beta) \quad \Rightarrow \quad \beta (1 - \theta_f) = 2h/\mu^2
\]

\[
\frac{d\theta}{d\xi}\bigg|_{\xi=0-} = e^{-\beta (1 - \theta_f)/2} \quad \Rightarrow \quad \mu = \exp(-h/\mu^2)
\]

\[\mu^2 \ln \mu^2 = -2h\]

C-shaped curve: no solution for \(2h > 1/e\)
quenching at finite flame velocity \(U_L/U_{Ladia} = 1/\sqrt{e}\)
Lecture 6: **Thermal quenching and flammability limits**

6-1. Extinction through thermal loss

6-2. Basic concepts in chemical kinetics

*Combustion of hydrogen*

*Two-step model. Crossover temperature*

*One-step model with temperature cutoff*

6-3. Flame speed near flammability limits
6-2. Basic concepts in chemical kinetics

Combustion of hydrogen

C.K. Law; Cambridge University Press (2006)

units: moles/cm³, s⁻¹ and Kelvin

dc_ij/dt = -ω_j

ω_j = ̇k_jc_i1c_j2 or ω_j = ̇k_jc_i1c_j2c_j3

̇k_j = ̇B_jT^ν e⁻^T_ω_j/T

<table>
<thead>
<tr>
<th>Label</th>
<th>Reaction</th>
<th>̇k_j</th>
<th>̇B_j</th>
<th>ν_j</th>
<th>T_ω_j</th>
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<tbody>
<tr>
<td>1</td>
<td>O₂ + H ⇌ OH + O</td>
<td>̇k_{1f}</td>
<td>3.52 × 10^{16}</td>
<td>-0.7</td>
<td>8590</td>
</tr>
<tr>
<td>2</td>
<td>H₂ + OH ⇌ H₂O + H</td>
<td>̇k_{2f}</td>
<td>1.17 × 10^9</td>
<td>1.3</td>
<td>1825</td>
</tr>
<tr>
<td>3</td>
<td>H₂ + O ⇌ OH + H</td>
<td>̇k_{3f}</td>
<td>5.06 × 10^4</td>
<td>2.67</td>
<td>3165</td>
</tr>
<tr>
<td>4f</td>
<td>O₂ + H + M → HO₂ + M</td>
<td>̇k_{4f}</td>
<td>5.79 × 10^{19}</td>
<td>-1.4</td>
<td>0</td>
</tr>
<tr>
<td>5f</td>
<td>H + H + M → H₂ + M</td>
<td>̇k_{5f}</td>
<td>1.30 × 10^{18}</td>
<td>-1</td>
<td>0</td>
</tr>
<tr>
<td>6f</td>
<td>H + OH + M → H₂O + M</td>
<td>̇k_{6f}</td>
<td>4.00 × 10^{22}</td>
<td>-2</td>
<td>0</td>
</tr>
<tr>
<td>7f</td>
<td>HO₂ + H → OH + OH</td>
<td>̇k_{7f}</td>
<td>7.08 × 10^{13}</td>
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<td>148</td>
</tr>
<tr>
<td>8f</td>
<td>HO₂ + H → H₂ + O₂</td>
<td>̇k_{8f}</td>
<td>1.66 × 10^{13}</td>
<td>0</td>
<td>414</td>
</tr>
<tr>
<td>9f</td>
<td>HO₂ + OH → H₂O + O₂</td>
<td>̇k_{9f}</td>
<td>2.89 × 10^{13}</td>
<td>0</td>
<td>-250</td>
</tr>
</tbody>
</table>

shuffle reactions
(1f), (2f), (3f) chain branching

O₂ + 3H₂ → 2H₂O + 2H
rate: ω_{1f} = c_{HCO₂}k_{1f}

(4f) chain breaking
M + H + O₂ → M + HO₂;
rate: ω_{4f} = c_{HCO₂}nk_{4f}

k_{4f} = B_{4f}

(8b) initiation
H₂ + O₂ → HO₂ + H


Simplified two-step model: crossover temperature

Clavin, Searby; Cambridge University Press (2014) p. 390-393

(B) R + X → 2X, \ ω_B = c_{RCX}B_Be^{-E/k_BT}, E \gg k_BT

(R) M + X → P + Q, \ ω_R = c_Xn_B, \ E_R = 0

\[ c_{RB_B}e^{-E_1/k_BT^*} = n_B \]

hydrogen combustion: \[ k_{1f}(T^*) = B_{1f}e^{-E_1/k_BT^*} = n_B \]

Flammability limit

\[ T_b = T^* \Rightarrow q_RY_u^* = c_p(T^* - T_u) \]
Methane-air flame

\[ \phi = \frac{N_F}{N_{O_2}} \]

Equivalence ratio

\[ \phi = 1 : \text{stoichiometry} \]
\[ \phi > 1 : \text{fuel rich} \]
\[ \phi < 1 : \text{fuel lean} \]

near to the flammability limit

\[ \phi = 0.65 \]

”thicker flame”
Two-step model for rich hydrogen flames near the flammability limit

\begin{align*}
\text{O}_2 + 3\text{H}_2 & \rightarrow 2\text{H}_2\text{O} + 2\text{H}, \\
\omega_{1f} & = c_H c_{\text{O}_2} k_{1f}(T), \quad k_{1f}(T) = B_1 e^{-E_1/k_B T} \\
\text{H} + \text{H} & \rightarrow \text{H}_2 + Q, \\
\omega_{4f} + \omega_{5f} & = n c_H c_{\text{O}_2} B_{4f} + n c_H^2 B_{5f} \\
\end{align*}

\[
\frac{dc_H}{dt} = \left[ B_1 e^{-E_1/k_B T} - n B_{4f} \right] c_{\text{O}_2} c_H - n B_{5f} c_H^2
\]

\[(B_1 e^{-E_1/k_B T} - n B_{4f})/n B_{4f} \ll 1\]

tri molecular recombination reaction \((5f) \Rightarrow \text{H} \text{ in quasi-steady state}\)

\[T > T^* : \quad c_H \approx c_{\text{O}_2} \frac{[B_1 e^{-E_1/k_B T} - n B_{4f}]}{n B_{5f}}\]

\[T < T^* : \quad c_H = 0\]

**One-step model (near the flammability limit)**

\[n B_{4f} = B_1 e^{-E_1/k_B T^*}\]

\[
1/\tau^* \equiv (n B_{4f}^2 c_{\text{O}_2}^*)/B_{5f}
\]

\[
\begin{align*}
\frac{m d\theta}{dx} - \rho D_T \frac{d^2 \theta}{dx^2} & \approx \frac{\rho \tau^*}{\tau^*} \psi^2 J(T) \\
\frac{m d\psi}{dx} - \rho D_{\text{O}_2} \frac{d^2 \psi}{dx^2} & \approx -\frac{\rho \tau^*}{\tau^*} \psi^2 e^{-E/k_B (1-1/\tau^*)} J(T)
\end{align*}
\]

\[
\begin{cases}
T > T^* : \quad J(T) \equiv \frac{T_u}{T} \left[e^{-E/k_B (1-1/\tau^*)} - 1\right] \\
T < T^* : \quad J(T) = 0
\end{cases}
\]

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

reaction of order 2 with a temperature cutoff

very close to the flammability limit

\[
\frac{T_b - T^*}{T^*} \ll \frac{k_B T^*}{E} \quad \Rightarrow \quad [e^{-E/k_B (1-1/\tau^*)} - 1] \approx \frac{E}{k_B} \left(\frac{1}{T^*} - \frac{1}{T}\right) \ll 1
\]
6-3. Flame speed near flammability limits

\[ \theta \equiv \frac{(T - T_u)}{(T_b - T_u)} \in [\theta^*, 1] \quad \theta^* \equiv \frac{(T^* - T_u)}{(T_b - T_u)} \quad T_b > T^* \Rightarrow \theta^* < 1 \text{ but close to } 1 \\

\[ m \frac{d\theta}{dx} - \rho_b D_T \frac{d^2 \theta}{d^2 x} \approx \frac{\rho_b}{\tau^*} \psi^2 j(\theta) \]

\[ m \frac{d\psi}{dx} - \rho_b D_{O_2} \frac{d^2 \psi}{d^2 x} \approx -\frac{\rho_b}{\tau^*} \psi^2 j(\theta) \]

\[ \begin{align*}
\theta > \theta^* &: j(\theta) \approx b^*(\theta - \theta^*) \\
\theta < \theta^* &: j(\theta) = 0
\end{align*} \]

reaction zone: \( \psi = Le(1 - \theta) \), \[ D_T \frac{d^2 \theta}{d^2 x} = \frac{Le^2 b^*}{\tau^*}(1 - \theta)^2[(\theta - 1) - (\theta^* - 1)] \]

\[ Le \equiv \frac{D_T}{D_{O_2}} \]

\[ \times \frac{d\theta}{dx} + \int_{\theta^*}^{1} d\theta + \text{matching} \Rightarrow D_T \frac{d\theta}{dx} \bigg|_{-} \approx Le \sqrt{\frac{b^*}{6}} (1 - \theta^*)^2 \sqrt{\frac{D_T}{\tau^*}} \quad \rho_u \frac{U_L}{\rho_b \sqrt{D_T/\tau^*}} \approx \frac{\sqrt{b^*}}{6} (1 - \theta^*)^2 \]

\[ 0 < \frac{T_b - T^*}{T_b - T_u} \ll 1 \Rightarrow \rho_u \frac{U_L}{\rho^* \sqrt{D_T/\tau^*}} \approx \frac{\sqrt{b^*}}{6} \left( \frac{T_b - T^*}{T^* - T_u} \right)^2 \]

the flame velocity decreases smoothly to zero when approaching the flammability limit \( T_b \rightarrow T^* \)

the flame thickness \( d_L^* \) diverges, \( T_b \rightarrow T^* \): \[ \frac{d^*_L}{d_L} \propto \frac{1}{\beta^2} \left( \frac{T^* - T_u}{T_b - T^*} \right)^2 \]

Divergence of the thermal sensitivity: Thermal quenching

\[ \frac{T_b}{U_L} \frac{dU_L}{dT_b} = \frac{2T_b}{T_b - T^*} \rightarrow \infty \]

the least heat loss quenches the flame at a non zero velocity
Dynamics of Combustion Waves in Premixed Gases

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Lecture VII
Flame kernels and quasi-isobaric ignition
Lecture 7: Flame kernels and quasi-isobaric ignition

7-1. Introduction

7-2. Zeldovich critical radius

7-3. Critical radius near the flammability limits

7-4. Dynamics of slowly expanding flames
Introduction

Flammability limits × Critical conditions of ignition

Some hydrocarbon lean mixtures that are flammable cannot be ignited quasi-isobarically
Some hydrocarbon rich mixtures that are non-flammable can sustain curved flames

Upward propagation limit is different from downwards

Ignition in turbulent flows

Turbulence facilitates ignition of hydrocarbon lean mixtures
Turbulence may suppress ignition of hydrocarbon rich mixtures
Lecture 7: **Flame kernels and quasi-isobaric ignition**

7-1. Introduction
7-2. Zeldovich critical radius
7-3. Critical radius near the flammability limits
7-4. Dynamics of slowly expanding flames
VII-2) Zeldovich critical radius

Flame kernel for a flame far from the flammability limits

Unstable **steady spherical solution** for the one-step model of adiabatic flames

\[ \theta \equiv (T - T_u)/(T_b - T_u) \quad \psi \equiv Y/Y_u \]

\[ \tau_{rb} \equiv \tau_r(T_b) \quad c_p(T_b - T_u) = q_R Y_u \]

\[ \Delta \theta = \frac{1}{R^2} \frac{d}{dR} \left( R^2 \frac{d\theta}{dR} \right) \quad \Delta \psi = \frac{1}{R^2} \frac{d}{dR} \left( R^2 \frac{d\psi}{dR} \right) \]

No flow

\[ -D_T \frac{1}{R^2} \frac{d}{dR} \left( R^2 \frac{d\theta}{dR} \right) = D \frac{1}{R^2} \frac{d}{dR} \left( R^2 \frac{d\psi}{dR} \right) = \frac{\psi}{\tau_{rb}} e^{-\beta(1-\theta)} \]

\[ R \leq R_f : \quad \theta = \theta_f, \quad \psi = 0; \quad R \to \infty : \quad \theta = 0, \quad \psi = 1 \]

**Flame temperature**

\[ \text{Le} \neq 1 \Rightarrow T_f \neq T_b \]

\[ D_T \frac{d}{dR} \left( R^2 \frac{d\theta}{dR} \right) + D \frac{d}{dR} \left( R^2 \frac{d\psi}{dR} \right) = 0 \]

(conservation energy)

double integration from \( R = 0 \) to \( R = \infty \)

\[ D_T \theta = D(1 - \psi) \quad \Rightarrow \quad \theta_f = 1/\text{Le} \]

\[ \text{Le} \equiv D_T/D \]

\[ \text{Le} < 1 \Rightarrow T_f > T_b \]

\[ \text{Le} > 1 \Rightarrow T_f < T_b \]
Unstable steady spherical solution for the one-step model of adiabatic flames

\[ \theta \equiv (T - T_u)/(T_b - T_u) \quad \psi \equiv Y/Y_u \quad \tau_{rb} \equiv \tau_r(T_b) \quad c_p(T_b - T_u) = q_R Y_u \]

\[-D_T \frac{1}{R^2} \frac{d}{dR} \left( R^2 \frac{d\theta}{dR} \right) = D \frac{1}{R^2} \frac{d}{dR} \left( R^2 \frac{d\psi}{dR} \right) = \frac{\psi}{\tau_{rb}} e^{-\beta(1 - \theta)} \]

\[ R \leq R_f : \quad \theta = \theta_f, \quad \psi = 0; \quad R \to \infty : \quad \theta = 0, \quad \psi = 1 \]

Asymptotic analysis \( \beta \gg 1 \)

Thin reaction zone \( \beta \to \infty \) thickness \( \ll \) flame radius \( R_f \)

\[ x \equiv R - R_f, \quad |x| \ll R_f : \quad -D_T \frac{d^2 \theta}{dx^2} = D \frac{d^2 \psi}{dx^2} = \frac{\psi}{\tau_{rb}} e^{-\beta(1 - \theta)} \]

\[ \eta \equiv \beta(x/R_f) = O(1), \quad \eta \in [-\infty, +\infty] \quad \psi \equiv \text{Le}(\theta_f - \theta) \quad \psi e^{-\beta(1 - \theta)} = e^{\beta(\theta_f - 1)}(\text{Le}/\beta)\Theta e^{-\Theta} \]

\[ \Theta \equiv \beta(\theta_f - \theta) = O(1) \quad \Theta \in [0, \infty] \]

Inner variables

\[ \times \frac{d\Theta}{d\eta} + \int_0^\Theta d\Theta \Rightarrow \beta \to \infty : \quad -\lim_{\Theta \to \infty} D_T \frac{d\theta}{dR} = e^{\beta(\theta_f - 1)/2} \sqrt{2 \text{Le} \frac{D_T}{\beta^2 \tau_{rb}}} \]

External zones

\[ \frac{d}{dR} \left( R^2 \frac{d\theta}{dR} \right) = 0 \quad R \geq R_f : \quad \theta = \frac{1}{\text{Le} \frac{R_f}{R}} \quad R = R_f : \quad \frac{D_T \frac{d\theta}{dR}}{\frac{1}{\text{Le} \frac{R_f}{R}}} = -\frac{1}{\frac{1}{\text{Le} \frac{R_f}{R}}} \quad R < R_f : \theta = \theta_f \]

Radius of the kernel

\[ \text{matching} \Rightarrow \frac{1}{\text{Le} \frac{R_f}{R}} \frac{D_T}{\frac{1}{\text{Le} \frac{R_f}{R}}} = e^{\frac{\beta}{2}(1 - \frac{1}{\text{Le} \frac{R_f}{R}})} \sqrt{\text{Le} \frac{D_T}{\tau_{rb}}} \leftrightarrow \frac{R_f}{d_L} = \text{Le}^{-3/2} e^{\frac{\beta}{2}(1 - \frac{1}{\text{Le} \frac{R_f}{R}})} \]

\[ \tau_{rb} \equiv \beta^2 \tau_{rb}/2, \quad d_L \equiv \sqrt{\frac{D_T}{\tau_{rb}}} \]

\[ \text{Le} < 1 : \quad R_f \ll d_L \quad \text{Le} > 1 : \quad R_f \gg d_L \]
Quasi-isobaric ignition as a nucleation problem

\[
\frac{\bar{R}_f}{d_L} = \frac{1}{\text{Le}^{3/2}} e^{\frac{\theta}{2}} (1 - \frac{1}{\text{Le}})
\]

\[
\text{Le} < 1 : \quad \bar{R}_f \ll d_L \\
\text{Le} > 1 : \quad \bar{R}_f \gg d_L
\]

Lean hydrocarbon mixtures \( \text{Le} > 1 \) are difficult to ignite \((R_f > d_L)\)

\[
D_{C_nH_m} < D_{O_2} \approx D_T, \quad \text{Le} \approx D_{O_2}/D_{C_nH_m} > 1
\]

**Instability?** (adiabatic condition)

\[
\theta = \theta_f R_f / R \\
\theta_f = 1/\text{Le} = \text{cst.} \\
\text{preheated zone at rest}
\]

\[
\frac{d\theta/dR}{|R=R_f} = -\theta_f/R_f
\]

heat flux towards the preheated zone  

\[
R_f \quad R_f > \bar{R}_f : \quad \text{diffusion fluxes} \propto 1/R \\
\text{convective flux } dR_f/dt > 0 \\
\text{positive feedback: amplification}
\]

\[
R_f \quad R_f < \bar{R}_f : \quad \text{diffusion fluxes} \propto 1/R \\
\text{convective flux } dR_f/dt < 0
\]

**Stability analysis**

**Stabilization** in the presence of heat loss for \( \text{Le} < 1 \)


**Flame balls in microgravity**  

lean hydrogen mixtures, diameter = 2 – 15 mm


**Ignition** by a constant energy source

Lecture 7: Flame kernels and quasi-isobaric ignition

7-1. Introduction
7-2. Zeldovich critical radius
7-3. Critical radius near the flammability limits
7-4. Dynamics of slowly expanding flames
Critical radius near the flammability limits


chemical-kinetics data: $T^*$ crossover temperature $\theta^* \equiv (T^* - T_u)/(T_b - T_u)$
composition: $T_b$ associated with the heat release $T_b - T_u = q/c_p$
flame temperature of a spherical flame: $T_f$, $\theta_f \equiv (T_f - T_u)/(T_b - T_u) = 1/Le$

$$-D_T \frac{1}{R^2} \frac{d}{dR} \left( R^2 \frac{d\theta}{dR} \right) = \frac{D}{R^2} \frac{d}{dR} \left( R^2 \frac{d\psi}{dR} \right) = \dot{W}$$

$R \leq R_f: \quad \theta = \theta_f, \quad \psi = 0$;
$R \to \infty: \quad \theta = 0, \quad \psi = 1$

$$\varepsilon \equiv \beta \frac{(T_b - T^*)}{(T_b - T_u)} > 0 \quad \beta \equiv \frac{E}{k_B T_b} \left( 1 - \frac{T_u}{T_b} \right) \gg 1 \left\{ \begin{array}{l} \varepsilon = O(1): \text{near to flammability limits } (\varepsilon = 0: \text{quenching } \dot{W} = 0) \\ \varepsilon \gg 1, e^{-\varepsilon} \approx 0: \text{far from flammability limits} \end{array} \right. \right.$$  

Thin reaction zone $\beta \to \infty$ (non-dimensional form $\zeta = x/d_L$, $d_L$ for $\varepsilon \gg 1$, $Le = 1$, $2^{nd}$ reaction order)

$$-d^2 \theta/d\zeta^2 = \dot{w}(\theta, \psi), \quad (1/Le)d^2 \psi/d\zeta^2 = \dot{w}(\theta, \psi)$$

$$\theta = \theta_f: \psi = 0$$

$$\dot{w} = \frac{\beta^3}{4} Le^2 e^{\beta(\theta_f - 1)} \left\{ (\theta_f - \theta) \left[ e^{\beta(\theta - \theta_f)} - e^{-\varepsilon - \beta(\theta_f - 1)} \right] \right\}$$

$$\frac{d\theta}{d\zeta} \Rightarrow \left( \frac{d\theta}{d\zeta} \right)^2 = \frac{Le^2}{2} e^{\beta(\theta_f - 1)} \int_{\theta^* = 1 - \varepsilon/\beta}^{\theta_f} \beta^3 (\theta_f - \theta)^2 \left\{ e^{\beta(\theta - \theta_f)} - e^{-\varepsilon - \beta(\theta_f - 1)} \right\} d\theta$$

at the exit of the reaction layer (entrance of the preheated zone)
\[
\left( \frac{d\theta}{d\zeta} \right)^2 = \frac{Le^2}{2} \beta(\theta_f - 1) \int_{\theta = 1 - \varepsilon / \beta}^{\theta_f} \beta^3 (\theta_f - \theta)^2 \left\{ e^{\beta(\theta - \theta_f)} - e^{-\varepsilon - \beta(\theta_f - 1)} \right\} d\theta
\]

\text{at the exit of the reaction layer (entrance of the preheated zone)}

\[
\Theta = \beta(\theta_f - \theta) \in [0, \Theta_f] \quad \text{measure of the distance from the flammability limit: } \Theta_f \in [0, \infty]
\]

\[
d\theta = -\beta d\Theta
\]

\[
(d\theta/d\zeta)^2 = Le^2 e^{\beta(\theta_f - 1)} J(\Theta_f)
\]

\[
J(\Theta_f) = \frac{1}{2} \int_0^{\Theta_f} \Theta^2 (e^{-\Theta} - e^{-\Theta_f}) d\Theta \in [0, 1]
\]

\[
J(\Theta_f) = 1 - e^{-\Theta_f} \left( 1 + \Theta_f + \frac{\Theta_f^2}{2!} + \frac{\Theta_f^3}{3!} \right)
\]

\[
\Theta_f \gg 1 : \quad J \approx 1
\]

\[
0 \leq \Theta_f \ll 1 : \quad J \approx \Theta_f^4 / (4!)
\]

\[
\text{Preheated zone and matching}
\]

flame temperature of the spherical flame

\[
R \geq R_f : \quad \frac{d\theta}{dR} = -\theta_f \frac{R_f}{R^2}, \quad \Theta_f = \frac{1}{Le}
\]

\[
d_L \text{ for } \varepsilon \gg 1, \ Le = 1, 2^{\text{nd}} \text{ reaction order}
\]

\[
\beta \to \infty : \quad \frac{d_L}{R_f} = Le^2 e^{\frac{\beta}{2} \left( \frac{1}{Le} - 1 \right)} \sqrt{J(\Theta_f)}
\]

\[
T_f \to T^* \Rightarrow R_f/d_L \to \infty
\]

\[
\Theta_f \to 0
\]
$T_b$ is determined by the composition of the mixture $Y_{Ru}$ (mass fraction of the limiting component)

$T^*$ is determined by the chemical kinetics $Y_{Ru}$

$\theta^* \text{ depends on the composition}$

\[ \theta^* = \frac{T^* - T_u}{T_b - T_u} \]

temperature of the planar flame depends on the composition

$\theta_f = 1/Le$

\[ \theta_f = \frac{T_f - T_u}{T_b - T_u} = \frac{1}{Le} \]

$T_b = T^*$

\[ \theta^* = 1 \]

$T_f = T^*$

\[ \theta^* = \frac{1}{Le} \]

$T_f = T^*$

\[ \frac{1}{Le} < \theta^* < \frac{1}{Le} < 1 \]

Le > 1 $\Rightarrow$ $T_f < T_b$

Le < 1 $\Rightarrow$ $T_f > T_b$

Flammability limit

flammable mixtures that cannot be ignited (infinite critical radius)

non-flammable mixtures that can be ignited (flame balls)

energetic mixtures

Flammable mixtures

energetic mixtures

Le > 1 : Heavy hydrocarbon lean mixtures

Hydrogen rich mixtures

Le < 1 : Heavy hydrocarbon rich mixtures

Hydrogen lean mixtures

Flammability limits ≠ Critical conditions of ignition

Some hydrocarbon lean mixtures that are flammable cannot be ignited quasi-isobarically
Some hydrocarbon rich mixtures that are non-flammable can sustain curved flames

Limits for upstream propagation ≠ downstream propagation

Buoyancy promoted curved flames

Ignition in turbulent flows


Turbulence facilitates ignition of hydrocarbon lean mixtures
Turbulence may suppress ignition of hydrocarbon rich mixtures

simplest explanation:

Turbulent diffusion coefficients are all equal ⇔ \( Le > 1 \) \( \text{laminar} \)
\( Le = 1 \) \( \text{turbulent} \)
Lecture 7: Flame kernels and quasi-isobaric ignition

7-1. Introduction
7-2. Zeldovich critical radius
7-3. Critical radius near the flammability limits
7-4. Dynamics of slowly expanding flames
Dynamics of slowly expanding flame kernels

Quasi-steady preheated zone of flame kernel?

preheated zone in the reference frame attached to \( R_f(t) \)
\[
\dot{R}_f \equiv \frac{dR_f}{dt}
\]

\[
\frac{\partial \theta}{\partial t} - \dot{R}_f \frac{\partial \theta}{\partial R} - D_T \frac{1}{R^2} \frac{\partial}{\partial R} \left( R^2 \frac{\partial \theta}{\partial R} \right) = 0
\]

quasi-steady state?
\[
t_{\text{relax}} \equiv \frac{R^2}{D_T} \ll t_{\text{evol}} \equiv \frac{R_f}{R_f} R \ll \sqrt{D_T t_{\text{evol}}} \text{, not valid at large distance}
\]

The evolution of spherical flame kernel cannot be quasi-steady at large distance

exact solution of the heat equation with a point energy source \( \partial T/\partial t = D_T \Delta T \) point source, \( R = 0, t > 0 : \dot{Q}(t) \)

\[
T(R, t) - T_u = \int_0^t \frac{\dot{Q}(t - \tau) \exp(-R^2/4D_T \tau)}{\rho c_p (4\pi D_T \tau)^{3/2}} d\tau
\]

\( \dot{Q} = \text{cst.} \)

\[
X' \equiv R/\sqrt{4D_T \tau} \quad \text{d}X' = -2D_T R \frac{d\tau}{(4D_T \tau)^{3/2}}
\]

\[
T - T_u = \frac{1}{4\pi D_T \rho c_p R} \frac{1}{\sqrt{\pi}} \int_{R/\sqrt{4D_T t}}^{\infty} dX' e^{-X'^2}
\]

relax time toward \((T - T_u) \propto 1/R\) increases with \( R \) like \( R^2/D_T \)

\[
R^2/(4D_T t) \to 0
\]
For $\text{Le} < 1$ and near to the Zeldovich radius the slow evolution of flame kernels is governed by the diffusion at large distance

$$\tau \equiv t/t_{\text{ref}} \quad \sqrt{t_{\text{ref}}} \equiv \frac{\beta (1 - \text{Le}^{1/2})}{\text{Le}} \frac{R_{fZ}}{(4\pi D_T)^{1/2}} \quad r_f \equiv R_f/R_{fZ}$$

Joulin’s equation (Joulin 1985)

$$\frac{\beta}{2} \left( \theta_f - \frac{1}{\text{Le}} \right) = -\int_0^\tau \frac{d\tau'}{\tau'\sqrt{2}} \dot{\theta}_f (\tau - \tau')$$

$$\frac{1}{r_f} = \exp \left[ -\int_0^\tau \frac{d\tau'}{\tau'\sqrt{2}} \dot{\theta}_f (\tau - \tau') \right]$$

The structure and the dynamics of flame kernels $\neq$ planar flames even for $R_f \gg d_L$ ($\theta \approx \theta_f/R$)

Extension to a short pulse of an energy source


Extension to the proximity of flammability limits + heat loss


Dynamical quenching of flame kernels in nonflammable mixtures for $\text{Le} < 1$

$$\frac{1}{\sqrt{r_f}} + H_b r_f^2 = 1 - I(\tau) \quad \text{where} \quad I(\tau) \equiv \int_0^\tau \frac{d\tau'}{\tau'^{1/2}} \dot{\theta}_f (\tau - \tau')$$

Self-extinguished flames in micro-gravity experiments of lean methane-air mixtures

Ronney P. *Combust. Flame* (1990) **82**, 1-14
Princeton Summer School on Combustion
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Dynamics of Combustion Waves in Premixed Gases

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Lecture VIII
Thermo-acoustic instabilities. Vibratory flames
Lecture 8: Thermo-acoustic instabilities

Lecture 8-1. Rayleigh criterion

Acoustic waves in a reactive medium
Sound emission by a localized heat source
Linear growth rate

Lecture 8-2. Admittance & transfer function

Flame propagating in a tube
Pressure coupling
Velocity and acceleration coupling

Lecture 8-3. Vibratory instability of flames

Acoustic re-stabilisation and parametric instability (Mathieu’s equation)
Flame propagating downward (sensitivity to the Markstein number)
Bunsen flame in an acoustic field
VIII-1) Rayleigh criterion

Acoustic waves in a reactive medium

Ideal gas

\[ p = (c_p - c_v) \rho T \]

\[ \frac{c_p}{c_p - c_v} \frac{Dp}{Dt} = c_p T \frac{D\rho}{Dt} + c_p \rho \frac{DT}{Dt} \]

\[ D/ Dt \equiv \partial / \partial t + \mathbf{u} . \nabla \]

\[ a^2 = \frac{c_p}{c_v} \frac{D}{c_p - c_v} \frac{Dp}{Dt} = \frac{c_p}{c_p - c_v} \frac{Dp}{Dt} - \frac{c_v}{c_p - c_v} a^2 \frac{D}{Dt} \rho \]

Energy conservation

\[ \rho c_p \frac{D}{Dt} T = \frac{Dp}{Dt} + \nabla . (\lambda \nabla T) + \sum_j Q^{(j)} \hat{W}^{(j)} \]

\[ \frac{c_v}{c_p - c_v} \frac{Dp}{Dt} - \frac{c_v}{c_p - c_v} a^2 \frac{D}{Dt} \rho = \nabla . (\lambda \nabla T) + \sum_j Q^{(j)} \hat{W}^{(j)} \]

\[ Dp / Dt - a^2 D\rho / Dt = \dot{q}_\gamma \]

isentropic acoustic

\[ \delta p = a^2 \delta \rho \]

\[ \dot{q}_\gamma \equiv (\gamma - 1) \left[ \nabla . (\lambda \nabla T) + \sum_j Q^{(j)} \hat{W}^{(j)} \right] \]

\[ \gamma \equiv c_p / c_v \]

\[ \dot{q}_\gamma (\mathbf{r}, t) = \text{heat transfer} + \text{heat release} \]

(rate of energy transfert per unit volume)
\[
Dp/Dt - a^2 D\rho/Dt = \dot{q}_\gamma
\]
\[
\dot{q}_\gamma \equiv (\gamma - 1) \left[ \nabla.(\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)} \right] \quad \gamma \equiv c_p/c_v
\]
Linearization around a uniform state \( \nabla \bar{a} \approx 0 \),
\[
\rho = \bar{\rho} + \rho', \quad p = \bar{p} + p', \quad u = \bar{u} + u', \quad \dot{q}_\gamma = \bar{\dot{q}}_\gamma + \dot{q}'_\gamma
\]
Mean flow velocity neglected in front of the sound speed \( \bar{u}.\nabla \approx 0 \),
\[
\frac{1}{\rho} \frac{D\rho}{Dt} = -\nabla u, \quad \rho \frac{Du}{Dt} = -\nabla p \Rightarrow \partial \rho' / \partial t = -\bar{\rho}\nabla u', \quad \bar{\rho} \partial u' / \partial t = -\nabla p',
\]
Approximations \( \partial / \partial t \)
\[
\partial^2 \rho' / \partial t^2 = \Delta p'
\]
\[
\partial^2 p' / \partial t^2 - \bar{a}^2 \partial \rho' / \partial t = \dot{q}'_\gamma
\]
elimination of \( \rho' \)
\[
\partial^2 p' / \partial t^2 - \bar{a}^2 \Delta p' = \partial \dot{q}'_\gamma / \partial t
\]

**Sound emission by a localized heat source in free space**

Acoustic wavelength \( \gg \) size of the combustion zone \( \partial \dot{q}'_\gamma (r, t) / \partial t = \delta(r)\dot{\Omega}(t) \), \( \dot{\Omega}(t) \equiv \partial \dot{\Omega}(t) / \partial t, \)
\[
\dot{\Omega}(t) = \iiint \dot{q}'_\gamma (r', t) d^3 r'
\]
Green's retarded propagator
\[
(1/\bar{a}^2) \partial^2 G / \partial t^2 - \Delta G = \delta(r)\delta(t), \quad G(r, t) = \bar{a} \delta(r - \bar{a}t)/4\pi r
\]
spherical geometry
\[
p'(r, t) = \frac{1}{4\pi \bar{a}^2} \iiint \frac{1}{r'} \frac{\partial}{\partial t} \dot{q}'_\gamma (r', t - r/\bar{a}) d^3 r' = \frac{\dot{\Omega}(t - r/\bar{a})}{4\pi \bar{a}^2 r}, \quad r = |r|
Liner growth rate

Retro-action loop:

Rocket engines, gas turbines...

Simplest retro-action mechanism: pressure coupling + 1-D geometry

\[
\begin{align*}
\delta q' &= b \delta p/\tau_{ins} \\
\delta p(x, t) &= \sum_{k=-\infty}^{\infty} \tilde{p}_k(t)e^{ikx} \quad k = 2\pi n/L \\
\frac{\partial^2 p'}{\partial t^2} - a^2 \Delta p' &= \partial q'_\gamma / \partial t \\
\frac{d^2 \tilde{p}_k}{dt^2} - \frac{b}{\tau_{ins}} \frac{d\tilde{p}_k}{dt} + a^2 k^2 \tilde{p}_k &= 0 \\
\tilde{p}_k(t) &\propto e^{\sigma(k)t}
\end{align*}
\]

\( \text{Im}(\sigma) = \omega_k + \ldots, \quad \text{Re}(\sigma) = b/(2\tau_{inst}) + \ldots \quad \Rightarrow \]

\[ \left\{ \begin{array}{l}
b > 0 \text{ fluctuations of heat release and pressure in phase: instability} \\
b < 0 \text{ fluctuations of heat release and pressure out of phase: stability}
\end{array} \right. \]

More general retro-action mechanism

\[
\begin{align*}
\delta q'_\gamma(x, t) &= \frac{1}{\tau_{ins}} \int_{-\infty}^{t} b(t - t')\delta p'(x, t')t' \\
b(\tau) &= \int_{-\infty}^{+\infty} r(\omega)e^{i\omega \tau_d(\omega)}e^{i\omega \tau}d\omega + c.c. \\
r(\omega) &> 0 \\
\omega \tau_d(\omega) &\text{ is the phase lag}
\end{align*}
\]

\[ -\pi/2 < \omega_k \tau_d(\omega_k) < +\pi/2 : \text{ Instability} \]

Nonlinear study: limit cycles in the unstable case
Lecture 8: **Thermo-acoustic instabilities**

Lecture 8-1. Rayleigh criterion

- Acoustic waves in a reactive medium
- Sound emission by a localized heat source
- Linear growth rate

Lecture 8-2. Admittance & transfer function

- Flame propagating in a tube
- Pressure coupling
- Velocity and acceleration coupling

Lecture 8-3. Vibratory instability of flames

- Acoustic re-stabilisation and parametric instability (Mathieu’s equation)
- Flame propagating downward (sensitivity to the Markstein number)
- Bunsen flame in an acoustic field
Admittance & transfer function

Flame propagating in a tube

thickness of the flame brush $\ll$ acoustic wavelength

gas expansion $\Rightarrow$ jump of the fluctuations of the flow velocity (acoustics)

$$\frac{\delta u_b - \delta u_u}{U_L} = O(1)$$

jump of pressure across the flame brush is negligible

$$\delta p = \rho a \delta u$$

$$\frac{\delta p_b - \delta p_u}{p} = O(U_L/a)$$

$$\delta p_f : \text{fluctuation of the pressure at the flame}$$

$$p/\rho a^2 = O(1)$$

averaged (per period) flux of combustion energy transferred to the acoustic wave

$$\dot{E}_t = (\delta u_b - \delta u_u)\delta p_f$$

mass conservation (quasi-isobaric combustion)

$$\nabla \cdot \mathbf{u} = \frac{1}{T} \frac{\text{D}\mathbf{T}}{\text{D}t} = \frac{\dot{q}_\gamma / (\gamma - 1)}{\rho c_p T} = \frac{\dot{q}_\gamma}{\rho a^2}$$

$$(\delta u_b - \delta u_u) = \int_{\text{flame brush}} \frac{\delta q_\gamma}{\rho a^2} \, dx$$
\[
\dot{E}_t = (\delta u_b - \delta u_u) \delta p_f \\
(\delta u_b - \delta u_u) = \int \frac{\delta q_\gamma}{\rho a^2} \, dx
\]

**Pressure coupling**

Definition of the admittance function \( Z(\omega) \)

\[
\delta u(t) = \text{Re} \left[ \hat{u}(\omega) e^{i\omega t} \right] \\
\delta p(t) = \text{Re} \left[ \hat{p}(\omega) e^{i\omega t} \right] \\
(\hat{u}_b - \hat{u}_u) = Z(\omega) \hat{p}_f / \rho_b a_b 
\]

\[
\dot{E}_t = \frac{1}{4\rho_b a_b} (Z \hat{p}_f \hat{p}_f^* + Z^* \hat{p}_f \hat{p}_f^*) = \frac{1}{2} \left[ \text{Re} \, Z(\omega) \right] |\hat{p}_f|^2 / \rho_b a_b
\]

instability : \( \text{Re}(Z) > 0 \)

Analytical study of a planar flame submitted to a fluctuation of pressure \( (\beta \rightarrow \infty) \) \( \delta T_f / T_f \propto \delta p_f / p_f \)

|\( Z | = O(M_b) \\
gaseous flame

\[
\frac{\tau_a}{\tau_{ins}} \propto (\gamma - 1) M_b \frac{L}{k_B T_b}
\]

coeff depends on the position in the tube as \( \delta p_f \) does

weak coupling

\[
\frac{\tau_a}{\tau_{ins}} \ll 1
\]

P. Clavin et al. (1990), *J. Fluid Mech.* 216, 299-322


**Solid propellant**


Velocity and acceleration coupling

fluctuating velocity ⇒ modification to flame geometry
⇒ fluctuation of heat release through the flame surface

Transfer function for a flame in a tube $T_r(\omega)$

\[ \hat{u} p_f^* = - \hat{u}^* p_f \]

phase quadrature (acoustic mode of a tube)

\[ \hat{E}_t = \text{Im} \, T_r(\omega)(i \hat{u} u^* p_f^*) / 2 \]

Real number (sign depends on position)

Weakly cellular flame propagating downward in an acoustic wave

acceleration of a curved flame ⇒ modulation of the flame surface

\[ S = \int dy \sqrt{1 + \alpha_y^2} \]

\[ \int \delta q \, dx = \rho_u U_L c_p (T_b - T_u) \delta S / S_o \]

\[ \delta u_b - \delta u_u = \int \frac{\delta q}{\rho a^2} dx \quad \Rightarrow \quad \delta u_b - \delta u_u = (T_b / T_u - 1) U_L \delta S / S_o \]

Consider a curved front slightly perturbed

\[ x = \alpha(y, t) \quad \alpha(y, t) = \tilde{\alpha}(t) \cos(ky) \quad \tilde{\alpha}(t) = \tilde{\alpha}_0 + \tilde{\alpha}_1 e^{i\omega t} + \text{c.c} \]

\[ k \tilde{\alpha}_0 \ll 1 \quad |\tilde{\alpha}_1| \ll \tilde{\alpha}_0 \quad \text{(linear response ok)} \quad \Rightarrow \quad \delta S / S_o = (k^2 / 2) \tilde{\alpha}_0 \tilde{\alpha}_1 e^{i\omega t} + \text{c.c.} \]

\[ \tilde{\alpha}_1 \text{ vs } \hat{u}_u \quad g'(t) = \text{Re} \left[ i \omega \hat{u}_u e^{i\omega t} \right] \quad \bar{g} > 0 \]

lecture IV: \[ \left( 1 + \frac{\rho_b}{\rho_u} \right) \frac{d^2 \tilde{\alpha}}{dt^2} + 2(U_L k) \frac{d\tilde{\alpha}}{dt} - \left( \frac{\rho_u}{\rho_b} - 1 \right) k \left[ -\frac{\rho_b}{\rho_u} [\bar{g} + g'(t)] + U_L^2 k \left( 1 - \frac{k}{k_m} \right) \right] \tilde{\alpha} = 0 \]

Analytical expression ($k = k_c$)

P. Pelcé and D. Rochwerger (1992), J. Fluid Mech. 239, 293-307

ok for the primary instability
Lecture 8: Thermo-acoustic instabilities

Lecture 8-1. Rayleigh criterion

*Acoustic waves in a reactive medium*
*Sound emission by a localized heat source*
*Linear growth rate*

Lecture 8-2. Admittance & transfer function

*Flame propagating in a tube*
*Pressure coupling*
*Velocity and acceleration coupling*

Lecture 8-3. Vibratory instability of flames

*Acoustic re-stabilisation and parametric instability (Mathieu’s equation)*
*Flame propagating downward (sensitivity to the Markestein number)*
*Bunsen flame in an acoustic field*
VIII-3) Vibratory instability of flames

Primary instability + re-stabilisation + parametric instability

**Acoustic instability in Premixed Flames**

![Acoustic instability in Premixed Flames](https://example.com/figure1.png)

**Acoustic re-stabilisation and parametric instability**

Markstein 1964

\[
\tau' \equiv t / \tau_h, \quad \tau_h \equiv 1 / (U_L k), \quad \omega \equiv \omega \tau_h, = (\omega \tau_L) / (k d_L) \quad \kappa = kd_L
\]

\[
v_b \equiv \rho_u / \rho_b > 1 \quad B \equiv \frac{v_b}{v_b + 1} \quad D \equiv v_b \left(\frac{v_b - 1}{v_b + 1}\right) \frac{N}{\kappa} \quad C \equiv \left(\frac{v_b - 1}{v_b + 1}\right) \frac{u_a}{\omega}
\]

Mathieu’s equation. Kapitza pendulum

\[
t \equiv \omega \tau' \quad Y(t) \equiv e^{B \tau'} \hat{\alpha}
\]

\[
\frac{d^2 Y}{dt^2} + \left\{ \Omega + h \cos(t) \right\} Y = 0
\]

\[
\Omega = -\frac{(D + B^2)}{\omega^2} \quad h = C
\]

\[ u_a = 0 \]

Kapitza 1951
Mathieu’s equation. Kapitza pendulum

\[ \Omega = \text{constant} \]

\[ \frac{d^2 Y}{dt^2} + \{\Omega + h \cos(t)\} Y = 0 \]

\( \Omega > 0 \): Oscillator whose frequency \( \sqrt{\Omega} \) is modulated  

Prametic instability (Faraday 1831)

\( \Omega < 0 \): Re-stabilization of an unstable position of a pendulum by oscillations (Kapitza 1951)

Stability limits of the solutions to Mathieus’s equation

White regions: stable. Grey regions unstable

Flame propagating downward

\[ \frac{d^2 \tilde{a}}{d\tau^2} + 2B \frac{d \tilde{a}}{d\tau} + \left[-D + \omega^2 C \cos(\omega \tau)\right] \tilde{a} = 0 \]

G.H. Markestein (1964) Nonsteady flame propagation New York: Pergamon

see §§ 2.5.5, 2.9.2-4 in P.Clavin & G.Searby (2016) Cambridge University Press
Sensitivity of the acoustic instability to the Markstein number and the acoustic frequency

Flattening of Bunsen flames in an acoustic field (Hahnemann Ehret 1943, Durox et al. 1997, Baillot et al. 1999)

Rich Bunsen methane flame + intense axial acoustic field

acoustic equipotential surface

140 Hz
Structure and Dynamics of Combustion Waves in Premixed Gases

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ECM & CNRS (IRPHE)

Lecture IX
Turbulent flames
Lecture 9: Turbulent flames

9-1. Introduction

9-2. Turbulent diffusion

\textit{Einstein-Taylor’s diffusion coefficient}

\textit{Rough model of turbulent transport}

\textit{Well-stirred flame regime}

9-3. Strongly corrugated flamelet regime

\textit{Kolmogorov’s laws}

\textit{Gibson’s scale}

\textit{Elements of fractal geometry}

\textit{Self similarity of strongly corrugated flames}

\textit{Co-variant laws}

9-4. Turbulent combustion noise

\textit{Monopolar sound emission}

\textit{Sound generated by a turbulent flame}

\textit{Blow torch noise}
9-1. Introduction

The problem of premixed flames in a turbulent flow is still widely open

Experiments are difficult. Experimental data are very scattered

Even the simplest model has no known solution (Nonlinear stochastic equation)

Reaction-diffusion wave in a turbulent flow (no gas expansion)

\[ \frac{\partial \theta}{\partial t} + v(r, t) \cdot \nabla \theta - D_T \Delta \theta = \omega'(\theta)/\tau_{rb}. \]

\[ \nabla \cdot v = 0 \]

prescribed turbulent flow (stochastic field)

Same model in the wrinkled flame regime \((l_{tur} \gg d_L, \tau_{tur} \gg \tau_L \Rightarrow U_n = U_L)\)

eq. flame surface \(G(r, t) = G_0\)

\[ \frac{\partial G}{\partial t} + (dr/dt) \cdot \nabla G = 0 \quad dr/dt = v(r, t) - U_n n \quad n = \nabla G/|\nabla G| \]

\[ v = (u, w_y, w_z) \]

\[ x = \alpha(y, z, t) \]

\[ G - G_0 = x - \alpha(y, z, t) \]

\[ \partial \alpha/\partial t - u(r_f, t) + w(r_f, t) \cdot \nabla \alpha = U_{tur} - U_n \sqrt{1 + |\nabla \alpha|^2} \]

\[ \langle S \rangle = \int \int dx dy \left( \sqrt{1 + |\nabla \alpha|^2} \right) \]

\[ U_{tur}/U_L = \frac{\langle \sqrt{1 + |\nabla \alpha|^2} \rangle}{\langle \sqrt{1 + |\nabla \alpha|^2} \rangle} \]

\[ U_{tur} S_0 = U_L \langle S \rangle \]

Unfortunately the condition of existence of \(\langle S \rangle\) is not known!

\[ |v| \ll U_L : \quad U_{tur}/U_L \approx 1 + (|v|/U_L)^2 \]

\[ |v| \gg U_L : \quad U_{tur} \approx |v| \]

(Damköler 1940)

Bending effect modification to the laminar flame structure
9.2. Turbulent diffusion

**Taylor’s diffusion coefficient** (analogy with Einstein random walk for molecular diffusion)

1-D for simplicity: \( \frac{dx}{dt} = v(t), \ x(t) = \int_0^t v(t') dt' \) \( v(t) = v(x(t), t) \)

\( \langle x^2(t) \rangle = \int_0^t dt' \int_0^t dt'' \langle v(t')v(t'') \rangle \)\[ \langle x^2(t) \rangle = 2 \int_0^t dt' \int_0^t d\tau \langle v(t')v(t' - \tau) \rangle \]

turbulence: homogeneous in time \( \langle v(t)v(t - \tau) \rangle = \langle v^2 \rangle g(\tau) \) \( g(0) = 1, \ \lim_{\tau \to \infty} g = 0 \)

integration by parts \( \langle x^2(t) \rangle = 2 \langle v^2 \rangle \int_0^t (t - \tau) g(\tau) d\tau \) where \( \int_0^\infty \tau g(\tau) d\tau = O(\tau_I^2) \)

\( t \gg \tau_I, 1-D: \langle x^2(t) \rangle = 2D_{tur} t, \quad 3-D: \langle x^2(t) \rangle = 6D_{tur} t \), where \( D_{tur} \) turbulent diffusion coefficient

Rough model for the turbulent transport (analogy with molecular diffusion)

\( \langle v\theta \rangle \approx -D_{tur} \nabla \langle \theta \rangle, \quad \langle \nabla \cdot (v\theta) \rangle \approx -D_{tur} \Delta \langle \theta \rangle \)

limited to scalar mixing with small displacement / size (blobs, sheets ..) \( l_I \ll L \) \( v_I \approx \langle v^2 \rangle^{1/2} \)

\( l_I \equiv v_I \tau_I \)

\( D_{tur} = l_I v_I \)

Well-stirred flame regime of Damköhler (1940) \( l_I \ll d_L \) and \( D_{tur} \gg D_T \)

little practical importance

\( U_{tur} \approx \sqrt{D_{tur}/\tau_b} \) \( \frac{U_{tur}}{U_L} \approx \sqrt{\left( \frac{l_I}{d_L} \right) \left( \frac{v_I}{U_L} \right)} \gg 1, \quad d_{tur} \approx D_{tur}/U_{tur} \gg d_L \)
9.3. Strongly corrugated flamelet regime

Kolmogorov’s laws
homogeneous, isotropic and fully developed turbulence

Richardson cascade

Decomposition in a continuos set of vortices
\[ l_i, \tau_i, v_i \equiv l_i/\tau_i \]

\[ \text{turn-over velocity} \quad \text{local Reynolds nb} \quad \nu \equiv \mu/\rho \]

Kolmogorov scale
\[ l_K, \tau_K, v_K \quad \text{Re}_K = 1 \quad l_i > l_K \quad v_i > v_K \quad \forall i \]

Integral scale
\[ l_I, \tau_I, v_I \quad \text{Re}_I \gg 1 \quad l_i > l_I \quad v_i > v_l \quad \forall i \]

Scaling laws (dimensional analysis)
\[ l_K \ll l_i \ll l_I \]

energy transfer in NS eqs:
\[ \rho (v \cdot \nabla) v^2 / 2 \]

\[ v_i^3 / l_i \equiv \epsilon \approx \text{cst} \]

\[ \Rightarrow \quad v_i \approx \epsilon^{1/3} l_i^{1/3}, \quad v_i^2 \approx \epsilon^{2/3} l_i^{2/3}, \quad \tau_i \approx \epsilon^{-1/3} l_i^{2/3} \]

dissipation rate of energy:
\[ \nu \nabla \cdot \nabla \nu \]

\[ \epsilon = \nu ^2 / l_K^2 \quad \Rightarrow \quad \epsilon = \nu_0^3 / l_I \]

\[ \text{Re}_K \equiv v_K l_K / \nu = 1 \quad \Rightarrow \quad l_I / l_K \approx \text{Re}_I^{3/4}, \quad v_I / v_K \approx \text{Re}_I^{1/4}, \quad \tau_I / \tau_K \approx \text{Re}_I^{1/2} \]

\[ \text{Re}_I \gg 1 \]

energy spectrum:
\[ \langle v^2 \rangle / 2 = \int_0^\infty dk \ E(k) \quad E(k) \approx \epsilon^{2/3} k^{-5/3} \quad K41 \ 	ext{scaling law} \]

definition of strongly corrugated flames
\[ v_K \ll U_L \ll v_I \]

\[ d_L \ll l_K, \quad \tau_L \ll \tau_K \quad \text{no modification to the laminar flame structure} \]

Gibson scale \[ l_G \quad (\text{Peters 1986}) \]

definition of the Gibson scale: smallest size of the wrinkles on the flame front

\[ \text{turn-over time} = \text{transit time across the vortex} \quad \tau_i \approx l_i / U_L \quad \Rightarrow \quad v_i \approx U_L \]

\[ l_G \equiv U_L^3 / \epsilon \quad \Rightarrow \quad l_K \ll l_G \ll l_I \]

\[ l_i < l_G \Rightarrow u_i < U_L \Rightarrow l_i / U_L < \tau_i = l_i / u_i \]

many scales of wrinkles \[ l_G \ll l_I \Rightarrow \text{fractal geometry of the flame front} \]

Elements of fractal geometry

Weaker resolution \( l_j, \quad l_G < l_j < l_i \)

nb of cubes of size \( l_j \) that intersect the surface within the volume \( l_i^3 \)

Total surface area in a cube of size \( l_i, \quad l_G < l_i < l_I \)

nb of cubes of size \( l_G \) that intersect the surface within the volume \( l_i^3 \)

Fractal dimension \( D_f > 2 \): \( N_{i,j} \approx \frac{l_j^2}{l_j} \)

\( S_{i,j}/l_i^2 \approx (l_i/l_j)^{D_f-2} \)

Regular surface: \( D_f = 2 \Rightarrow \) total area \( S_i \) in a box of size \( l_i \)

\( S_i/l_i^2 = \lim_{l_j \rightarrow 0} S_{i,j}/l_i^2 = \text{finite constant} \)

For a flame of thickness \( d_L \) its area is well defined for wrinkles whose scale is larger than \( d_L, \quad l_j > d_L \)

The fractal dimension \( D_f > 2 \) can concern only scales greater than the smallest wrinkles

Fractal dimension of a turbulent flame can be meaningful only for \( d_L < l_G < l_j < l_i < l_I \)
Self similarity of strongly corrugated flames

Assumption: the Kolmogorov cascade is not modified by gas expansion

\[ v_K \ll U_L \ll v_I \quad d_L \ll l_K \ll l_G \ll l_I \]

Contamination time vs combustion time

Kolmogorov cascade

\[ \tau_i \approx \epsilon^{-1/3} l_i^{2/3} \quad \text{ok for } l_i \gg l_G \]

Fastest contamination: integral scale \( v_I \gg v_i \). \( U_{\text{tur}} = v_i \)?

ok if the combustion time of the vortex is not longer than the turnover time

Self similar law

An effective front of thickness \( l_i \) is defined at each scale

A flame velocity \( U_i \) can be defined at each scale if

\[ U_i = \langle S_{i,j} / l_i^2 \rangle U_j \quad U_i / U_j = \langle S_{i,j} \rangle / l_i^2 \]

At the Gibson scale the combustion time of the vortex = turnover time \( U_L = v_G \implies l_G / U_L = l_G / v_G \)

Self similarity: same law at all scales \( \Rightarrow \) combustion time of the vortex = the turnover time \( \forall l_i \)

\[ l_i / U_i = \tau_i \implies U_i = v_i \]

Kolmogorov cascade \( \Rightarrow \) small vortices burn faster than larger ones

\[ U_{\text{tur}} = v_I, \quad l_{\text{tur}} = l_I \]

Fractal dimension of the flame surface:

Kolmogorov scaling \( v_i / v_j = (l_i / l_j)^{1/3} \)

\[ \langle S_{i,j} \rangle / l_i^2 \Rightarrow v_i / v_j = \langle S_{i,j} \rangle / l_i^2 \Rightarrow \langle S_{i,j} \rangle / l_i^2 = (l_i / l_j)^{1/3} \]

\[ \Rightarrow D_f = 7/3 \]

def fractal dimension The result is the same for all mixtures...??
Co-variant laws


More general law independent of the turbulent scaling and satisfying additivity

Turbulent energy contained in the range \([l_i, l_j]\): 
\[ v_{i,j}^2 \equiv \sum_{k=i}^{j-1} v_k^2 \quad v_k^2 : \text{energy in } [k, k+1] \]

Co-variant law = same for each couple of length scales \(l_i, l_j\)  \(l_i > l_j\)

The only co-variant law for the flame velocity \(U_i\) at scale \(l_i\) satisfying additivity is 
\[ U_i^2 = U_j^2 + c v_{i,j}^2 \]

Co-variance? \(l_i > l_k > l_j\), 
\[ v_{i,j}^2 = v_{i,k}^2 + v_{k,j}^2 \quad U_i^2 = U_j^2 + c v_{i,k}^2 + c v_{k,j}^2 = U_k^2 + c v_{i,k}^2 \]

co-variance ok 
\[ U_i^2 = U_k^2 + c v_{i,k}^2 \]

Not limited to a strong turbulence

The case \(c = 1\) covers the known results at low and large turbulence intensity

Reasonably good agreement with experiments

\[ v/U_L = O(1), \quad l I/l_K \approx 180 \]
9-4. Turbulent combustion noise

wavelength \( a/\omega \gg L \) size of the flame

**Monopolar sound emission**

Deformable (small) body with fluctuating volume \( V(t) \)

\[
\mathbf{u} = \nabla \phi(\mathbf{r}, t) \quad \text{acoustic potential} \quad \phi(\mathbf{r}, t) = -\frac{\dot{V}(t - a r)}{4\pi r} \quad r \equiv |\mathbf{r}|, \quad \dot{V}(t) \equiv \frac{dV}{dt}
\]

\( r \gg L : \quad \mathbf{v} = (4\pi ar)^{-1}\dot{V}(t - r/a), \quad \ddot{V}(t) \equiv \frac{d^2V(t)}{dt^2} \)

Radiated flux of energy (intensity of sound) \( \mathbf{I} = \rho a \langle v^2 \rangle \)

Total acoustic energy radiated/unit time \( I = (\rho/4\pi a)\left\langle (d^2V/dt^2)^2 \right\rangle \) mass flow rate of burned gas in the lab frame

**Sound generated by a turbulent flame** \( \frac{dV}{dt} = \dot{M}_b/\rho_b \)

\[
\dot{M}_b = \rho_b \int_S (\mathcal{D}_f + \mathcal{U}_b)d^2\sigma \quad \dot{M}_u = \rho_u \int_S (\mathcal{D}_f + \mathcal{U}_L)d^2\sigma \quad \rho_u \mathcal{U}_L = \rho_b \mathcal{U}_b
\]

normal flame velocity in the lab frame

elimination of \( \mathcal{D}_f \)

\( \frac{dV}{dt} = \dot{M}_b/\rho_b = \dot{M}_u/\rho_u + (\mathcal{U}_b - \mathcal{U}_L)S \)

\( \frac{d^2V}{dt^2} = (\mathcal{U}_b - \mathcal{U}_L)dS/dt \)

\( \int \) constant

\[ I = (\rho/4\pi a)(\mathcal{U}_b - \mathcal{U}_L)^2 \left\langle (dS/dt)^2 \right\rangle \]

intensity of sound

Strahle 1985

\[ \frac{d\tilde{I}(\omega)}{d\omega} = \frac{\rho}{4\pi a} (\mathcal{U}_b - \mathcal{U}_L)^2 \int_0^\infty dt \exp{i\omega t} \left\langle \dot{S}(t)\dot{S}(0) \right\rangle \]

power spectrum of sound

\( \dot{S}(t) \equiv dS/dt \)
total intensity of sound

\[ I = (\rho/4\pi a)(U_b - U_L)^2 \langle (dS/dt)^2 \rangle \]

Strongly corrugated regime with the Kolmogorov scaling

\[ D_f = 7/3 \quad \Rightarrow \quad I \approx \frac{1}{4\pi} \left( \frac{T_b}{T_u} - 1 \right)^2 (\rho\Delta V) \frac{v_I^4}{al_I} \]

\[ d\tilde{I}(\omega) \propto \omega^{-5/2} d\omega \]


in agreement with experiments on very large burners

(Abugov Obrezkov 1978)

Blowtorch noise

Combustion noise is two orders of magnitude higher

the noise is not resulting from the direct interaction of upstream turbulence on the flame front amplification by the intrinsic flame instability is essential

Searby et al. 2001 Phys. Fluids. 13, 3270-3275
Princeton Summer School on Combustion  
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Dynamics of Combustion Waves  
in Premixed Gases

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Lecture X  
Supersonic waves (shocks and detonations)
Lecture 10: Supersonic waves

10-1. Background

*Model of hyperbolic equations for the formation of discontinuity*

*Riemann invariants*

*Rankine-Hugoniot conditions for shock waves*

10-2. Inner structure of a weak shock wave

*Formulation*

*Dimensional analysis*

*Analysis*

10-3. ZND structure of detonations

10-4. Selection mechanism of the CJ wave
10-1. Background

PLANAR SHOCK WAVE
INERT GAS

SUPERSOONIC
FRONT

$\mathcal{D} > a_u$

MOVING
PISTON

$\nu_p$

GAS AT REST

UNIFORM FLOW

$\text{distance } \propto (\mathcal{D} - \nu_p) t$

Supersonic

Subsonic

$\mathcal{D} > a_u$

$U_N < a_N$

$U_N = \mathcal{D} - \nu_p$

thickness: few mean free paths

Poisson 1808, Stokes 1848, Riemann 1860, Rankine 1869, Hugoniot 1889, Rayleigh 1910
SHOCK WAVE AS A SINGULARITY OF THE EULER EQUATIONS

Riemann (1860)
shock wave \approx \text{discontinuity in the solution of the Euler equations}

**Model of hyperbolic equations for the formation of discontinuities**

\[
\frac{\partial u}{\partial t} + a(u) \frac{\partial u}{\partial x} = 0
\]

\(a(u)\) given function

**initial condition**

\[t = 0 : \quad u = u_o(x)\]

\[u = u(x, t)\]

Simple case: linear equation

\[a = a_o = \text{cst.} : \quad u = u_o(x - a_o t)\]

propagation at constant velocity without deformation

**Nonlinear equation** \(a(u)\) \(\frac{da}{du} \neq 0\)

**Method of characteristics**

The solution is conserved along any trajectory \(dx/dt = a(u)\) in the phase plan \((x, t)\).

\[u = u(x(t), t) \quad \frac{du}{dt} = 0 \quad \Rightarrow \quad \frac{dx}{dt} = \text{constant}\]

\(u(x, t)\) is constant along the straight lines \(x = a_o t + x_o\): \(u = u_o\) \(u_o \equiv u(a_o)\)

\(du_0/dx_0 \neq 0 \quad \Rightarrow \quad da_0/dx_0 \neq 0\) **Intersection of characteristics:** finite time singularity
Nonlinear equation \( \partial u/\partial t + a(u) \partial u/\partial x = 0 \)

\[ t = 0 : \quad u = u_o(x) \]
\[ u = u(x, t) \] ??

**Method of characteristics**

trajectories \( x(t) : \quad dx/dt = a(u) \quad u = u(x(t), t) \quad du/dt = 0 \)

\[ u(x, t) = \text{cst.} \Rightarrow a(x, t) = \text{cst.} \]

\( u(x, t) \) is constant along the straight lines; \( t = 0 : \ x = a_o t + x_o, \ u = u_o \)

\[ x = a_o t + x_o \quad u_o \equiv u(a_o) \]

Speed increases with increasing \( u \), \( da/du > 0 \)

\[ u_o(x) \equiv u(x, t = 0) \]

**Initial state**

\[ \text{da/du} > 0 : \text{larger values of } u \text{ run faster} \]

\( \Rightarrow \text{formation of singularities after a finite time} \)
\[ \partial u / \partial t + a(u) \partial u / \partial x = 0 \]

Speed increases with increasing \( u \), \( da / du > 0 \)

\[ \Rightarrow \text{formation of singularities after a finite time} \]

larger values run faster

\[ t > t_b : \text{multivalued solution. Wave breaking} \]

\( u(x, t) \) constant on straight trajectories in the phase plane \((t, x)\)

\[ x(x_0, t) = x_0 + a_0(x_0)t : \quad u(x, t) = u_0(x_0) \]

\[ \partial x / \partial x_0 = 1 + t(da_0 / dx_0) \quad \partial x_0 / \partial x = [1 + t(da_0 / dx_0)]^{-1} \]

\[ \frac{\partial u}{\partial x} = \frac{\partial x_0}{\partial x} \frac{du_0}{dx_0} \quad \frac{\partial u}{\partial x} = \frac{du_0}{dx_0} / [1 + t(da_0 / dx_0)] \]

diverges at time \( t = \frac{1}{-da_0 / dx_0} \) where \( da_0 / dx_0 < 0 \)

\[ t_b \equiv \text{time of wave breaking} \text{ (shortest time for the divergence of } \partial u / \partial x) \]

\[ t_b = \frac{1}{\max |da_0 / dx_0|} \]
\[ \frac{\partial u}{\partial t} + a(u)\frac{\partial u}{\partial x} = 0 \quad \text{conservative form} \quad \frac{\partial u}{\partial t} + \frac{\partial j}{\partial x} = 0 \]

\[ j(u) \quad \frac{dj}{du} = a(u) \]

\[ j(u) \equiv \int_{u_-}^{u} a(u')du' \]

**Discontinuous solution**

Are step functions \( u_+ \neq u_- \) propagating at constant velocity \( D \) solutions?

\[ u(\xi) \quad \xi = x -Dt \]

\[ \frac{\partial}{\partial t} = -D\frac{d}{d\xi} \quad \frac{\partial}{\partial x} = \frac{d}{d\xi} \]

\[ D? \]

\[ -D \frac{du}{d\xi} + \frac{dj}{d\xi} = 0 \quad \quad j - Du \quad \text{is a conserved scalar} \]

\[ j(u_+) - Du_+ = j(u_-) - Du_- \]

\[ D = \frac{j(u_+) - j(u_-)}{u_+ - u_-} \]

Infinite numbers of solutions !! **Ill posed problem**

\[ f(u) \times \left( -D \frac{du}{d\xi} + \frac{dj}{d\xi} \right) = 0 \quad \forall \text{ function } f(u) \]

Definition of \( F(u) \) and \( G(u) : \)

\[ \frac{dF}{du} \equiv f(u) \quad \frac{dG}{du} \equiv f(u)a(u) \]

\[ \frac{d}{du} [-DF(u) + G(u)] = 0 \quad \Rightarrow \]

\[ D = \frac{G(u_+) - G(u_-)}{F(u_+) - F(u_-)} \]
Discontinuous solutions

\[ \partial u/\partial t + a(u)\partial u/\partial x = 0 \]

Are step functions \( u_+ \neq u_- \) propagating at constant velocity \( D \) solutions?

\[ u(\xi) \quad \xi = x - Dt \]

Infinite numbers of solutions!! Ill posed problem

adding a dissipative term makes the problem well posed

\[ \frac{d}{d\xi} \left[ -uD + j(u) - \epsilon \frac{du}{d\xi} \right] = 0 \]

\[ \epsilon \frac{du}{d\xi} = j(u) - uD + \text{cst} \quad \frac{\xi}{\epsilon} = \int_0^u \frac{du}{j(u) - uD + \text{cst}} \]

\[ j(u) \equiv \int_{u_-}^u a(u')du' \]

\[ \xi = \pm \infty : \frac{du}{d\xi} = 0 \Rightarrow 2 \text{ expressions of the cst that should be equal} \Rightarrow \text{a single value of } D \]

\[ D = \frac{j(u_+) - j(u_-)}{u_+ - u_-} \]

\( u(\xi) \) continuous function \( \lim_{\epsilon \to 0} u = \text{step function} \)

\( a(u) = u \): Burgers equation. Analytical solution to the initial value problem

Riemann invariants (1860)

Euler equation + constant entropy + ideal gas: \( a^2 = \frac{dp}{d\rho} = \gamma \frac{p}{\rho} \Rightarrow \frac{2}{a} = \frac{dp}{d\rho} - \frac{d\rho}{\rho} \Rightarrow 2\frac{da}{a} = (\gamma - 1)\frac{d\rho}{\rho} \)

\[
\lambda \times \frac{\partial}{\partial t} \rho + u \frac{\partial}{\partial x} \rho + \rho \frac{\partial}{\partial x} u = 0 + a^2 \frac{\partial}{\partial t} \rho + u \frac{\partial}{\partial t} u + u \frac{\partial}{\partial x} u = 0
\]

\[
\lambda \frac{\partial}{\partial t} \rho + \left( \lambda u + \frac{a^2}{\rho} \right) \frac{\partial}{\partial x} \rho + \frac{\partial}{\partial t} u + (\lambda \rho + u) \frac{\partial}{\partial x} u = 0
\]

choose \( \lambda \) such that \( \lambda u + a^2/\rho = \lambda (\lambda \rho + u) \Rightarrow \lambda = \pm a/\rho \)

\( \lambda \rho = \pm a \)

\( \lambda \rho + u = u \pm a \)

2 characteristics:

\[
\lambda d\rho + du = 0 \quad \pm \frac{a}{\rho} d\rho + du = 0
\]

\[
J_+ = \frac{2}{\gamma - 1} a + u = \text{cst sur } C_+ \quad J_- = \frac{2}{\gamma - 1} a - u = \text{cst sur } C_-
\]

Simple waves

\( C_+ \) are straight lines

Rarefaction wave

Composition wave

formation of a singularity: shock wave
**Centred waves**

\[ t < 0 : \text{ piston velocity } = 0 \]
\[ t > 0 : \text{ piston velocity } = \text{cst} \neq 0 \]

Sel-similar solutions \( x/t \)

**Compression**

- Shock wave at constant velocity > piston velocity
- no discontinuity of \( u \)
- discontinuity of \( du/dx \) propagating at the local sound speed
- fully unsteady process: thickness \( \frac{u_p t}{2} \)

**Rarefaction**

- Uniform flow at piston speed
- Centred rarefaction wave
- Fluid at rest

\[ x < 0 : \text{ piston velocity } = 0 \]
\[ x > 0 : \text{ piston velocity } = \text{cst} \neq 0 \]
Rankine-Hugoniot conditions

(jumps across a shock wave)
Shock waves

Rankine-Hugoniot conditions for shock waves
(1870 – 1880)

Eqs for the conservation of mass, momentum and energy

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0 \quad \frac{\partial (\rho u)}{\partial t} = -\frac{\partial}{\partial x} \left( p + \rho u^2 - \rho \frac{\partial u}{\partial x} \right) \quad \frac{\partial (\rho u_{\text{tot}})}{\partial t} = -\frac{\partial}{\partial x} \left[ \rho u(h + u^2/2) - \lambda \frac{\partial T}{\partial x} - \mu u \frac{\partial u}{\partial x} \right]
\]

Written in the moving frame of the shock at velocity \(D\)

Steady problem

\[
p_u - p_N = m^2 \left[ \frac{1}{\rho_N} - \frac{1}{\rho_u} \right] \quad h_u - h_N = m^2 \left[ \frac{1}{\rho_N^2} - \frac{1}{\rho_u^2} \right]
\]

\[
h(\rho_u, p_u) - h(\rho_N, p_N) + \frac{1}{2} \left( \frac{1}{\rho_u} + \frac{1}{\rho_N} \right) (p_N - p_u) = 0
\]

Hugoniot curve \( (p - 1/\rho) \)

\[h(p, \rho) - h(p_u, \rho_u) - \frac{1}{2} \left( \frac{1}{\rho_u} + \frac{1}{\rho} \right) (p - p_u) = 0\]

Michelson-Rayleigh line

\[p - p_u = -m^2 \left( \frac{1}{\rho} - \frac{1}{\rho_u} \right)\]
Ideal (polytropic) gas \( \gamma \equiv \frac{c_p}{c_v} \)

\[
p = (c_p - c_v) \rho T, \quad h = c_p T = \frac{\gamma}{\gamma - 1} \frac{p}{\rho}
\]

\[
h(p, \rho) - h(p_u, \rho_u) - \frac{1}{2} \left( \frac{1}{\rho_u} + \frac{1}{\rho} \right) (p - p_u) = 0
\]

\[
\mathcal{P} \equiv \frac{(\gamma + 1)}{2\gamma} \left( \frac{p}{p_u} - 1 \right), \quad \mathcal{V} \equiv \frac{(\gamma + 1)}{2} \left( \frac{\rho_u}{\rho} - 1 \right)
\]

Hugoniot curve \( (\mathcal{P} + 1)(\mathcal{V} + 1) = 1 \)

Michelson-Rayleigh line \( \mathcal{P} = -M_u^2 \mathcal{V} \)

quadratic equation for \( \mathcal{V} \), 2 solutions: \( \mathcal{V} = 0 \), \( \mathcal{V} = \mathcal{V}_N \)

**Shock wave (Neumann state) vs \( M_u \)**

<table>
<thead>
<tr>
<th>( u_N )</th>
<th>( \rho_u = \frac{(\gamma - 1)M_u^2 + 2}{(\gamma + 1)M_u^2} )</th>
<th>( p_N = \frac{2\gamma M_u^2 - (\gamma - 1)}{(\gamma + 1)} )</th>
<th>( T_N = \frac{2\gamma M_u^2 - (\gamma - 1)}{(\gamma + 1)^2 M_u^2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho_N = \frac{(\gamma - 1)M_u^2 + 2}{(\gamma + 1)M_u^2} )</td>
<td>( p_a = 2\gamma M_u^2 - (\gamma - 1) )</td>
<td>( T_a = \frac{2\gamma M_u^2 - (\gamma - 1)}{(\gamma + 1)^2 M_u^2} )</td>
<td></td>
</tr>
</tbody>
</table>

\( M_N = \frac{u_N}{a_N} < 1 \), \( M_N^2 = \frac{(\gamma - 1)M_u^2 + 2}{2\gamma M_u^2 - (\gamma - 1)} \) \( \iff \) \( 2\gamma M_u^2 M_N^2 - (\gamma - 1)(M_u^2 + M_N^2) - 2 = 0 \)

**General comments**

The Hugoniot curve is tangent to the isentropic

the entropy change along the Hugoniot curve is of third order \( \Rightarrow M_u \equiv \mathcal{D}/a_u > 1 \)

\[
\begin{align*}
\delta s &= s - s_u, & \delta p &= p - p_u, \\
\delta s &\neq \delta p \\
\frac{\delta s}{\delta p} &= \frac{1}{12T_u} \left( \frac{\partial^2 s}{\partial p^2} \right)_s (\delta p)^3
\end{align*}
\]

The Hugoniot relation is not an iso-function of state

\[
h(p, \rho) - h(p_u, \rho_u) - \frac{1}{2} \left( \frac{1}{\rho_u} + \frac{1}{\rho} \right) (p - p_u) = 0 \quad \text{cannot be written in the form} \quad H(1/\rho, p) = H(1/\rho_u, p_u)
\]

\[
h(p, \rho) - h(p_N, \rho_N) - \frac{1}{2} \left( \frac{1}{\rho_N} + \frac{1}{\rho} \right) (p - p_N) = 0 \neq h(p, \rho) - h(p_u, \rho_u) - \frac{1}{2} \left( \frac{1}{\rho_u} + \frac{1}{\rho} \right) (p - p_u) = 0
\]

Rarefaction shock does not exist. The entropy of the fluid increases through the shock

\[\text{Irreversibility}\]

\[\rho u \frac{ds}{dx} = \frac{d}{dx} \left( \frac{\lambda}{T} TX \right) + \dot{\omega}_s, \quad \dot{\omega}_s > 0\]

P. Clavin X
10-2. Inner structure of a weak shock wave

Clavin, Searby (2014) Cambridge University Press, pp. 219-222

\[
\frac{\partial p}{\partial t} + \frac{\partial(pu)}{\partial x} = 0 \quad \frac{\partial(pu)}{\partial t} = -\frac{\partial}{\partial x} \left( p + \rho u^2 - \mu \frac{du}{dx} \right) \quad \frac{\partial(\rho e_{\text{tot}})}{\partial t} = -\frac{\partial}{\partial x} \left[ \rho u(h + \frac{u^2}{2}) - \lambda \frac{dT}{dx} - \mu u \frac{du}{dx} \right]
\]

Formulation

( reference frame attached to the shock wave )

\[
\rho u = m, \quad p + \rho u^2 - \mu \frac{du}{dx} = \text{cst.} \quad m \left( h + \frac{u^2}{2} \right) - \lambda \frac{dT}{dx} - \mu u \frac{du}{dx} = \text{cst.}
\]

\( x \to -\infty : \quad p = p_u, \quad \rho = \rho_u, \quad u = D \quad x \to \infty : \quad dp/dx = 0, \quad dp/dx = 0, \quad du/dx = 0
\]

\[
m = \rho_u D \quad \frac{p}{\rho} = (\gamma - 1)c_v T \quad h = \frac{\gamma}{\gamma - 1} \frac{p}{\rho}
\]

Two coupled equations for \( p \) and \( \nu \equiv 1/\rho, m \) given \( \quad (u = mv, \quad c_v T = pv/(\gamma - 1)) \)

\[
(p - p_u) + m^2(v - v_u) = \mu m \frac{dv}{dx}, \quad \frac{\gamma}{\gamma - 1} (pv - p_u v_u) - \frac{1}{2} (p - p_u)(v + v_u) = \frac{\gamma}{\gamma - 1} \frac{\lambda}{mc_p} \frac{d(pv)}{dx} + \frac{\mu m}{2} (v - v_u) \frac{dv}{dx}
\]

\( x \to \infty : \quad dp/dx = 0, \quad dv/dx = 0 \)

Dimensional analysis

\[
u/a = O(1), \quad \text{mean free path} \quad \mu/\rho = \text{viscous diffusion coefficient} \approx \ell/a \implies \text{thickness of shock waves} \approx \text{mean free path}
\]

macroscopic equations not valid ?

ok for weak shock!
\[ M_u \equiv \frac{D}{a_u} > 1 \quad \text{Analysis for} \quad \epsilon \equiv M_u - 1 \ll 1 \quad \text{(weak shock)} \quad \frac{D}{a_u} = 1 + \epsilon \]

\[
(p - p_u) + m^2(v - v_u) = \mu m \frac{d\nu}{dx},
\]

\[
\frac{\gamma}{\gamma - 1} (p v - p_u v_u) - \frac{1}{2} (p - p_u)(v + v_u) = \frac{\gamma}{\gamma - 1} \frac{\lambda}{mc_p} \frac{d(p v)}{dx} + \frac{\mu m}{2} O(\epsilon^3) \frac{dv}{dx}
\]

\[ x \rightarrow -\infty : p = p_u, \quad v = v_u \quad \quad x \rightarrow \infty : dp/dx = 0, \quad dv/dx = 0 \]

**Non-dimensional equations**

\[ v \equiv 1/\rho \quad \nu \equiv (v - v_u)/v_u = O(\epsilon) \quad \pi \equiv (p - p_u)/p_u = O(\epsilon) \]

\[ \lambda/mc_p = D_{Tu}/(\rho_u D) \approx D_{Tu}/(\rho_u a_u) \quad \text{Pr} \equiv \mu/\rho_u (\rho_u D_{Tu}) \]

\[ \xi \equiv x/\ell \quad \ell \equiv D_{Tu}/a_u \quad a_u = \sqrt{\gamma p_u/\rho_u} \quad \quad M_u^2 = 1 + 2\epsilon + .. \]

\[
\begin{aligned}
\frac{1}{\gamma} \pi + (1 + 2\epsilon) \nu &= \text{Pr} \frac{d\nu}{d\xi} + O(\epsilon^3), \\
\left(\frac{\gamma + 1}{2\gamma}\right) \pi \nu + \frac{1}{\gamma} \pi + \nu &= \frac{d\pi}{d\xi} + \frac{d\nu}{d\xi} + O(\epsilon^3), \\
\frac{1}{\gamma} \pi + \nu &= \text{Pr} \frac{d\nu}{d\xi} - 2\epsilon \nu + O(\epsilon^3), \quad \Rightarrow \quad \left(\frac{\gamma + 1}{2\gamma}\right) \pi \nu + \text{Pr} \frac{d\nu}{d\xi} - 2\epsilon \nu &= \frac{d\pi}{d\xi} + \frac{d\nu}{d\xi} + O(\epsilon^3),
\end{aligned}
\]

\[ \pi = -\gamma \nu + O(\epsilon^2), \quad \Rightarrow \quad [(\gamma - 1) + \text{Pr}] \frac{d\nu}{d\xi} = \left(\frac{\gamma + 1}{2} \nu + 2\epsilon\right) \nu \]

**Rankine-Hugoniot**

\[ \nu_N = -4\epsilon \frac{1}{\gamma + 1} \quad \pi_N = -4\epsilon \frac{\gamma}{\gamma + 1} \]

\[ \nu_N = -\frac{4\epsilon}{\gamma + 1} \quad \pi_N = \frac{\gamma}{\gamma + 1} \quad \text{shock thickness} \]
\( M_u \equiv \frac{D}{a_u} > 1 \)  \textbf{Analysis for} \( \epsilon \equiv M_u - 1 \ll 1 \)  \textbf{(weak shock)}

\[
[(\gamma - 1) + Pr] \frac{d\nu}{d\xi} = \left(\frac{\gamma + 1}{2} \nu + 2\epsilon\right) \nu
\]

\[
\frac{2}{\gamma + 1} [(\gamma - 1) + Pr] \frac{d\nu}{d\xi} = \nu(\nu - \nu_N) \leq 0
\]
\( \xi = -\infty : \) initial state, \( \nu = 0, \quad \xi = +\infty : \) shocked gas, \( \nu = \nu_N = -4\epsilon/(\gamma + 1) \)

\[
\nu_N = -\frac{4\epsilon}{\gamma + 1}
\]

\( Y \equiv \frac{(\gamma + 1)}{4\epsilon} \nu \in [0, -1] \)
\( \zeta \equiv \frac{2}{[(\gamma + 1) + Pr]} \epsilon \xi = \frac{2}{[(\gamma + 1) + Pr]} \frac{x}{(\ell/\epsilon)} \)

\[
\zeta = O \left(\frac{x}{\ell/\epsilon}\right)
\]

\[
\frac{dY}{d\zeta} = Y(Y + 1) < 0
\]

\( \zeta = -\infty : Y = 0, \quad \zeta = +\infty : Y = -1 \)

\[
\zeta = \int \frac{dY}{Y(Y + 1)} \quad Y(\zeta) = -\frac{e^\zeta}{e^\zeta + 1}
\]

\text{shock thickness} = \text{mean free path}/(M_u - 1)

\text{microscopic length if} \( M_u - 1 = O(1) \)
\text{macroscopic length if} \( (M_u - 1) \ll 1 \)

\[
x = O(l/\epsilon)
\]
10-3. Gaseous detonations

OVERDRIVEN DETONATION REACTING GAS

PISTON SUPPORTED SUPersonic WAVE

SUPersonic FRONT

$\mathcal{D} > a_u$

MOVING PISTON

$\nu_p$

FRESH MIXTURE AT REST

UNIFORM FLOW OF BURNED GAS

FIRE

$\mathcal{D} > a_u$

$U_b < a_b$

$U_b = \mathcal{D} - \nu_p$

C-J REGIME $U_{b_{CJ}} = a_{b_{CJ}}$

lead shock reaction zone

Abel 1870, Berthelot et Vielle 1881, Mallard et Le Chatelier 1881, Mikhail’son 1893, Chapman 1899, Jouguet 1904, Vielle 1900, Zel’dovich 1940, von Neumann 1942, Döring 1943,
JUMP ACROSS A DETONATION

(ZND inner structure of the detonation wave in steady state)

Mikhelson condition for the CJ detonation (1893)

\[
\frac{\partial p}{\partial t} = -\frac{\partial (\rho u)}{\partial x}, \quad \frac{\partial (\rho u)}{\partial t} = -\frac{\partial}{\partial x} \left( p + \rho u^2 - \mu \frac{\partial u}{\partial x} \right), \quad \frac{\partial (\rho e_{tot})}{\partial t} = -\frac{\partial}{\partial x} \left[ \rho u T + \frac{u^2}{2} - q_m \right] - \lambda \frac{\partial T}{\partial x} - \mu \frac{\partial u}{\partial x}.
\]

\[c_p(T_b - T_u) + (u_b^2 - D^2)/2 = q_m\]

\[\frac{\gamma}{\gamma - 1} \left( \frac{p_b}{\rho_b} - \frac{p_u}{\rho_u} \right) - \frac{1}{2} (p_b - p_u) \left( \frac{1}{\rho_u} + \frac{1}{\rho_b} \right) = q_m\]

\[\mathcal{P} = -M_u^2 \mathcal{V} \]

\[\mathcal{P} = \frac{(\gamma + 1)}{2\gamma} \left( \frac{p}{p_u} - 1 \right), \quad \mathcal{V} = \frac{(\gamma + 1)}{2} \left( \frac{\rho_u}{\rho} - 1 \right)\]

\[(\mathcal{P} + 1)(\mathcal{V} + 1) = 1 + Q\]

\[Q = \frac{\gamma + 1}{\gamma - 1} \frac{q_m}{2 c_p T_u}\]

Lower bound of propagation velocity \(D = D_{CJ}\)

(called Chapmann-Jouguet 1899 – 1904)

\[(M_u^2 - 1)^2 \geq 4Q M_u^2\]

\[M_u \geq M_{uCJ} \equiv \sqrt{Q} + \sqrt{Q + 1}, \quad \text{Mikhelson (1893)}\]

In the CJ wave the velocity of the burned gas is sonic in the frame of the wave \(u_{bCJ} = a_{bCJ}\) (self-sustained wave)

(Rayleigh line is tangent)

In the overdriven detonations \(D > D_{CJ}\) the velocity of the burned gas is subsonic in the frame of the wave \(u_b < a_b\)

(piston-supported detonation)

see next slide
Planar detonation

Detonation Front

N
Shock

Detonation velocity

End of heat release zone

Piston velocity

Zoom

Detonation

Front

\( D \)

\( U_N \)

\( T_N \)

Shock

Neumann state

Reaction rate

\( T_b \)

\( U_b \)

\( U_b = a_b \)

Detonation thickness

\( p_b \)

\( p_N \)

\( U \)

\( p_u \)

\( p_b_CJ \)

\( B_{CJ} \)

\( B' \)

\( N_{CJ} \)

\( U_N \)

\( U_{b,CJ} \)

\( U_{b,CJ} \)

\( U_{b,CJ} \)

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ZND structure of detonations
Zeldovich (1940) Neumann (1942) Döring (1944)

Detonation = Shock-driven combustion wave
conjectured by Vieille (1900)

structure of the detonation: inert shock followed by a much larger reaction zone

Combustion = large activation energy
order of magnitude

\[
\frac{E}{k_B T_N} \gg 1 \Rightarrow \frac{1}{\tau_r(T_N)} \approx \frac{e^{-E/k_B T_N}}{\tau_{\text{coll}}} \ll \frac{1}{\tau_{\text{coll}}} \quad \text{and} \quad \frac{u_N}{a_N} = O(1), \quad d_N \equiv u_N \tau_r(N) \gg a_N \tau_{\text{coll}} \approx \ell
\]

thickness of the reaction zone \(\gg\) thickness of the lead (inert) shock

\[
D_T \approx a_N^2 \tau_{\text{coll}}, \quad \frac{D_T}{d_N^2} = \frac{D_T}{(u_N \tau_r)^2} = \left( \frac{a_N}{u_N} \right)^2 \left( \frac{\tau_{\text{coll}}}{\tau_r} \right) \frac{1}{\tau_r}, \quad \Rightarrow \quad 1 < \frac{a_N}{u_N} = O(1) \quad \Rightarrow \quad \frac{D_T}{d_N^2} \ll \frac{1}{\tau_r}
\]

diffusion rate \(\ll\) reaction rate \(\Rightarrow\) diffusion terms are negligible in the reaction zone behind the shock
ZND structure of detonations

Zeldovich (1940) Neumann (1942) Döring (1944)

structure of the detonation: inert shock followed by a much larger reaction zone

\[
\frac{D_T}{d_T^2} \approx \frac{a_N^2 \tau_{\text{coll}}}{d_N^2} \approx \frac{\tau_{\text{coll}}}{(T_N)^2} \approx \frac{e^{-E/k_b T_N}}{\tau_r(T_N)} \ll \frac{1}{\tau_r(T_N)}
\]

diffusion rate \ll reaction rate \Rightarrow diffusion terms are negligible

Formulation

Reference frame of the lead shock \((x = 0)\)

\[
\frac{\gamma}{\gamma - 1} \frac{d}{dx} \left( \frac{p}{\rho} \right) + u \frac{du}{dx} - q_m \frac{d\psi}{dx} = 0 \quad \frac{dp}{dx} + \rho u \frac{du}{dx} = 0
\]

\[
\frac{\gamma}{\gamma - 1} \frac{d}{dx} \left( \frac{p}{\rho} \right) + u \frac{du}{dx} - q_m \frac{d\psi}{dx} = 0 \quad \rho u \frac{d\psi}{dx} = \rho \frac{\dot{w}(T, \psi)}{\tau_r(T_N)}
\]

\[
\psi \in [0, 1] \quad \dot{w}(T, \psi = 1) = 1 \quad \dot{w}(T, \psi = 0) = 0.
\]

\[
x = 0: \quad u = u_N, \quad \rho = \rho_N, \quad p = p_N, \quad \psi = 1, \quad \dot{w} = 1
\]

\[
x \to \infty: \quad u = u_b, \quad \rho = \rho_b, \quad p = p_b, \quad \psi = 0, \quad \dot{w} = 0
\]

detonation thickness \(d_N = u_N T_r(T_N)\)

\[
a^2 = \gamma \frac{p}{\rho}
\]

\[
\frac{d}{dx} \left( \frac{p}{\rho} \right) = p \frac{d}{dx} \left( \frac{1}{\rho} \right) + \frac{1}{\rho} \frac{dp}{dx} = \frac{p}{\rho u} \frac{du}{dx} + \frac{1}{\rho} \frac{dp}{dx} = \frac{a^2}{\gamma u} \frac{du}{dx} - \frac{u}{\gamma} \frac{du}{dx} \quad \Rightarrow \quad \frac{\gamma}{\gamma - 1} \frac{d}{dx} \left( \frac{p}{\rho} \right) + u \frac{du}{dx} = \frac{1}{\gamma - 1} \frac{a^2 - u^2}{(a^2 - u^2)} \frac{du}{dx}
\]

\[
(a^2 - u^2) \frac{du}{dx} = (\gamma - 1) q_m u \frac{d\psi}{dx}, \quad \Rightarrow \quad \frac{du^2}{d\psi} = 2(\gamma - 1) q_m \frac{u^2}{(a^2 - u^2)}
\]
Phase portrait in the plan $\psi - u^2$

$$\frac{du^2}{d\psi} = 2(\gamma - 1)q_m \frac{u^2}{(a^2 - u^2)}$$

Initial state $\psi = 0$: $u^2 = D^2$, $a^2 = a_u^2$

Neumann state $\psi = 0$: $u^2 = u_N^2$, $a^2 = a_N^2$

energy eq.

$$\frac{1}{\gamma - 1}a^2 + \frac{1}{2}u^2 - q_m \psi = \frac{1}{\gamma - 1}a_u^2 + \frac{1}{2}D^2$$

$C_p T$

zero reaction rate

no supersonic wave without a leading shock

OK with the Vieille’s conjecture
C-J Detonation = self-propagating wave

\[ U_b \leq a_b \]

\[ U_{bCJ} = a_{bCJ} \]

\[ u_b = D - U_b \]

\[ u_{bCJ} = D_{CJ} - a_{bCJ} \]

10-4. Selection mechanism of the CJ wave

Rarefaction wave in the burnt gas when the piston is suddenly stopped

leading edge of the rarefraction wave = speed of sound /gas flow
\[
\sqrt{\frac{dx_f}{dt} - D_{CJ}} \propto \frac{x_f}{t}
\]

\[
\frac{D_{CJ}}{x_f(t) - D_{CJ}t} \propto \frac{1}{t} + \text{constant}
\]

\[
\lim_{t \to \infty} x_f(t) = D_{CJ}t + \text{constant}
\]
Dynamics of Combustion Waves in Premixed Gases

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Lecture XI
Initiation of detonations
Lectures 11: Initiation of detonation

Lecture 11-a: Direct initiation
- Background
- Rarefaction wave behind a CJ detonation
- Critical energy
- Critical dynamics

Lecture 11-b: Spontaneous initiation and quenching
- Initiation at high temperature
- Spontaneous quenching

Lecture 11-c: Deflagration to Detonation Transition
- Basic ingredients
- Experiments
- Runaway phenomenon
- Intrinsic DDT mechanism of laminar flames
What is the direct initiation of detonation?

Formation of a detonation in open space produced by the rapid deposition of a powerful concentrated energy source.

**Detonable mixtures**

Mixtures in which self-sustained planar detonations can propagate. The Neumann temperature (just behind the lead shock) of the CJ detonation should be larger than the crossover temperature:

$$T_{NC,J} > T_c$$

**Composition**

$$\left(\gamma - 1\right)M_{u_{C,J}}^2 > 1 \Rightarrow T_{NC,J} \propto \frac{q_m}{c_p}$$

**Crossover temperature**

$$850 \text{ K} < T_c < 1250 \text{ K}$$

**Chemical kinetics**

Heat release per unit mass of the deficient species (fuel or oxygen in lean and rich mixtures respectively)
Planar detonations in steady state. Self-sustained regime: CJ wave

(flow velocity in the laboratory frame)

reference frame of the lead shock wave

\[ \rho_u D = \rho_b U_b \quad \Rightarrow \quad u_b = \left(1 - \frac{\rho_u}{\rho_b}\right) D \]

Conservation of mass, momentum and energy across the wave lead to a quadratic equation for

\[ \begin{align*}
\gamma & = \frac{(\gamma + 1)}{2} \left( \frac{\rho_u}{\rho_b} - 1 \right) = -\frac{(\gamma + 1)}{2} \frac{u_b}{D} \\
M_u^2 \nu^2 + (M_u^2 - 1) \gamma + Q &= 0 \\
Q & = \frac{(\gamma + 1)}{2} \frac{q_m}{c_p T_u} \\
M_u & = \frac{D}{a_u}
\end{align*} \]

\(u_b = D - U_b\)

laboratory frame

CJ detonation

Lower bound of propagation velocity \(D = D_{CJ}\)

marginal solution

\[ \nu_{CJ} = -\frac{(M_{u_{CJ}}^2 - 1)}{2M_{u_{CJ}}^2} \quad M_{u_{CJ}}^2 \gg 1 \quad \Rightarrow \quad \nu_{CJ} \approx -1/2, \quad u_{b_{CJ}} \approx D_{CJ}/(\gamma + 1) \]

sonic condition

\[ U_{b_{CJ}} = a_{b_{CJ}} \quad u_{b_{CJ}} = D_{CJ} - a_{b_{CJ}} \]
Lecture 11-a: Direct initiation

**Rarefaction wave behind a CJ detonation**

Flow velocity in the laboratory frame

Reference frame of the lead shock wave

**CJ DETONATION: SELF PROPAGATING**

Stop the piston ⇒ Rarefaction wave

Flow of burned gas behind a CJ detonation viewed as a discontinuity

**self-similar form** Zeldovich (1942) Taylor (1950)

\[ u(r, t) = v(x) \quad x \equiv r/t \]

Flow velocity in the laboratory frame
Rarefaction wave behind a planar CJ detonation  
(discontinuous model)

**self-similar form**

\[ u(r, t) = v(x) \]

\[ x \equiv r/t \]

flow velocity in the laboratory frame

\[
\frac{\partial}{\partial r} = \frac{1}{t} \frac{d}{dx}, \quad \frac{\partial}{\partial t} = -\frac{r}{t^2} \frac{d}{dx} = -\frac{x}{t} \frac{d}{dx}
\]

Euler eqs. in a planar geometry \( \Rightarrow \)

\[
(v - x) \frac{1}{\rho} \frac{d\rho}{dx} + \frac{dv}{dx} = 0
\]

\[
a^2 \frac{1}{\rho} \frac{d\rho}{dx} + (v - x) \frac{dv}{dx} = 0
\]

\[
\begin{bmatrix}
1 - \left(\frac{v - x}{a}\right)^2
\end{bmatrix} \frac{dv}{dx} = 0
\]

Riemann invariant \( J_+ \)

\[
\frac{2a}{\gamma - 1} - v = \frac{2a_{bcJ}}{\gamma - 1} - v_{bcJ} \Rightarrow a = \frac{\gamma - 1}{2} (v - v_{bcJ}) + a_{bcJ}
\]

\[
\frac{\gamma + 1}{2} (v - v_{bcJ}) = x - (a_{bcJ} + v_{bcJ})
\]

elimination of \( a \)

rarefaction wave = straight line

sonic condition

\[ a_{bcJ} + v_{bcJ} = D_{CJ} \]

\[
(\gamma + 1) \frac{v - v_{bcJ}}{D_{CJ}} = 2 \left( \frac{x}{D_{CJ}} - 1 \right)
\]

Planar

\[ \frac{v}{D_{CJ}/(\gamma + 1)} \]

core of burned gas at rest

weak discontinuity: sonic velocity \( x = a_b, \ r = a_b t \)

\[ a_{bcJ} \approx \frac{\gamma}{\gamma + 1} D_{CJ}, \quad v_{bcJ} = \frac{D_{CJ}}{\gamma + 1} \]

\[ v = 0: a_b = -\frac{\gamma - 1}{2} v_{bcJ} + a_{bcJ} \approx \frac{D_{bcJ}}{2} \]

\[ v = 0: x = -\frac{\gamma + 1}{2} v_{bcJ} + D_{bcJ} \approx \frac{D_{bcJ}}{2} \]
Rarefaction wave behind a spherical CJ detonation
(discontinuous model)

\[ M_{u_{CJ}}^2 \gg 1 \quad \text{for simplicity} \]

self-similar solution for the flow of burned gas = rarefaction wave

\[ v(x) \equiv r/t \]
flow velocity in the laboratory frame

\[
\frac{\partial}{\partial r} = \frac{1}{t} \frac{d}{dx}, \quad \frac{\partial}{\partial t} = -\frac{r}{t^2} \frac{d}{dx} = -\frac{x}{t} \frac{d}{dx}
\]

\[
\frac{1}{\rho} \frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial r} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u) = 0
\]

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} = -\frac{a^2}{\rho} \frac{\partial \rho}{\partial r}
\]

\[ \Rightarrow \left\{ \begin{array}{l}
(v - x) \frac{1}{\rho} \frac{d\rho}{dx} + \frac{d\rho}{dx} + \frac{2v}{x} = 0 \\
 a^2 \frac{1}{\rho} \frac{d\rho}{dx} + (v - x) \frac{dv}{dx} = 0
\end{array} \right. \]

\[ \Rightarrow \frac{x}{v} \frac{dv}{dx} = \frac{2}{1 - \left(\frac{v-x}{a}\right)^2} \]

self-similar solution of the first kind (Zeldovich-Barenblatt 1958)

\[ \xi \equiv r/(D_{CJ} t), \quad v = v_{b_{CJ}} U(\xi), \quad \rho = \rho_{b_{CJ}} R(\xi) \]

\[ M_{u_{CJ}}^2 \gg 1 \quad \text{strong shock approximation: } D_{b_{CJ}}/v_{b_{CJ}} = \gamma + 1, \quad a/v_{b_{CJ}} = \gamma R^{(\gamma - 1)/2} \]

\[ [U - (\gamma + 1)\xi] \frac{1}{R} \frac{dR}{d\xi} + \frac{dU}{d\xi} + \frac{2U}{\xi} = 0 \quad \gamma^2 R^{\gamma - 1} \frac{1}{R} \frac{dR}{d\xi} + [U - (\gamma + 1)\xi] \frac{dU}{d\xi} = 0 \]

\[ \xi = 1: U = 1, R = 1. \]

\[ \lim_{\xi \to 1} (1-U)^2 = \frac{2\gamma}{\gamma + 2} (1 - \xi) \]

Start the numerical integration at \( \xi = 1: U = 1, \frac{dU}{d\xi} = \sqrt{\frac{\gamma}{2(\gamma + 2)} \frac{1}{(1 - \gamma)}} \)

Stop the calculation at \( \xi_o \) at which \( U = 0; \) uniform solution in \( 0 \leq \xi \leq \xi_o \)

spherical kernel of burnt gas at rest whose radius increasing linearly with time
**Direct initiation ?**

Initiation by releasing quasi *instantaneously* an amount of energy in a quasi *point*. (e.g. explosive charge) Successful initiation occur above a critical energy

\[ E > E_c \]

At early time after deposition, the size of the spherical wave is very small and the energy liberated by the exothermal reaction is negligible in front of the energy that has been deposited.

Therefore, the initial condition for the study of direct initiation is a *point blast wave* which is described by a spherical *self-similar* solution of inert *Euler equations* (no time and space scale).
Point blast wave explosion in an inert gas (spherical geometry) 
(Taylor 1941 Sedov 1946)

The shock velocity $D(t)$ varying with the time $\Rightarrow$ the entropy jump across the shock is not constant however the dissipation can be neglected outside the shock.

The flow is solution of the Euler equations completed by the entropy wave equation

$$\text{Euler eqs. } + \left( \frac{\partial}{\partial t} + v \frac{\partial}{\partial r} \right) \left( \frac{p}{\rho^\gamma} \right) = 0$$

and satisfies to the Rankine-Hugoniot condition on the lead shock treated as a discontinuity:

Strong shock $M_u \equiv D/a_u \gg 1 \Rightarrow v_N = \frac{2}{\gamma+1}D(t), \quad \rho_N = \frac{\gamma+1}{\gamma-1}\rho_u, \quad p_N = \frac{2}{\gamma+1}\rho_u D^2(t)$ \quad where $D(t) \equiv \frac{dr_f}{dt}$

look for a self similar solution in the form $\xi \equiv \frac{r}{r_f(t)}, \quad v = D(t)V(\xi), \quad \rho = \rho_u R(\xi), \quad p = \rho_u D(t)^2 P(\xi)$

$\Rightarrow$ 3 o.d.e. for $V(\xi), R(\xi), P(\xi)$ with $\xi = 1: \quad V = 2/(\gamma + 1), \quad R = (\gamma + 1)/(\gamma - 1), \quad P = 2/\gamma + 1$,

The trajectory of the lead shock $r = r_f(t)$ is obtained by the following dimensional analysis:

2 dimensional parameters $E$ and $\rho_u \Rightarrow$ a single non-dimensional parameter can be built with $r$ and $t$: $r(\rho_u/E t^2)^{1/5}

$$r_f(t) = b(\gamma) \left( \frac{E}{\rho_u} \right)^{1/5} t^{2/5} \Rightarrow D(t) = \dot{r}_f(t) = \frac{2 b(\gamma)}{5} \left( \frac{E}{\rho_u} \right)^{1/5} t^{-3/5}$$

$$\rho_u D^2 r^3 \approx (2/5)^2 E$$

conservation of energy:

$$4\pi \int_0^{r_f(t)} \rho \left[ \frac{1}{\gamma - 1} \frac{p}{\rho} + \frac{v^2}{2} \right] r^2 dr = E \Rightarrow b = 1.0033 \ldots \text{ for } \gamma = 1.4$$

Dimension of $E = \frac{\text{mass} \times \text{length}^2}{\text{time}^2}$

Dimension of $\rho = \frac{\text{mass}}{\text{length}^3}$

Flow field of the Taylor-Sedov blast wave

![Flow field of the Taylor-Sedov blast wave](image-url)
Point blast wave explosion in a combustible gas

Successful direct initiation: Transition between 2 self-similar solutions

\[ E > E_c : \begin{cases} \text{point blast explosion} \\ \text{Sedov-Taylor} \end{cases} \quad \text{spherical CJ wave} \quad \text{Zeldovich-Taylor} \quad \begin{cases} D_f(t) \\ \mathcal{D}_{CJ} \end{cases} \quad \begin{cases} D_f(t) \\ \infty \end{cases} \]

\[ E < E_c : \begin{cases} \text{point blast explosion} \\ \text{fluid at rest } v = 0 \end{cases} \quad \begin{cases} D_f(t) \\ a_u \end{cases} \]

\[(\text{Detonation} = \text{discontinuity}) \Rightarrow \text{no criticality!} \]
\[(\text{no length scale}) \Rightarrow \text{no ignition failure}\]

(Korobeinikov 1971, Liñan et al. 2012)

\[ D_f(t) \xrightarrow{\mathcal{D}_{CJ} \quad \forall E} \quad \text{at } r_f \approx r_f^* \text{ and } t \approx t^* \text{ corresponding to } \rho_u r_f^* 3 \mathcal{D}_{CJ}^2 \approx E, \ t^* \approx r_f^*/\mathcal{D}_{CJ} \]
First numerics in a spherical geometry

Korobeinikov (1971)
Detonation = discontinuity

( zero detonation thickness: )
No critical energy !

 Conclusion: the critical energy is due to modifications of the inner structure of the detonation
Direct numerical simulations of the flow in spherical geometry including the unsteady inner structure of the detonation show that there is a critical energy for a successful initiation; below, the initiation fails and the shock velocity decreases to the sound speed in an inert mixture.

He Clavin JFM (1994) 277 p. 227-248
Eckett et al. JFM (2000) 421 p. 147-183
Critical energy: Zeldovich criterion (1965)

Order of magnitude estimate for the critical energy by dimensional analysis

the time of the blast wave velocity to reach $D_{CJ} = $ reaction time at the Neumann state of the CJ wave

criticality: $\tau^*_{CJ} = \tau_{NCJ}$

self-similar blast wave

$\mathcal{D}(t) \approx (E/\rho_u)^{1/5} / t^{3/5}$

strong shock

$\mathcal{D}/u_N = (\gamma + 1)/\gamma - 1$

strong CJ wave

$\mathcal{D}^2_{CJ} \approx 2(\gamma^2 - 1)q_m$

$E_c \approx 2\rho_u q_m \frac{(\gamma + 1)^4}{(\gamma - 1)^2} d_{CJ}^3$

Smaller by many orders of magnitude than in experiments! $10^{-5} - 10^{-6}$

Lee (1984)

Nonlinear curvature induced modification to the inner structure and fully unsteady effects are essential for a correct estimation of the critical energy
Lecture 11-a: **Direct initiation**

*Critical energy*

*Nonlinear curvature effect in spherical geometry*

He Clavin *JFM* (1994) **277** p. 227-248

*Quasi-steady analysis for large activation energy*
Non linear curvature effect steady state approximation of the spherical detonation structure

**Turning point in the parameter space «radius-velocity »:**
there is no spherical CJ detonation below a critical radius

Generic equation of a turning point: \[ \Theta e^{-\Theta} = K \]
unknown solution: \( \Theta \) parameter K

\[ \Theta \equiv 2\beta_N \left( \frac{\overline{D}_{CJ} - D_{CJ}}{\overline{D}_{CJ}} \right) \]
\[ K \equiv \frac{16\gamma^2}{\gamma^2 - 1} \frac{\beta_N \overline{d}_{CJ}}{R} \]

collapsing for \( K = K^* \): \( \Theta_\pm = \Theta^* = 1 \)

\[ \Theta e^{-\Theta} \]

\( R < R_c \)
No spherical CJ: overdriven regimes that are damped by the rarefaction wave!

\[ K^* = 1/e \Rightarrow R_c/\overline{d}_{CJ} \approx 10^2 \]
OK with DNS
**Details of the asymptotic analysis**

*He Clavin JFM (1994) 277 p. 227-248*

**Nonlinear curvature effect of a spherical CJ detonation**

\[
\nabla j = \frac{1}{r^2} \frac{\partial (r^2 j)}{\partial r} = \frac{\partial j}{\partial r} + \frac{2}{r} j
\]

Reference frame of the lead shock \( x = r_f(t) - r \) \( u = D - v \) \( \frac{dr_f(t)}{dt} = D \) \( \partial / \partial r \rightarrow - \partial / \partial x \) \( \partial / \partial t \rightarrow \partial / \partial t + D \partial / \partial x \)

**Euler eqs.**

- **Mass**
  \[
  \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{2}{r_f} \rho (D - u) = 0
  \]

- **Momentum**
  \[
  \left( \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} \right) u = - \frac{1}{\rho} \frac{\partial p}{\partial x} + \frac{dD}{dt} + \rho (D - u) u - \rho \nabla j \]

- **Energy**
  \[
  \left[ \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} \right] \left( c_p T - q_m \psi \right) - \frac{1}{\rho} \frac{\partial p}{\partial x} = \frac{\partial (\rho u^2 + p)}{\partial x} - \frac{\partial (\rho u u)}{\partial x} = 0
  \]

Quasi-steady state approximation: Large radius \( \epsilon \equiv d_{CJ}/r_f \ll 1 \)

Integration across the inner structure \( x = 0 \): Neumann state, \( \rho_N u_N = \rho_u D \) \( x = d \): burnt gas

**First order approximation**

\[
\frac{(\rho_b u_b - \rho_u D)}{\rho_u D} \approx - I_1
\]
\[
\frac{(\rho_b u_b^2 + p_b) - (\rho_u D^2 + p_u)}{\rho_u D^2} \approx - I_2
\]

Unperturbed planar solution: \( \bar{p}(x) \bar{u}(x) = \rho_u D \)

\[
I_1 \approx 2 \epsilon \int_0^d \left( \frac{\bar{p}(x)}{\rho_u} - 1 \right) \frac{dx}{d_{CJ}} \quad \left( \frac{\gamma}{\gamma - 1} \frac{p_b}{\rho_b} + \frac{u_b^2}{2} \right) \approx \left( \frac{\gamma}{\gamma - 1} \frac{p_u}{\rho_u} + \frac{D^2}{2} + q_m \right)
\]

\[
I_2 \approx 2 \epsilon \int_0^d \left( 1 - \frac{\rho_u}{\bar{p}(x)} \right) \frac{dx}{d_{CJ}}
\]

Square-wave model: thickness of the reaction zone \( \ll \) thickness of the induction zone \( d_{ind} \), \( I_1,2 \propto \epsilon d_{ind}/d_{CJ} \)

**Arrhenius law**

\( \beta_N \equiv \frac{E}{k_B T_{NCJ}} \gg 1 \)

\[
d_{ind} = d_{CJ} \exp \left[ -2\beta_N \left( \frac{D - D_{CJ}}{D_{CJ}} \right) \right] \quad \frac{D - D_{CJ}}{D_{CJ}} = O(1/\beta_N)
\]

\[
(d - D_{CJ}) = O(1/\beta_N)
\]

\( (\gamma - 1) M_u^2 \gg 1 \Rightarrow \frac{\rho_u}{\rho_N} \approx \frac{\gamma - 1}{\gamma + 1}, \quad \frac{T_N}{T_u} \approx 2 \gamma M_u^2 \frac{(\gamma - 1)}{(\gamma + 1)^2}, \quad \frac{T_N}{T_{NCJ}} \approx \left( \frac{D}{D_{CJ}} \right)^2
\]

\[
I_1(D) \approx \frac{4}{(\gamma - 1) \gamma} \frac{d_{CJ}}{r_f} \exp \left[ -2\beta_N \left( \frac{D - D_{CJ}}{D_{CJ}} \right) \right] \quad I_2 \approx \frac{\gamma - 1}{\gamma + 1} I_1
\]

**Lead Shock**

\( x = 0 \)

**Deduction of the asymptotic analysis**

**Large radius**

**Initial conditions**

**Equation of state**

**Lead shock**

**Detonation thickness**

**Reaction rate**

**Curved detonation**

**Integration across the inner structure**

**Details of the asymptotic analysis**

**Nonlinear curvature effect of a spherical CJ detonation**

**Quasi-steady state approximation**

**First order approximation**

**Square-wave model:** thickness of the reaction zone \( \ll \) thickness of the induction zone \( d_{ind} \), \( I_1,2 \propto \epsilon d_{ind}/d_{CJ} \)
Small modification of the burnt gas state

$$\frac{\delta \rho_b}{\rho_{b,cJ}} + \frac{\delta u_b}{a_{b,cJ}} = \frac{\delta D}{D_{CJ}} - I_1 \quad \Rightarrow \quad I_1 = O(1/\beta_N) \quad \Rightarrow \quad \frac{\delta u_b(D)}{a_{b,cJ}} = O(1/\beta_N), \quad \frac{\delta \rho_b(D)}{\rho_{b,cJ}} = O(1/\beta_N), \quad \frac{\delta p_b(D)}{p_{b,cJ}} = O(1/\beta_N) \quad \delta u_b \equiv u_b - a_{b,cJ}, \quad \delta \rho_b \equiv \rho_b - \rho_{b,cJ}, \quad \delta p_b \equiv p_b - p_{b,cJ}$$

Small variations of the continuity eq, the Euler eqs and the energy eq yield

$$\frac{\delta \rho_b}{\rho_{b,cJ}} + \frac{\delta u_b}{a_{b,cJ}} = \frac{\delta D}{D_{CJ}} - I_1 \quad \Rightarrow \quad I_1 = O(1/\beta_N) \quad \Rightarrow \quad \frac{\delta u_b(D)}{a_{b,cJ}} = O(1/\beta_N), \quad \frac{\delta \rho_b(D)}{\rho_{b,cJ}} = O(1/\beta_N), \quad \frac{\delta p_b(D)}{p_{b,cJ}} = O(1/\beta_N) \quad \delta u_b \equiv u_b - a_{b,cJ}, \quad \delta \rho_b \equiv \rho_b - \rho_{b,cJ}, \quad \delta p_b \equiv p_b - p_{b,cJ}$$

Small variations of the continuity eq, the Euler eqs and the energy eq yield

$$\frac{\delta \rho_b}{\rho_{b,cJ}} + \frac{\delta u_b}{a_{b,cJ}} = \frac{\delta D}{D_{CJ}} - I_1 \quad \Rightarrow \quad I_1 = O(1/\beta_N) \quad \Rightarrow \quad \frac{\delta u_b(D)}{a_{b,cJ}} = O(1/\beta_N), \quad \frac{\delta \rho_b(D)}{\rho_{b,cJ}} = O(1/\beta_N), \quad \frac{\delta p_b(D)}{p_{b,cJ}} = O(1/\beta_N) \quad \delta u_b \equiv u_b - a_{b,cJ}, \quad \delta \rho_b \equiv \rho_b - \rho_{b,cJ}, \quad \delta p_b \equiv p_b - p_{b,cJ}$$

Sonic condition in the burnt gas:

$$u_b^2 = \gamma p_b/\rho_b \quad \Rightarrow \quad \frac{\delta \rho_b}{\rho_{b,cJ}} + \frac{\delta u_b}{a_{b,cJ}} = \frac{\delta D}{D_{CJ}} - I_1 \quad \Rightarrow \quad I_1 = O(1/\beta_N) \quad \Rightarrow \quad \frac{\delta u_b(D)}{a_{b,cJ}} = O(1/\beta_N), \quad \frac{\delta \rho_b(D)}{\rho_{b,cJ}} = O(1/\beta_N), \quad \frac{\delta p_b(D)}{p_{b,cJ}} = O(1/\beta_N) \quad \delta u_b \equiv u_b - a_{b,cJ}, \quad \delta \rho_b \equiv \rho_b - \rho_{b,cJ}, \quad \delta p_b \equiv p_b - p_{b,cJ}$$

$$\begin{align*}
\frac{\delta D}{D_{CJ}} & = \frac{1}{\gamma - 1} \rho_{b,cJ} - \frac{1}{\gamma - 1} \rho_{p,cJ} + \frac{\delta u_b}{a_{b,cJ}} = \left( \frac{D_{CJ}}{a_{b,cJ}} \right)^2 \frac{\delta D}{D_{CJ}} \\
\frac{\rho_{b,cJ}}{\rho_{b,cJ}} & \approx \frac{\gamma + 1}{\gamma} \left[ 1 + \frac{1}{\gamma - 1} \left( \frac{D_{CJ}}{a_{b,cJ}} \right)^2 \right] - 2 \frac{\delta D}{D_{CJ}} \quad \frac{\delta D}{D_{CJ}} = \frac{\gamma + 1}{\gamma - 1} \rho_{b,cJ} - \frac{\delta D}{D_{CJ}} I_1(D) - \frac{\delta D}{D_{CJ}} I_2(D)
\end{align*}$$

is a C-shaped curve with a turning point at

$$2 \beta_N \left( \frac{D_{CJ} - D}{D_{CJ}} \right) e^{-2 \beta_N \left( \frac{D_{CJ} - D}{D_{CJ}} \right)} = \frac{16 \gamma^2}{\gamma^2 - 1} \beta_N \frac{d_{CJ}}{d_f}$$

$$r^* = \frac{16 \gamma^2}{\gamma^2 - 1} \beta_N \frac{d_{CJ}}{d_f} \quad D^* = \left( 1 - \frac{1}{2 \beta_N} \right) \frac{D_{CJ}}{D_{CJ}}$$

there is no spherical CJ detonation with a radius $$r_f < r^*$$

$$r^*/d_{CJ} \approx 10^3$$

ok with DNS of He Clavin (1994)

ok with the experiments of Lee (1984)

Limitations of the analysis: Square-wave model. Quasi-steady state

No change in order of magnitude

$$Ec \approx (5/2)^2 \rho_u D_{CJ}^{3/2} r^* \approx (5^2/2)(\gamma^2 - 1) q_m \rho_u r^* \approx 10^8 - 10^9 \times \text{Zeldovich value}$$

(1956)
Curvature effect on the detonation structure

(\textit{steady state} approximation)

\begin{align*}
\frac{\text{critical radius}}{\text{detonation thickness}} & \approx 10^2 \quad \Rightarrow \quad \frac{\text{critical energy}}{\text{Zeldovich value}} \approx 10^6 \\
\text{Arrhenius factor}
\end{align*}

Good order of magnitude but the critical energy is overestimated !

\textbf{Weakness of the analysis:}

\textit{quasi-steady state approximation}

\textit{unsteadiness} induced re-ignition for $R < R_c$
**Lecture 11-a: Direct initiation**

**Critical dynamics**

**Unsteady analysis** of the direct initiation in a spherical geometry in the limit of **small heat release** enlightening the **qualitative** behavior

\[ \epsilon \equiv q/c_p T_u < 1 \]

Clavin, Denet *JFM* (2020) Vol. 897, A30

Clavin, Hernandez-Sanchez and Denet *JFM* (2021) Vol. 915, A 122

**1st step:** Asymptotic analysis of the **rarefaction wave** in the **discontinuous** model

- **Self-similar** solution behind a **spherical CJ wave**
- **Unsteady rarefaction wave** behind **overdriven detonations** approaching CJ
- **Transient flow** when reaching the CJ velocity

**2nd step:** **Unsteady inner structure** of the detonation taken into account

- **Two-length scales** problem: **matching condition**
- **Critical dynamics:** the role of the trajectory of the **sonic point**
1st step: Asymptotic analysis of the rarefaction wave in the discontinuous model (detonation = discontinuity)

**Self-similar solution for the reaction wave behind a spherical CJ wave**

Asymptotic analysis in the limit of small heat release \( \epsilon \equiv q/c_p T_u < 1 \)

\[ \frac{D_{oC,J} - a}{a} \approx \epsilon \ll 1, \quad D_{oC,J} \approx (1 + \epsilon)a, \]

the result is qualitatively similar to the limit of large Mach number \( M \gg 1 \) by Zeldovich (1942) Taylor (1945)

**Detonation front:**
\[ r = r_f(t) > r_0(t) \quad \text{dr}_f/\text{dt} = D_{oC,J} > a_o \]

**Inert core:**
\[ r_0 \leq r \leq r_f(t) : \quad \frac{u}{\epsilon a} = V \left( \frac{r - r_f(t)}{\epsilon r_0(t)} \right) \]

Analytical solution of the flow field

\[ V(z) \ln V(z) - V(z) + (z + 1) = 0 \]

**Same singularity** on the detonation front as in Zeldovich Taylor!
1st step: Asymptotic analysis of the rarefaction wave in the discontinuous model limit of small heat release

- **Unsteady rarefaction wave** behind *overdriven detonations* approaching CJ

\[ 0 < \frac{u_{fi}}{\epsilon a} - 1 \ll 1, \quad r_0(t) \leq r \leq r_f(t) : \]
\[
\frac{u(r,t)}{u_f(t)} = \frac{r - r_0(t)}{r_f(t) - r_0(t)}
\]
\[
r_0(t) = a_o t + r_{0i}, \quad u_f(t) \equiv u(r_f, t)
\]

\[ u_f(t) \geq 1 : \]
\[
\frac{u_f(t)}{u_{fi}} = \frac{r_f(t) - r_0(t)}{r_f(t)} \left[ \frac{r_f(t) - r_{0i}}{r_{fi}} + \frac{u_{fi}}{a_o} \ln \left( 1 + \frac{a_o t}{r_{fi}} \right) \right]^{-1}
\]

*linear velocity profile* (strictly limited to overdriven regimes)

- **Transient flow** of the rarefaction wave *as soon as the CJ velocity* is reached

*Overdriven solution* \[\rightarrow\] *Self similar CJ solution*

**Abrupt transition** of the gradient on the detonation front
**Two length scales problem.** Flame thickness = small scale. Rarefaction wave = long scale
(internal flame structure) (external flow)

In the limit of small heat release, the problem is reduced to a **single nonlinear** differential equation of first order for the flow field that has to be solved by **matching** the solution in the burned gas side of the inner flame structure with a **point blast wave**. The **Arrhenius law** governing the reaction rate is truncated below a **crossover temperature** denoting the chemical kinetics induced **quenching** at low temperature.
Critical dynamics: Role of the trajectory of the sonic point

Propagation velocity (relative to the lead shock) of the disturbances associated with \( C_+ \) is

\[
\frac{dx_{C_+}}{dt} = u + a - D
\]

Sonic point: \( D - u = a \)

The sonic point separates the flow in two regions:
- **ahead**, the flow is subsonic (relative to the lead shock), \( D - u < a \);
- **behind**, the flow is supersonic, \( D - u > a \).

The rarefaction wave is not disturbed behind the exit of the reaction zone by the heat-release: it is the same as behind an overdriven detonation of zero thickness for which the flow gradient is uniform and decreases continuously. The flow of burned gas adjacent to the reaction zone being subsonic the detonation regime is overdriven. The reaction rate is decreased by the rarefaction wave and the detonation is slowed down.

The flow gradient of the rarefaction wave decreasing continuously, the sonic point get closer and closer to the exit of the reaction zone. The damping is stopped as soon as the sonic point catches the exit of the reaction zone protecting the reaction rate of further damping since the flow relative to the reaction zone becomes sonic. This is possible if the gas temperature in the rarefaction wave has not decreased below the cross over temperature...
When the sonic point enters the reaction zone, it stays stuck near the end of the reaction and the sonic condition makes the detonation free from further damping by the rarefaction wave. The inner structure of the detonation (initially slaved by the external flow) becomes isolated in a state out of equilibrium. The equilibrium state is restored through an increase in reaction rate, producing a re-acceleration of the detonation front towards the spherical CJ regime. This re-acceleration occurs near the critical radius characterizing the quasi-steady spherical detonations.

Therefore, the critical energy is overestimated (of an order unity) by the nonlinear curvature effect of the spherical CJ detonation in quasi-steady state but the critical radius is not modified.

Sketch of the flow field of an overdriven detonation for a velocity of the lead shock below the planar CJ value, for a radius smaller than the critical radius.

\[ \frac{(D - D_{\text{CJ}})}{a} \]

\[ x \equiv r_f/(be^{-1}l_{\text{CJ}}) \]
The trajectories « velocity of the lead shock versus radius » are obtained near the critical condition by the numerical study of the single equation of the asymptotic analysis. Typical results are plotted below for different initial conditions corresponding to blast waves with different deposited energy.

Success of initiation occurs if the sonic point reaches the reaction zone before the reaction gets thermally quenched. Otherwise failure is produced.
Numerical solution of the equation

Damping by the rarefaction wave stops as soon as the sonic point enters the reaction zone and protects the detonation structure from further damping by the burnt gas flow, then the front re-accelerates.
Lectures 11: Initiation of detonation

Lecture 11-a: Direct initiation

Flow of burnt gas in spherical CJ detonations
Point blast explosions
Critical energy
Critical dynamics

Lecture 11-b: Spontaneous initiation and quenching

Initiation at high temperature
Spontaneous quenching

Lecture 11-c: Deflagration to Detonation Transition

Basic ingredients
Experiments
Runaway phenomenon
Intrinsic DDT mechanism of laminar flames
**Spontaneous initiation of detonation at high temperature**


J.H.S. Lee et al. (1978) *Acta Astronautica* 5, pp. 971-982

Gaseous detonations are difficult to ignite: a large increase of pressure is required $p_{NCJ} \approx 30 – 50\text{atm}$

Not possible with an homogeneous explosion of a gaseous pocket at constant volume $(\Delta p/p < 10) \quad (T_N < T_c)$

Possible with gradients of $T$

Induction delay (Ignition time) $\tau_{ind}(T, p)$ is highly sensitive to $T$

$t = 0$: initial gradient of $T \Rightarrow$ gradient of $\tau_{ind}$

1-D: hot slides ignite before cold slides $\dot{q}_v = q_v \omega (t - \tau_{ind}(x))$ (rate of heat release per unit volume) $\Rightarrow$ propagation of an induction front at a speed $\approx (d\tau_{ind}/dx)^{-1}$

Mechanism spontaneous initiation: combustion $\Rightarrow$ pressure pulses that propagate with about the speed of sound $a$

synchronisation: $$(d\tau_{ind}/dx)^{-1} = a$$

$$d\tau_{ind}/dx \approx \text{cst.} \Rightarrow \tau_{ind}(x) \approx \tau_{ind}^0 + x(d\tau_{ind}/dx)$$

$$\dot{q}_v = q_v \omega (t - \tau_{ind}^0 - x(d\tau_{ind}/dx)) \approx q_v \omega (t - \tau_{ind}^0 - x/a)$$

$$\frac{\partial^2 p}{\partial t^2} - a^2 \frac{\partial^2 p}{\partial x^2} = (\gamma - 1) \frac{\partial \dot{q}_v}{\partial t}$$ 

simple wave: \[ \frac{\partial}{\partial t} \delta p + a \frac{\partial}{\partial x} \delta p = (\gamma - 1) q_v \omega (t - \tau_{ind}^0 - x/a) \]

run away (secular solution) $\delta p = t (\gamma - 1) q_v \omega (t - \tau_{ind}^0 - x/a)$

The amplitude of the pressure pulse increases linearly with time at the rate of the reaction rate.
P.Clavin XI

\[(d\tau_{\text{ind}}/dx)^{-1} = a\]

Spontaneous initiation has been observed in experiments and numerics

---

**Spontaneous quenching**

Liberman et al. (1994) Combust. Theory Model. 23 (3)p. 4183-4193

Spontaneous ignition at high \(T\) may be followed by sudden quenching at lower \(T\)

Theoretical analysis:

\[
\begin{align*}
\text{square-wave model} & \quad \text{ quasi-steady induction zone : } d_{\text{ind}}/dx & \approx e^{-2\beta_N (D-\overline{D})} \\
\frac{dd_{\text{ind}}}{dt} \neq 0 & \Rightarrow \text{ mass flux in reaction zone } \neq \rho_u D \\
\frac{\delta D_{\text{CJ}}}{D_{\text{CJ}}} & \approx (2M^2_{u_{\text{CJ}}})^{-1} \frac{\delta T_u}{T_u} \Rightarrow \frac{d}{dt} d_{\text{ind}} \propto e^{-2\beta_N \frac{(D-\overline{D})}{\overline{D}}} L \frac{dD}{dx}
\end{align*}
\]

gemeotrical construction:

difference of mass flux = difference of slopes of \(UN\) and \(NB \propto (D-\overline{D})/\overline{D}\) \((\gamma - 1)M^2_u \gg 1\)

\[
(\gamma - 1)M^2_u \gg 1 : \quad \frac{d}{dt} d_{\text{ind}} \propto \overline{u}_N \frac{(D-\overline{D})}{\overline{D}} \\
\]

C-shaped curve \(\mathcal{D}\) vs \(dT_u/dx\) with a turning point

\[
2\beta_N \left( \frac{D_{\text{CJ}} - \mathcal{D}}{D_{\text{CJ}}} \right) e^{-2\beta_N \frac{D_{\text{CJ}} - \mathcal{D}}{D_{\text{CJ}}}} = K
\]

critical condition for sudden quenching \(K^* = 1/e\)

where \(K \equiv 4\beta_N \tau_{\text{ind}}(T_{\text{CJ}}) \left( -\frac{dD_{\text{CJ}}}{dx} \right) = O(1)\)

A CJ detonation cannot survive to a strong temperature gradient at low temperature \((K > 1/e)\) \(\frac{dK}{dT_u} < 0\)

The non-uniform pocket of hot gas should have a proper shape for initiating a detonation

---

\(\gamma\) - 1 \(M^2_u\) \(\overline{u}_N\) \(\overline{D}\) \(\mathcal{D}\) \(K^*\) \(K\)
Lectures 11: Initiation of detonation

Lecture 11-a: Direct initiation

Flow of burnt gas in spherical CJ detonations
Point blast explosions
Critical energy
Critical dynamics

Lecture 11-b: Spontaneous initiation and quenching

Initiation at high temperature
Spontaneous quenching

Lecture 11-c: Deflagration to Detonation Transition

Basic ingredients
Shchelkin scenario
Runaway phenomenon
Intrinsic DDT mechanism of laminar flames
Lecture 11-c: **Deflagration to Detonation Transition (DDT)**

*Basic ingredients*

DDT is an **abrupt** transition between two **opposite** regimes of propagation.

Flame = reaction-diffusion wave markedly subsonic, \( \frac{U_L}{a_u} \ll 1 \)

Detonation = shock driven **supersonic combustion** wave without diffusion behind the lead shock, \( \frac{D}{a_u} > 1 \)

No intermediate quasi steady propagation regime!
Despite more than a century of researches, DDT remains a poorly understood problem.

Since the pioneering experiments of Oppenheim (1965), DDT has been known to develop in various forms (viscous effects in the boundary layers, unsteady compression waves, thermal gradients, local explosion…)

There is no mechanism of DDT that is generally agreed upon as being universal!

However it is now well established that DDT is a local and sudden explosion of a small centre either on the flame front or ahead of it, either inside or outside the boundary layer on the wall (Urtiew and Oppenheim (1966) *Proc. R. Soc. London A* 295 pp 13-28)

Here the attention will be limited to an intrinsic DDT mechanism of laminar flames: DDT of elongated laminar flames propagating in tubes.

Turbulence can promote an early transition but is not an essential DDT mechanism.
First, few words about DDT induced by local explosions in the boundary layer
(Oppenheim’s experiments 1966-1973)


Hot spots in the boundary layer between the lead shock and the flame

Heating by viscous dissipation in the boundary layers at the wall

+ compressional heating

\[ \nabla T \neq 0 \quad \nabla \text{induction time} \neq 0 \]

**local explosion** ahead of the flame by the **spontaneous ignition** of Zeldovich

(we will come back to this case at the end of the lecture)

---

Here the attention will be limited to the DDT near the tube axis on the leading edge of an elongated front of a laminar flame propagating in a tube

**Experiments in** $50 \times 50 \text{ mm}^2$ tubes:


Basic ingredients of the intrinsic DDT mechanism of laminar flames ignited on the closed wall of a tube

-1) **Piston effect**: fresh gas put in motion ahead of the flame

\[ U_{\text{tur}} = s U_b \]

-2) **Flame acceleration** through an increase of the flame surface area

\[ s = \frac{\text{flame surface area}}{\text{cross section}} \]

-3) **Heating** of the fresh mixture by compressible effects
   (through a shock wave or a compression wave and/or viscous dissipation)

-4) **High sensitivity** of the flame velocity to the temperature
1-D flame in a tube

Piston effect \( \frac{\rho_u}{\rho_b} = \frac{T_b}{T_u} = \frac{U_b}{U_u} > 1 \)

Turbulent wrinkled flame \( U_L \rightarrow sU_L \)

folding factor: \( s = \frac{\text{flame surface area}}{\text{cross section}} \)

Turbulence-induced DDT

the flow upstream of the flame becomes turbulent

the wrinkling of the flame front increases

Runaway mechanism

Shchelkin scenario (1940-1950)
Lecture 11-c: **Deflagration to Detonation Transition**

*Shchelkin scenario*

**Turbulence induced DDT** (Shchelkin 1940-1945)

<table>
<thead>
<tr>
<th>Turbulent flow of fresh mixture</th>
<th>$\Rightarrow$</th>
<th>$s$</th>
<th>$\Rightarrow$</th>
<th>$U_{\text{tur}}$</th>
<th>$\Rightarrow$</th>
<th>flow velocity</th>
<th>$\Rightarrow$</th>
<th>turbulence intensity</th>
<th>$\Rightarrow$</th>
<th>$s$</th>
<th>$\Rightarrow$</th>
<th>$U_{\text{tur}}$</th>
<th>(positive feedback)</th>
</tr>
</thead>
</table>

Strong shock wave $M \geq 5$ $\Rightarrow$ short induction time

Ignition of the compressed gas

Not observed in the DDT experiments of elongated flames in tubes $> 1960$

Sudden DDT for $M \approx 3$ temperature of the gas in the fresh mixture too small

fast self-ignition is not possible ($T_N < T_c$)

Sudden DDT not explained

Recent advances
The turbulence-induced DDT scenario is not observed in the 2010-2011 experiments

Millimeter-scale tubes, Wu et al. (2007-2011)
Centimeter-scale tubes, Liberman et al. (2010-2011)
(experiments and and DNSs)
Very energetic stoichiometric $H_2 - O_2$ mixtures: $U_L(T_u) \approx 9 \text{ m/s }, T_b \approx 3000 \text{K}$
$\mathcal{D}_{CJ} \approx 2800 \text{ m/s } T_{b_{CJ}} \approx 3600 \text{ K}$

Sudden transition at the flame front in the laminar regime
with a jump of the velocity of the combustion front from $\approx 300 \text{ m/s}$
to $\approx 3000 \text{ m/s}$ during $10^{-6}$ s.
X
$10^{-3}$ s.

at a temperature of the fresh mixture not high enough $T \approx 650 \text{ K}$
and a Mach number of the lead shock not large enough $M \approx 2.4$
for self-ignition behind the lead shock

This sudden transition was left unexplained. This is the topic of the rest of this lecture
Nonlinear thermal loop


*enlightening theoretical analysis ignored up to 2017*

Self-similar solution (1-D) of the double discontinuity model for a turbulent flame in the wrinkled flame regime

- Piston effect of the planar flame: $U_b \rightarrow s U_b$
- Piston effect of the wrinkled flame:
- Folding factor: $s = \frac{\text{flame surface area}}{\text{cross section}}$
- Quasi-steady solution: $U_b = \text{constant}, \quad \mathcal{D} = \text{constant}$
- Uniform 1-D flow: $s (U_b - U_L) = \mathcal{D} - U_N$

**Constant speed:** $U_f = s U_b$

- Flame brush: $\mathcal{D} > U_f$
- Shock wave:

\[(\mathcal{D} - U_f) t\]
1-D self-similar solution of a shock wave generated by a flame brush propagating at a constant velocity $U_{turb}$ from the closed end of a tube

$$U_{turb} = s U_b \quad s \text{ degree of folding}$$

Flame $\equiv$ semi-permeable piston

$$v = s(U_b - U_L) = \left( 1 - \frac{\rho_b}{\rho_u} \right) s U_b$$

Lead shock: RH conditions

$$v = D - U_N \approx \frac{a_o}{\gamma - 1} \left( \frac{T_N}{T_{uo}} - 1 \right)$$

weak shock

$$T_N = T_u \approx \frac{a_o}{\gamma - 1} \left( \frac{T_b}{T_{bo}} - 1 \right)$$

$$(1 - \frac{\rho_b}{\rho_u}) s U_b \approx \frac{a_o}{\gamma - 1} \left( \frac{T_b}{T_{bo}} - 1 \right)$$

ZFK flame velocity

$$U_b/U_{bo} \approx e^{\frac{E}{2k_B T_{bo}}} \left( \frac{T_b - T_{bo}}{T_{bo}} \right)$$

$$\frac{a_o}{\gamma - 1} \left( \frac{T_b}{T_u} - 1 \right) = \left( 1 - \frac{\rho_u}{\rho_b} \right) s U_b(0) e^{\frac{E}{2k_B T_{bo}(0)}} \left( \frac{T_b(t) - T_{bo}(t)}{T_{bo}(t)} \right)$$

Nonlinear solution $T_b(s)$ with a turning point

flame temperature versus degree of folding

$$X \equiv \frac{E}{2k_B T_{bo}} \left( \frac{T_b}{T_{bo}} - 1 \right)$$

$$K = \kappa s, \quad \kappa \equiv (\gamma - 1) \frac{(T_{bo} - T_{uo}) U_{bo}}{T_{bo}} a_o \frac{E}{2k_B T_{bo}}$$
Nonlinear solution $T_b(s)$ with a turning point

Flame temperature versus degree of folding

$$X e^{-X} = K$$

$$X \equiv \frac{E}{2kBT_{bo}} \left( \frac{T_b}{T_{bo}} - 1 \right) \quad \text{flame temperature}$$

$$K = \kappa s, \quad \kappa \equiv (\gamma - 1) \frac{(T_{bo} - T_u0)}{T_{bo}} \frac{U_{bo}}{a_o} \frac{E}{2kBT_{bo}} \quad \text{degree of folding}$$

Critical folding factor $s^* \approx 10 - 15$

No solution for $K > 1/e$ i.e when the folding is too large $s > s^*$

If $s < s^*$: No more self-similar solution

**DDT ?**

Numerical solutions of planar flames with a reaction rate multiplied by $s^2 > s^{*2} \approx 10^2 - 10^3$ show a runaway corresponding to DDT (Sivashinsky et al. 2017-2021) (non-physical model!)

Weaknesses of the Deshaies Joulin analysis

Weak shock wave

Unsteadiness of the compression wave induced by the self-acceleration of the flame neglected
DDT of elongated flames propagating in **closed** channels  
**laminar regime**

**Experiments in** $50 \times 50$ mm$^2$ **tubes:**


**Theoretical analyses**

P. Clavin, J. Fluid Mech. (2023) vol. 974, A46  

(no assumption of small heat release !)

There is also DDT in **long open ended** channels (not treated in these lectures)

**Experiment:** V. Bykov, et al. (2022) *Combust. Flame*, 238 111913  
**Theory:** P. Clavin, V. Bykov (2024) in preparation
In addition of the high thermal sensitivity there are two key mechanisms for the DDT of elongated flames in tubes (laminar regime)

Self-accelerating elongated flame (laminar) of a flame ignited at the centre of the closed end of a tube

-1) Back-flow


-2) Very energetic mixtures: $U_b/U_L = T_b/T_u \approx 10$
The back flow of burned gas towards the flame tip is well documented by PIV experiments and DNS

Ponizy et al. (2014) *Combust. Flame*, **161** 3051-3062

Figure 1: The streamlines and temperature field
The back-flow of burned gas plays an important role for DDT at the tip of a laminar finger-flame

**ONE-DIMENSIONAL PISTON MODEL ON THE TIP**

considering the local solution on the tip as quasi-planar

Clavin, Tofaili *Combustion and Flame* 232 (2021)111522

back-flow of burned gas at the tip $u_{bf}$

1-D piston model at the tip

$$u_{bf} = 2(L/R) U_b$$

$$U_f = u_{bf} + U_b = \sigma U_b$$

$$\sigma = 2(L/R) + 1$$

$$u_{uf} = U_f - U_L$$

the flows $u_{bf}$ and $u_{uf}$ are functionals of the laminar flame velocity $U_L(T_{uf})$

speed of the piston $U_f(t) = \sigma(t) U_b(t)$

flow velocity $T_{uf}(t)$

burned gas flow

semi-permeable piston

reference frame of the flame
Self-similar solution of the one-dimensional piston model

Clavin, Tofaili *Combustion and Flame* **232** (2021)111522

The solution is similar to Deshaies Joulin

but for a very energetic flame and a back flow

folding factor → elongation \( \sigma = 2L/R + 1 \) \( U_f = \sigma U_b \)

For very energetic mixtures the turning point corresponds to a critical elongation easily accessible by

the elongation front usually observed in tubes

\[
\frac{U_L(T_u)}{U_L(T_o)} = \left( \frac{T_b}{T_{bo}} \right)^2 \left( \frac{T_u}{T_o} \right)^{3/2} \exp \left[ -\frac{E}{2k_B} \left( \frac{1}{T_b} - \frac{1}{T_{bo}} \right) \right], \quad T_b/T_u > 10
\]

\[
\frac{U_f(T_u)}{U_f(T_{uo})} = \frac{T_b/T_u}{T_{bo}/T_{uo}} \frac{U_L(T_u)}{U_L(T_{uo})}
\]

The critical conditions are in good agreement with DDT of experiments

\( T_u^* \approx 650 \text{ K}, \quad U_L^* \equiv U_L(T_u^*) \approx 40 \text{ m/s}, \quad U_f^* \approx 890 \text{ m/s}, \)

\( M^* \equiv D^*/a_o \approx 2.5 \quad L^*/R \approx 1.8 \)
Limit (weakness) of self-similar solutions of the double-discontinuity model

Constant flame velocity self-similar solution

\[ U \]

\[ D \neq U_f \]

\[ v = D - U_N \]

\[ T_b \]

\[ T_N \]

\[ T_u \]

\[ (D - U_f) t \]

Unsteady compression waves launched ahead of the flame front by the acceleration of the tip when the elongation increases is an essential mechanism of DDT that is ignored by the self-similar solutions

unburned gas

impermeable wall

tongues of unburned gas

back-flow

plane compression wave

unburned gas

burned gas

\[ u = 0 \]

\[ U_P = U_b + u_b \]

\[ U_f \]

\[ T_b \]

\[ T_N \]

\[ T_u \]

\[ (D - U_f) t \]

unsteady flow
flame elongation

\[ \frac{dL(t)}{dt} > 0 \quad L(t) \rightarrow U_f(t) \]

\[ \sigma = 2(L/R) + 1 \quad \sigma(t) \]

**One-dimensional piston model beyond self similarity**


\[ U_f = [2(L/R) + 1]U_b \]

\[ U_L = (T_u/T_b)U_b \]

\[ u_{uf} = U_f - U_L \]

energetic mixture \( T_u/T_b < 1/10, \; 2(L^*/R) + 1 \approx 5 \)

\[ u_{uf} \approx U_f \]

the piston is quasi-impermeable near the turning point

\[ \frac{d\sigma}{dt} > 0 \]

**Start the increase in elongation** from an initial state in steady state constituted by a self-similar solution close to the turning point

\[ \sigma(t) = \sigma(0)[1 + t/t_e] \]

The initial lead shock is assumed far ahead the flame

\[ \frac{u_{uf}^* - u_{uf}(0)}{a_{uf}(0)} \ll 1 \quad \Rightarrow \quad \text{compression waves} \approx \text{downstream running acoustic waves} \]
Beyond self similarity


\[
\frac{u_{uf}(t) - u_{uf}(0)}{a_{uf}(0)} \ll 1 \quad \text{compression waves} \approx \text{downstream running acoustic waves}
\]

Riemann:

\[
\frac{T_{uf}(t)}{T_{uf}(0)} - 1 \approx (\gamma - 1) \left[ \frac{u_{uf}(t) - u_{uf}(0)}{a_{uf}(0)} \right]
\]

\[
\sigma(t) = \sigma(0)[1 + t/t_e] \quad 1/t_e \ll 1/\tau_L \quad \text{flame structure in quasi-steady state}
\]

Z FK:

\[
\frac{U_{b}(t)}{U_{b}(0)} = \exp \left[ \frac{1}{2k_B T_{b}(0)} \left( \frac{T_{uf}(t) - T_{uf}(0)}{T_{b}(0)} \right) \right]
\]

\[
u_{uf}(t) = \sigma(t)U_{b}(t) \quad \Rightarrow \quad \text{turning point of the function } \quad u_{uf}(\sigma)
\]

\[
\sigma(t^*) = \sigma^* \quad u_{uf}(t^*) = u_{uf}^*
\]

there is no more dynamical solution after a finite time

\[
\sigma > \sigma^* \iff t > t^*
\]

What happens when approaching \(\sigma^*\)?

Strong unsteady effects: finite time singularity of the dynamical solution!

(as shown in the rest of the lecture)
Dynamics close to the critical point when the flame and the burned gas are in steady state, retaining only unsteadiness in the unburned gas: strongly unsteady effects of the compression wave develop when approaching the critical point.

**generic expression for** \( U_f(\sigma) : \frac{\sigma - \sigma^*}{\sigma^*} \propto -\frac{(U_f - U_f^*)^2}{U_f^*} \) \( U_f \approx u_{uf} \)

\( \sigma(t) = \sigma(0)[1 + t/t_e] \)

\( t - t^* \to 0^+ : \frac{(U_f^* - U_f)}{U_f^*} = \sqrt{\frac{t^* - t}{t_e}} \Rightarrow \frac{t_e}{U_f^*} dU_f = \sqrt{\frac{t_e}{t^* - t}} \)

**finite-time singularity of the flame acceleration**

What about the flow field?

\( \frac{u(x,t)}{u_{uf}} \approx 1 - \sqrt{\frac{(t^* - t)}{t_e} + \frac{(x - X_f(t))}{a(0)t_e}} \)

Riemann: Burgers equation

\( \frac{\partial u}{\partial t} + \left( \frac{\gamma + 1}{2} u + a(0) \right) \frac{\partial u}{\partial x} = 0 \)

\( x = X_f(t) : u = U_f(t) = u_{uf}(t) \)

\( \frac{1}{u_{uf}^*} \left| \frac{\partial u}{\partial x} \right| \bigg| _{x=X_f(t)} = -\frac{1}{2a(0)t_e} \frac{1}{\sqrt{t_e^*}} \sqrt{t^* - t} / t_e^* \)

**singularity of the flow gradient on the piston at** \( t = t^* \)

\( t = t^* \quad u_{uf}/a(0) \approx [2\beta(\gamma - 1)]^{-1} \)

**ONSET OF A SHOCK IN THE FLAME STRUCTURE: DDT?**
Limitation of the analysis near the critical point: strong acceleration

⇒ neither the flame structure nor the burned gas flow are in quasi-steady state

**Unsteady** analysis by a perturbation analysis (small elongation rate):

approximate analysis of the full dynamics when approaching the critical point


Non dimensional equations are obtained with the initial state of the burned gas used as reference reference

\[ \tau \equiv t/t_L(0) \quad \text{where} \quad t_L(0) \equiv d_L(0)/U_b(0), \quad \xi \equiv (x - X_f)/d_L(0), \]

\[ r \equiv \frac{p}{p_b(0)}, \quad v \equiv \frac{u}{U_b(0)}, \quad \pi \equiv \frac{p}{p(0)}, \quad \theta \equiv \frac{T}{T_b(0)}, \]

\[ \varepsilon \equiv \frac{t_L(0)}{t_e}, \quad \sigma(\tau) = 1 + \epsilon \tau, \]

small elongation rate \( \varepsilon \ll 1 \) elongation

small Mach number \( \varepsilon \ll 1 \)

Mass-weighted coordinate: \((\xi, \tau) \rightarrow (z, \tau), \quad z \equiv \int_0^\xi r(\xi', \tau) d\xi', \quad \frac{\partial}{\partial \xi} = r \frac{\partial}{\partial z}\)

Asymptotic analysis with the ZFK model of flame: up to order \( \varepsilon \) included for retained the pressure effect

Equations outside the reaction sheet for \( \theta, \pi_1, v, \psi \)

mass+energy+ideal gas

\[ \frac{\partial v}{\partial z} = [1 - \varepsilon \pi_1] \frac{\partial^2 \theta}{\partial z^2} - \varepsilon 1 \frac{\partial \pi_1}{\partial \tau} m(\tau) \equiv \frac{D(1/\rho)}{Dt} = \frac{\partial u}{\partial z} - 1/\rho = (c_p - c_u)T/p \]

momentum

\[ \frac{\partial v}{\partial \tau} - m(\tau) \frac{\partial v}{\partial z} - \frac{\partial^2 v}{\partial z^2} = -\frac{1}{\gamma} \frac{\partial M_1}{\partial \tau} m(\tau) \equiv \rho \frac{D u}{Dt} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left[ \mu \frac{\partial u}{\partial x} \right] \]

species

\[ \frac{\partial \psi}{\partial \tau} - m(\tau) \frac{\partial \psi}{\partial z} - \frac{\partial^2 \psi}{\partial z^2} = 0, \quad \psi(z, \tau) \in [0, 1] \]

energy

\[ \frac{\partial \theta}{\partial \tau} - m(\tau) \frac{\partial \theta}{\partial z} - \frac{\partial^2 \theta}{\partial z^2} = \varepsilon \frac{(\gamma - 1)}{\gamma} \theta \left[ \frac{\partial \pi_1}{\partial \tau} - m(\tau) \frac{\partial \pi_1}{\partial z} \right], \quad \frac{\partial \pi_1}{\partial z} = O(\varepsilon) \]

Boundary conditions

**hyperbolic problem in the external zone**: \( z \rightarrow \pm \infty \): initial conditions

\[ z = 0: \quad v = v_b = \sigma(0)[1 + \epsilon \tau] m + \quad \text{ZFK jump conditions for } \theta, \psi \]
Formulation. Equations outside the reaction zone

details of the calculation

\[ m(\xi, \tau) = r(\xi, \tau) [V_f(\tau) - v(\xi, \tau)] > 0, \quad V_f \equiv U_f(\tau)/U_0(0), \quad r \equiv \pi/\theta \]

mass flux across the reaction sheet \( \xi = 0 \):

\[
m(\tau) \equiv m(0, \tau) = r(0, \tau) [V_f(\tau) - v(0, \tau)]
\]

change of variables:

\[
(\xi, \tau) \rightarrow (z, \tau)
\]

\[
z \equiv \int_0^\xi r(\xi', \tau) d\xi', \quad \frac{\partial}{\partial \xi} = r \frac{\partial}{\partial z} = \pi \frac{\partial}{\partial z} \quad \frac{\partial}{\partial \tau} = \frac{\partial}{\partial \tau} + \left[ \int_0^\xi \frac{\partial r(\xi', \tau)}{\partial \tau} d\xi' \right] \frac{\partial}{\partial \tau} z = \frac{\partial}{\partial \tau} \left[ m(\xi, \tau) - m(\tau) \right] \frac{\partial}{\partial z} \]

mass:

\[
\frac{\partial p}{\partial t} = -\frac{\partial (\rho u)}{\partial x} + \frac{\partial}{\partial x} \left[ \mu \frac{\partial u}{\partial x} \right]
\]

velocity:

\[
\frac{\partial v}{\partial \tau} - V_f(\tau) \frac{\partial r}{\partial \xi} = -\frac{\partial [r(\xi, \tau) v(\xi, \tau)]}{\partial \xi}
\]

momentum:

\[
\rho \frac{D u}{D t} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left[ \mu \frac{\partial u}{\partial x} \right]
\]

energy:

\[
\rho c_p \frac{D T}{D t} = \frac{D p}{D t} + \frac{\partial}{\partial x} \left[ \lambda \frac{\partial T}{\partial x} \right] + \frac{\partial(\rho u)}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial(\rho v)}{\partial x} \frac{\partial v}{\partial x} + \frac{\partial(\rho r)}{\partial x} \frac{\partial r}{\partial x} - m(\tau) \frac{\partial \theta}{\partial \tau} - \frac{\partial}{\partial \tau} \left( \frac{\partial^2 \theta}{\partial x^2} \right) = \frac{(\gamma - 1) \theta}{\gamma} \left[ \frac{\partial}{\partial \tau} (\frac{m(\tau)}{\partial \tau} \frac{\partial \pi}{\partial \tau} \frac{\partial \theta}{\partial \tau} \frac{\partial^2 \theta}{\partial \tau^2} \right] + (\gamma - 1) \theta^2 \left( \frac{\partial \theta}{\partial z} \right)^2
\]

mass + energy:

\[
\frac{\partial \nu}{\partial \tau} = \frac{\partial^2 \theta}{\partial \tau^2} + O(\epsilon)
\]

integration across the preheated zone:

\[
\beta \rightarrow \infty, \quad (1 - 0_0) = O(1/\beta), \quad \theta_{0_0} \equiv \theta|_{z=0} = O(1/\beta), \quad z = O(1), \quad \lim_{z \rightarrow \infty} \frac{\partial \theta}{\partial z} = O(1/\beta), \quad \int_{0^+}^{\infty} \frac{\partial \nu}{\partial z} \, dz = v_{u} - v_{b} - \frac{\partial \theta}{\partial z}|_{z=0^+} + O(\epsilon)
\]

instantaneous back flow:

\[
v_{b}(\tau) = \sigma(0)(1 + \epsilon \tau) e^{\beta[\theta_{b}(\tau) - 1]/2}
\]

jump conditions across the reaction sheet:

\[
\frac{\partial \theta}{\partial z}|_{z=0^+} = q_0 \theta_0(1 - \theta_{0_0})/2 + O(1/\beta), \quad q \equiv \frac{T_b(0) - T_u(0)}{T_b(0)} \quad \frac{\partial \theta}{\partial z} + \frac{1}{Le} \frac{\partial \psi}{\partial z}|_{z=0^+} = O(1/\beta^2), \quad Le = 1
\]

ZFK limit \( \beta \equiv E/k_BT_b(0) \rightarrow \infty \)

\[
\epsilon \ll \xi \ll 1, \quad (\gamma - 1) \beta \varepsilon \sigma(0) = O(1), \quad \pi = 1 + \varepsilon \pi_1(\epsilon z, \tau)
\]

multiple scale:

\[
\frac{\partial v}{\partial \tau} + \frac{(1 - 0_0) v}{x} = O(\epsilon)
\]

pressure uniform inside the flame structure

\[
\nu_u(0) \quad \nu_u(t) \quad T_u(t) \quad T_0 \quad T_b(0) \quad T_a(0) \quad u_b(t) \quad u_u(t) \quad T_b(t) \quad T_f(t) \quad (T - T_0)(T - T_b) \]

burnt gas outer flow
flame structure inner flow
fresh mixture isentropic compression wave
back flow flame thickness \( \xi(t) \) reaction sheet
Dynamics of Combustion Waves in Premixed Gases

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Lecture XII
Galloping detonations
Lecture 12: Galloping detonations

12-1. Physical mechanisms

*Instability mechanism*

*Two limiting cases*

12-2. General formulation

*Constitutive equations*

*Strong shock in the Newtonian approximation*

12-3. Strongly overdriven regimes in the limit \((\gamma - 1) \ll 1\)

*Distinguished limit*

*Integral-differential equation for the dynamics*

*Oscillatory instability*

12-4. CJ detonations for small heat release

*Reactive Euler equations in 1-D geometry*

*Near CJ regimes for small heat release. Transonic reacting flows*

*Slow time scale*

*Asymptotic model for CJ or near CJ regimes*

*Results for simplified chemical kinetics*
XII-1) Physical mechanisms

Detonation = inner shock followed by an exothermal reaction zone
Inner structure = uniform induction zone + zone of heat release
Galloping detonation = oscillatory instability: oscillation of the velocity of the lead shock

\[ \frac{\dot{\alpha}}{\alpha(t)} = 0 \]

reference frame of the unperturbed detonation

Instability mechanism

\[ \delta D = -\dot{\alpha}_t \neq 0 \Rightarrow \delta T_N \Rightarrow \delta l_{ind} \]
motion of the heat release zone produces a piston like effect
the unstable character depends on the phase shift

Two different coupling mechanisms:
- acoustic waves
- entropy wave

Two limiting cases

Strongly overdriven regimes for \((\gamma - 1) \ll 1\): quasi-isobaric flow, the delay by the acoustic waves is negligible
CJ regime for \(q_m/c_p T_u \ll 1\) and \((\gamma - 1) \ll 1\): transonic flow, the entropy wave is negligible

Lehr 1972
Lecture 12: Galloping detonations

12-1. Physical mechanisms
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   Two limiting cases

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   Strong shock in the Newtonian approximation

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12-4. CJ detonations for small heat release
   Reactive Euler equations in 1-D geometry
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   Results for simplified chemical kinetics
Reactive Euler equations in 1-D geometry

\[
\begin{aligned}
\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + u \cdot \nabla \\
\frac{1}{\rho} \frac{D \rho}{Dt} = -\nabla \cdot u, \\
\frac{D \psi}{Dt} = \frac{\dot{\psi}}{\tilde{t}_N}, \\
1-D \text{ Euler (compressible) eqs.}
\end{aligned}
\]

\[D \equiv \frac{\partial}{\partial t} + u \frac{\partial}{\partial x}\]

\[\dot{w}(\psi, T)\]

\[
\frac{1}{\gamma p} \left[ \frac{\partial}{\partial t} + (u \pm a) \frac{\partial}{\partial x} \right] p \pm \frac{1}{\gamma p} \left[ \frac{\partial}{\partial t} + (u \pm a) \frac{\partial}{\partial x} \right] u = \frac{q_m}{c_p T \tilde{t}_N} \frac{\dot{\psi}}{\tilde{t}_N}
\]

\[
1-D : \quad D^{\pm}/Dt \equiv \frac{\partial}{\partial t} \pm (a \pm u) \frac{\partial}{\partial x}
\]

entropy equation

generalized acoustic eqs.
\((\delta p = \pm \rho a \delta u)\)

Continuous set of feed back loops

upstream running acoustic wave

\[\frac{1}{\gamma p} \left[ \frac{\partial}{\partial t} + (u - a) \frac{\partial}{\partial x} \right] p - \frac{1}{\gamma p} \left[ \frac{\partial}{\partial t} + (u - a) \frac{\partial}{\partial x} \right] u = \frac{q_m}{c_p T \tilde{t}_N} \frac{\dot{\psi}}{\tilde{t}_N}\]

downstream running acoustic wave

\[\frac{1}{\gamma p} \left[ \frac{\partial}{\partial t} + (u + a) \frac{\partial}{\partial x} \right] p + \frac{1}{\gamma p} \left[ \frac{\partial}{\partial t} + (u + a) \frac{\partial}{\partial x} \right] u = \frac{q_m}{c_p T \tilde{t}_N} \frac{\dot{\psi}}{\tilde{t}_N}\]

entropy wave

downstream running acoustic wave

upstream running acoustic wave
Galloping detonation = pulsating instability of the 1-D solution

velocity of the shock oscillates
\[ D(t) = \bar{D} - \dot{\alpha}_t, \]

reaction rate oscillates
\[ \bar{\alpha} = 0, \quad \alpha(t) \quad \text{oscillations} \]

Reduced equations

**Reactive Euler equations**

\[
\begin{align*}
\frac{1}{\rho} \frac{D \rho}{Dt} &= -\nabla \cdot \mathbf{u}, \\
\frac{Du}{Dt} &= -\nabla p, \\
p &= (c_p - c_v)\rho T \\
\frac{1}{T} \frac{DT}{Dt} - \left( \frac{\gamma - 1}{\gamma} \right) \frac{1}{p} \frac{Dp}{Dt} &= \frac{q_m}{c_p T} \frac{\dot{w}}{\bar{T}_N}, \\
\frac{D\psi}{Dt} &= \frac{\dot{w}(\psi, T)}{\bar{T}_N}, \\
\bar{T}_N &= \tau_r(T_N)
\end{align*}
\]

**Reduced mass weighted distance from the shock** (useful for unsteady 1-D problems)

\[
x = \alpha(t), \quad \bar{T}_N = \tau_r(T_N)
\]

\[
x = \frac{1}{\rho_u \bar{T}_N} \int_{\alpha(t)}^{x} \rho(x', t) dx', \quad t = \frac{t}{\bar{T}_N}, \quad \bar{\alpha}_t \equiv \frac{d\alpha}{dt}
\]

\[
\frac{D}{Dt} \left( \frac{\rho_u}{\rho} \right) = \frac{\partial}{\partial t} \left( \frac{u}{\bar{D}} \right) + m(t) \frac{\partial}{\partial x}, \quad \text{where} \quad m(t) = \left[ \frac{\rho(x, t)[u(x, t) - \dot{\alpha}_t]}{\rho_u \bar{D}} \right]_{x=\alpha(t)} = 1 - \frac{\dot{\alpha}_t}{\bar{D}}
\]

\[
\begin{align*}
\frac{D}{Dt} \left( \frac{\rho_u}{\rho} \right) &= \frac{\partial}{\partial t} \left( \frac{u}{\bar{D}} \right) + m(t) \frac{\partial}{\partial x}, \\
\frac{D}{Dt} \left( \frac{u}{\bar{D}} \right) &= -\frac{\partial}{\partial x} \left( \frac{p}{\rho_u \bar{D}^2} \right), \\
\frac{D}{Dt} \left( \bar{T}_N \right) &= \frac{\partial}{\partial t} \left( \frac{u}{\bar{u}_N} \right), \\
\frac{1}{\bar{T}} \frac{DT}{Dt} - \frac{\gamma - 1}{\gamma} \frac{1}{p} \frac{Dp}{Dt} &= \frac{q_m}{c_p T} \frac{\dot{w}}{\bar{T}_N}, \\
\frac{D\psi}{Dt} &= \frac{\dot{w}(\psi, T)}{\bar{T}_N}
\end{align*}
\]
\[
\begin{align*}
\frac{\partial}{\partial t} \frac{\rho}{\rho} = \frac{\partial}{\partial x} \left( \frac{u}{\bar{D}} \right) & \iff \frac{\partial}{\partial t} \left( \frac{\bar{u}_N}{\rho} \right) = \frac{\partial}{\partial x} \left( \frac{\bar{u}}{\bar{u}_N} \right), \\
m(t) = 1 - \frac{\dot{\alpha}_t}{\bar{D}} & \iff m(t) \text{ unknown}.
\end{align*}
\]

**Boundary conditions**

Neumann state \( x = 0 : \) \( \rho = \rho_N(t), \ p = p_N(t), \ T = T_N(t) \) \( \rho_N(t)(u - \dot{\alpha}_t) = \rho_u \bar{D} m(t) \) \( \psi = 0 \)

expressed in terms of \( m(t) \) by the RH conditions

\[
\begin{align*}
\frac{u_N}{\bar{D}} &= \frac{(\gamma - 1)M^2_u + 2}{(\gamma + 1)M^2_u}, \\
\frac{T_N}{T_u} &= \left[ \frac{2\gamma M^2_u}{(\gamma + 1)^2} \right] \left[ \frac{(\gamma - 1)M^2_u + 2}{(\gamma + 1)^2 M^2_u} \right], \\
\frac{p_N}{p_u} &= \frac{2(\gamma M^2_u - (\gamma - 1))}{(\gamma + 1)}, \\
M^2 &= \frac{(\gamma - 1)M^2_u + 2}{2\gamma M^2_u - (\gamma - 1)}.
\end{align*}
\]

\( M_u = [1 - m(t)]\bar{M}_u \)

Burnt gas \( x \to \infty : \) \( \begin{cases} \text{overdriven regimes: } \ u = \bar{u}_b \\
\text{CJ regime: } \ p - \bar{p}_b = \bar{p}_u \bar{u}_b (u - \bar{u}_b) \text{ i.e. outgoing acoustic waves (radiation condition)} \end{cases} \)

**Analytical solutions are obtained in limiting cases**

**Strong shock in the Newtonian approximation**

\( \bar{M}_u \gg 1, \ (\gamma - 1) \ll 1 \) \( \Rightarrow \ \bar{M}_N^2 \approx \frac{\gamma - 1}{2} + \frac{1}{\bar{M}_u^2} \ll 1 \)

**Distinguished limit:**

\( \bar{M}_u \gg 1, \ (\gamma - 1)M_u^2 = O(1) \)

\[
\bar{M}_u^2 \ll 1, \quad \bar{M}_u^2 = O(1/\varepsilon^2), \quad (\gamma - 1) = O(\varepsilon^2)
\]

\[
\begin{align*}
\bar{u}_N/\bar{D} &= \bar{p}_u/\bar{p}_N \approx \varepsilon^2, \\
\bar{p}_N/\bar{p}_u &\approx \bar{M}_u^2 = O(1/\varepsilon^2), \\
\bar{u}_N/\bar{D} &\approx \varepsilon, \\
(\bar{u}_N/\bar{u}_u)^2 &\approx [2 + (\gamma - 1)\bar{M}_u^2]/2 = O(1)
\end{align*}
\]

\[
\begin{align*}
\bar{p}_u - \bar{p}_N \bar{u}_N &= 0, \\
d\bar{p}/dx + \bar{p}_u d\bar{u}/dx &= 0
\end{align*}
\]

and \( a^2/\gamma = p_N/\rho_N \) \( \Rightarrow \) \( (\bar{p}/\bar{p}_N - 1) = -\varepsilon^2 (\bar{u}/\bar{u}_N - 1), \)

Quasi-isobaric approximation of the shocked gas.
Lecture 12: Galloping detonations

12-1. Physical mechanisms
   Instability mechanism
   Two limiting cases

12-2. General formulation
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12-3. Strongly overdriven regimes in the limit \((\gamma - 1) \ll 1\)
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Strongly overdriven detonations in the limit \((\gamma - 1) \ll 1\)

Distinguished limit

\[\epsilon^2 \equiv \overline{M}_N^2 \ll 1, \quad \overline{M}_u^2 = O(1/\epsilon^2), \quad (\gamma - 1) = O(\epsilon^2)\]

\[q_N \equiv q_m/c_p\overline{T}_N = O(1) \quad \Leftrightarrow \quad \text{strongly overdriven regime}\]

\[M_{ucJ} = \sqrt{Q} + \sqrt{Q + 1} \quad \text{where} \quad Q = \frac{\gamma + 1}{2} \frac{q_m}{c_p T_u}\]

\[T_N/T_u = O(1) \Rightarrow M_{ucJ} = O(1) \Rightarrow M_u \gg M_{ucJ}\]

Negligible adiabatic compression

\[
\frac{1}{T} \frac{DT}{Dt} - \frac{(\gamma - 1) \overline{p}}{p} \frac{D\overline{p}}{Dt} = \frac{q_m}{c_p \overline{T}} \dot{\omega},
\]

\[
\Rightarrow \quad \left\{ \begin{array}{l}
\frac{\partial T}{\partial t} + m(t) \frac{\partial T}{\partial x} = \frac{q_m}{c_p} \dot{\omega}(\psi, T), \\
\frac{\partial \psi}{\partial t} + m(t) \frac{\partial \psi}{\partial x} = \dot{\omega}(\psi, T)
\end{array} \right.
\]

\[x = 0: \quad \psi = 0, \quad T = T_N(t)\]

\[T_N/T_u \approx [(\gamma - 1)M_u^2 + 2]/2 \quad \text{where} \quad M_u^2 = \overline{M}_u^2(1 - \dot{\alpha}_t/D)^2\]

The solution yields \(T(x,t)\) and \(\psi(x,t)\) in terms of \(m(t) = 1 - \dot{\alpha}_t/D\)
\[ Distinguished \ limit \quad (\gamma - 1)\beta_N = O(1) \quad \Leftrightarrow \quad \beta_N = O(1/\epsilon^2) \]

\[ m(t) = 1 - \dot{\alpha}_t / D, \quad \dot{\alpha}_t / D = O(1/\beta_N) \Rightarrow \]
\[
\frac{D}{Dt} \approx \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \sum \left[ \frac{\partial T}{\partial t} + \frac{\partial T}{\partial x} = \frac{q_m}{c_p} \dot{w}(\psi, T), \right.
\frac{\partial \psi}{\partial t} + \frac{\partial \psi}{\partial x} = \dot{w}(\psi, T) \]
\[ x = 0 : T = T_N(t), \psi = 0, \]

\[ (T_N - \overline{T}_N)/T_N = O(1/\beta_N) \Rightarrow \]
\[ \Theta_N(t) \equiv \beta_N(T_N(t) - \overline{T}_N)/T_N = O(1), \quad \ddot{w} - \widetilde{w} = O(1) \]

\[ Steady \ state \ solutions \]
\[
\left\{ \begin{array}{l}
\frac{dT}{dx} = \frac{q_m}{c_p} \dot{w}(\psi, T), \\
\frac{d\psi}{dx} = \dot{w}(\psi, T)
\end{array} \right. \]
\[ x = 0 : T = \overline{T}_N, \psi = 0, \]
\[ T = T(\Theta_N, x), \quad \psi = \mathcal{Y}(\Theta_N, x), \quad \Omega(\Theta_N, x) \equiv \dot{w}(\mathcal{T}, \mathcal{Y}) \]

\[ Unsteady \ solution \ (retarded \ functions) \]
\[ T(x, t) = T(\Theta_N(t - x), x), \quad \psi(x, t) = \mathcal{Y}(\Theta_N(t - x), x), \quad \dot{w} = \Omega(\Theta_N(t - x), x) \]
Distinguished limit $$(\gamma - 1)\beta_N = O(1) \iff \beta_N = O(1/\epsilon^2)$$

$$m(t) = 1 + O(1/\beta_N) \quad \left[ \frac{\partial}{\partial t} + m(t) \frac{\partial}{\partial x} \right] \approx \left[ \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right]$$

Rankine-Hugoniot

$$\frac{T_N}{T_u} = \left\{ \begin{array}{l} \frac{2\gamma M^2_u - (\gamma - 1)}{(\gamma + 1)^2 M^2_u + 2} \\
\frac{M^2_u}{M^2_u(1 - \alpha_t/D)^2} \end{array} \right\} \Rightarrow \frac{T_N(t) - T_N}{T_N} \approx - (\gamma - 1)\alpha_t/\bar{u}_N \ll 1, \Rightarrow \frac{u_N}{\bar{u}_N} \approx 1 + \frac{\alpha_t}{\bar{u}_N}$$

Quasi-isobaric approximation in the shocked gas + Continuity

$$\left[ \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right] \frac{T}{T_N} \approx \left[ \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right] \frac{\bar{p}_N}{\rho} = \frac{\partial}{\partial x} \left( \frac{u}{\bar{u}_N} \right)$$

Energy

$$\left[ \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right] \frac{T}{T_N} = \frac{q_m}{c_p T_N} \dot{\bar{w}}$$

$$\frac{u_b}{\bar{u}_N} - \frac{u_N}{\bar{u}_N} = \frac{q_m}{c_p T_N} \int_0^\infty \dot{\bar{w}}(x, t) dx$$

$$\dot{\bar{w}} = \Omega(\Theta_N(t - x), x)$$

Nonlinear integral-equation

$$1 + b\Theta_N(t) = \int_0^\infty \Omega(\Theta_N(t - x), x) dx, \quad b^{-1} = \beta_N(\gamma - 1) \frac{q_m}{c_p T_N} = O(1)$$

(Clavin He 1996)
strongly overdriven detonations in the Newtonian limit

quasi-isobaric approximation in the shocked gases

+ energy eq. for $T$

heat release per unit mass

progress variable

$$\left( \frac{\partial}{\partial t} + u \frac{\partial}{\partial r} \right) \left[ \ln T - \frac{(\gamma - 1)}{\gamma} \ln p \right] = \frac{q_m}{c_p T} \frac{\dot{w}(T, Y)}{t_r}$$

$\dot{w}$: non-dimensional reaction rate

chemical kinetics

$$\left( \frac{\partial}{\partial t} + u \frac{\partial}{\partial r} \right) Y = \frac{\dot{w}(T, Y)}{t_r}$$

$\rho T \approx$ cst.

unsteady / steady distribution of the rate of heat release

$$\Theta_N(t) = \frac{\beta(T_N(t) - T_N)}{T_N}$$

$$x \equiv \frac{1}{t_r \rho_a D} \int_{\alpha(t)}^{T_N} \rho(x) dx \quad t \equiv \frac{t}{t_r}$$

conservation of mass and boundary conditions

Rankine-Hugoniot at $x = 0$:

$$\frac{D(t) - \overline{D}}{\overline{D}} \Leftrightarrow \Theta_N(t) \quad \downarrow$$

$x \rightarrow \infty$ : boundedness

integral equation for $\Theta_N(t)$

$$1 + b \Theta_N(t) = \int_0^\infty \Omega(\Theta_N(t - x), x) dx, \quad b^{-1} \equiv \frac{\beta_N(\gamma - 1)}{c_p T_N} \frac{q_m}{T_N}$$
strongly overdriven detonations in the Newtonian limit
quasi-isobaric approximation in the shocked gas

\[ 1 + b \Theta_N(t) = \int_0^\infty \Omega(\Theta_N(t - x), x) \, dx, \]

\[ \Omega(\Theta_N, x) \approx e^{\Theta_N} \Omega(e^{\Theta_N} x), \]

\[ l/l = e^{-\Theta_N} \]

\[ l/l = e^{-\Theta_N} \]

\[ \hat{\mathcal{S}} \]

\[ \hat{\omega} = O(1) \Leftrightarrow \omega = O(\bar{t}_N) \]

\[ \text{high thermal sensitivity, } \beta_N \]

and/or

stiffness of the distribution of heat release \( \Omega(\Theta_N, x) \)

intermittency

nonlinear effects: stochasticity + dynamical quenching

OK with DNS
Lecture 12: Galloping detonations

12-1. Physical mechanisms
   Instability mechanism
   Two limiting cases

12-2. General formulation
   Constitutive equations
   Strong shock in the Newtonian approximation

12-3. Strongly overdriven regimes in the limit \((\gamma - 1) \ll 1\)
   Distinguished limit
   Integral-differential equation for the dynamics
   Oscillatory instability

12-4. CJ detonations for small heat release
   Reactive Euler equations in 1-D geometry
   Near CJ regimes for small heat release. Transonic reacting flows
   Slow time scale
   Asymptotic model for CJ or near CJ regimes
   Results for simplified chemical kinetics
Reactive Euler equations in 1-D geometry

\[
\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + u \nabla \quad \frac{1}{\rho} \frac{D\rho}{Dt} = -\nabla u, \quad \frac{D\psi}{Dt} = \frac{\dot{\psi}}{t_N},
\]

\[
\frac{Dp}{Dt} = \frac{\partial p}{\partial t} + \nabla \cdot u = \frac{q_m \dot{\psi}}{c_p T \dot{t}_N}.
\]

\[
\frac{1}{a^2} = \frac{\gamma p}{\rho} \quad 1-D: \quad \frac{D\pm}{Dt} \equiv \frac{\partial}{\partial t} \pm (a \mp u) \frac{\partial}{\partial x} \quad \Rightarrow \quad \frac{1}{\gamma p} \frac{Dp}{Dt} \pm \frac{1}{a} \frac{Du}{Dt} = \frac{q_m \dot{\psi}}{c_p T \dot{t}_N}
\]

- Entropy equation
- Generalized acoustic eqs.
- $\delta p = \pm \rho a \delta u$

**CJ detonations for small heat release**


Near CJ regimes for small heat release. Transonic reacting flows

**CJ and overdriven regimes**

\[
M_{u,CJ} = \sqrt{Q} + \sqrt{Q + 1} \quad Q = \frac{(\gamma + 1)}{2} \frac{q_m}{c_p T_u} \quad f = \frac{(M_u - M_{u,CJ}^{-1})^2}{4Q}
\]

CJ regime: $f = 1$, overdriven regime: $f > 1$

**Small heat release approximation** (transonic regimes)

\[
Q \ll 1
\]

Small parameter: $\epsilon^2 \equiv Q \ll 1 \quad M_{u,CJ}^2 \approx 1 + 2\epsilon$

Overdriven regime near CJ: $f = O(1)$

\[
M_u^2 \approx 1 + 2\epsilon \sqrt{f} \quad M_u^2 - M_{u,CJ}^2 \approx 2\epsilon(\sqrt{f} - 1)
\]
\( q_N \equiv \frac{q_m}{c_p T_N} = O(\epsilon^2) \quad f = O(1) \)

**Rankine-Hugoniot conditions**

\[ \frac{T_N}{T_u} \approx 1 + (\gamma - 1)(M_u^2 - 1), \quad \frac{p_N}{p_u} \approx \frac{\rho N}{\rho u} \approx 1 + (M_u^2 - 1), \quad \psi = 0 \]

\( (M_u^2 - 1) \ll 1 \)

**Steady state**

\[ (\bar{M}_u^2 - 1) \approx (1 - \bar{M}_N^2) \approx 2 \epsilon \sqrt{f} \]

crossover temperature: \( T_u < T^* < T_N \)

separation of scale: \( \tau_{coll/\hat{t}_N} \ll (\bar{M}_u - 1) \Rightarrow e^{-E/k_B T_N} \ll \epsilon \)

**Distinguished limit**

\[ (\gamma - 1) = O(\epsilon) \Rightarrow (T - T_N)/T_N = O(\epsilon^2) \]

**Non-dimensional equations**

\[ t \equiv \frac{t}{\hat{t}_N}, \quad x \equiv \frac{x}{a_u \hat{t}_N}, \quad \bar{u} \equiv \frac{u}{a_u}, \quad \bar{p} \equiv \frac{p}{p_u} = O(1) \gamma \ln \left( \frac{p}{p_u} \right), \quad \bar{\theta} \equiv \frac{\bar{T} - \hat{T}_u}{\hat{T}_u} \]

\[ \begin{array}{c}
\bar{\theta} = O(\epsilon^2) \quad a/a_u = 1 + O(\epsilon^2) \\
1 - \bar{u} = O(\epsilon) \quad \bar{\pi} = O(\epsilon)
\end{array} \]

the variation of \( a \) is negligible in

\[ \frac{1}{\gamma p} \left[ \frac{\partial}{\partial t} + (u \pm a) \frac{\partial}{\partial x} \right] p \pm \frac{1}{a} \left[ \frac{\partial}{\partial t} + (u \pm a) \frac{\partial}{\partial x} \right] u = \frac{q_m}{c_p T \hat{t}_N} \]

\[ \begin{align*}
\frac{\partial}{\partial t} + (1 + \bar{u}) \frac{\partial}{\partial x} \left( \bar{\pi} + \bar{u} \right) = \epsilon^2 \bar{w}, & \quad \frac{\partial}{\partial t} + \bar{u} \frac{\partial}{\partial x} \left[ \bar{\theta} - (\gamma - 1) \bar{\pi} \right] = \epsilon^2 \bar{w} \\
\frac{\partial}{\partial t} - (1 - \bar{u}) \frac{\partial}{\partial x} \left( \bar{\pi} - \bar{u} \right) = \epsilon^2 \bar{w} & \quad \frac{\partial}{\partial t} + \bar{u} \frac{\partial}{\partial x} \left( \psi = \bar{w} \right)
\end{align*} \]
Slow time scale

\[ M_u^2 - 1 = O(\epsilon) \Rightarrow \text{transonic flow: } u/a = 1 + O(\epsilon) \]

time scale of the downstream propagating acoustic wave: \( l_{\text{ind}}/a = \tilde{t}_N \)

\[
\frac{1}{\gamma p} \left[ \frac{\partial}{\partial t} + (u + a) \frac{\partial}{\partial x} \right] p + \frac{1}{a} \left[ \frac{\partial}{\partial t} + (u + a) \frac{\partial}{\partial x} \right] u = \frac{q_m}{c_p T} \frac{w}{\tilde{t}_N}
\]

time scale of the upstream propagating acoustic wave: \( l_{\text{ind}}/(a - u) \approx \tilde{t}_N/\epsilon \)

\[
\frac{1}{\gamma p} \left[ \frac{\partial}{\partial t} + (u - a) \frac{\partial}{\partial x} \right] p - \frac{1}{a} \left[ \frac{\partial}{\partial t} + (u - a) \frac{\partial}{\partial x} \right] u = \frac{q_m}{c_p T} \frac{w}{\tilde{t}_N}
\]

longest delay in the feedback loop \( \approx \tilde{t}_N/\epsilon \)

Scaling

\[ \tau \equiv \frac{t}{t_N/\epsilon} = \epsilon t \quad \leftarrow \quad t \equiv t/\tilde{t}_N \]

Period of oscillation = \( O(\tilde{t}_N/\epsilon) \)

non dimensional time of order unity
instantaneous position of the lead shock wave \( x = \alpha(\epsilon t/\tilde{t}_N) \quad a \equiv \alpha(t)/(a_u \tilde{t}_N) \leftarrow \) non dimensional position

non dimensional variable of order unity \( \mu, \pi, \theta : \)

\[
\begin{align*}
\hat{u} & \equiv \frac{u}{a_u} = 1 + \epsilon \mu, \\
\hat{\pi} & \equiv \frac{1}{\gamma} \ln \left( \frac{\hat{p}}{\hat{p}_u} \right) = \epsilon \pi, \\
\hat{\theta} & \equiv \frac{T - \hat{T}_u}{T_u} = \epsilon^2 \theta
\end{align*}
\]

\[ \tau \equiv \epsilon t, \quad \xi \equiv x - a(\tau), \quad \frac{\partial}{\partial \xi} = \epsilon \left( \frac{\partial}{\partial t} - \hat{\alpha}_\tau \frac{\partial}{\partial \xi} \right) \]

Reference frame of the moving shock:

\[ x \equiv x/(a_u \tilde{t}_N) \]

\[ \begin{align*}
\frac{\partial}{\partial t} + (1 + \hat{u}) \frac{\partial}{\partial x} (\hat{\pi} + \hat{u}) &= \epsilon^2 \hat{w}, \\
\frac{\partial}{\partial t} - (1 - \hat{u}) \frac{\partial}{\partial x} (\hat{\pi} - \hat{u}) &= \epsilon^2 \hat{w}, \\
\frac{\partial}{\partial \tau} + \hat{\alpha}_\tau \frac{\partial}{\partial \xi} \psi &= \hat{w},
\end{align*} \]

Arrhenius law: \( \hat{w}(\psi, \theta) = (1 - \psi)e^{\beta_e(\theta - \bar{\theta}_N)} \) with \[ \beta_e \equiv \frac{E}{k_B T_N} \epsilon^2 = O(1) \]

oscillations
heat release
entropy wave
induction
acoustic waves

\[ h \equiv (\gamma - 1)/\epsilon = O(1), \quad \hat{\alpha}_\tau \equiv \alpha(\tau)/d\tau \]
Asymptotic model for CJ or near CJ regimes

$\epsilon^2 \equiv q_m/c_B T_u \ll 1, \quad (\gamma - 1) = O(\epsilon), \quad E/k_B T_N = O(1/\epsilon^2)$

(Clavin Williams 2002)

\[
\frac{\partial (\pi + \mu)}{\partial \xi} = 0, \quad \frac{\partial (\theta - h\pi - \psi)}{\partial \xi} = 0,
\]

\[
\left[ \frac{\partial}{\partial \tau} + (\mu - \dot{\alpha}_\tau) \frac{\partial}{\partial \xi} \right] (\pi - \mu) = \dot{\psi}, \quad \frac{\partial \psi}{\partial \xi} = \dot{\psi}
\]

$\dot{\alpha}_\tau \equiv \text{da}(\tau)/d\tau$

$M_u = (\overline{D} - \dot{\alpha}_t)/\alpha_u = M_u - \epsilon \dot{\alpha}_\tau$

**Boundary conditions at the Neumann state**

\[
\frac{T_N}{T_u} \approx 1 + (\gamma - 1)(M_u^2 - 1),
\]

\[
\frac{p_N}{p_u} \approx \frac{\rho_N}{\rho_u} \approx 1 + (M_u^2 - 1)
\]

\[
M_u^2 - 1 \approx 2(M_u - 1) - 2\epsilon \dot{\alpha}_\tau
\]

$\rho_u(\overline{D} - \dot{\alpha}_t) = \rho_N(u|_{x=\alpha} - \dot{\alpha}_t)$

\[\mu + \pi = \sqrt{f} \quad \theta = h\sqrt{f} - h\mu + \psi\]

The problem is reduced to solve two equations for $\mu$ and $\psi$

\[
\left[ \frac{\partial}{\partial \tau} + (\mu - \dot{\alpha}_\tau) \frac{\partial}{\partial \xi} \right] \mu = -\dot{\psi}, \quad \frac{\partial \psi}{\partial \xi} = \dot{\psi}(\psi, \theta)
\]

$\xi = 0: \quad \mu = -\sqrt{f} + 2\dot{\alpha}_\tau$ and $\psi = 0,$

**Boundary condition in the burnt gas**

$\xi \to \infty: \quad \psi = 1, \quad \mu = \overline{\mu}_b = -\sqrt{f} - 1$

yields an integral equation for $\dot{\alpha}_\tau(\tau)$
Nonlinear equation for a transonic reacting flow

\[
\left[ \frac{\partial}{\partial \tau} + (\mu - \dot{a}_\tau) \frac{\partial}{\partial \xi} \right] \mu = -\dot{w}, \quad \frac{\partial \psi}{\partial \xi} = \dot{w}(\psi, \theta)
\]

\[
\xi = 0: \quad \mu = -\sqrt{f} + 2\dot{a}_\tau \quad \text{and} \quad \psi = 0,
\]

\[
\xi \to \infty: \quad \psi = 1, \quad \mu = \bar{\mu}_b = -\sqrt{f - 1}
\]

\[\dot{w}(\psi = 1) = 0\]

Result for simplified chemical kinetics

Simplification:

The reaction rate depends only on \(T_N(t)\)

The stability analysis is similar to that of strongly overdriven regimes!

Similar integral equation but with a delay controlled by the upstream running acoustic wave

\[
\Delta(\xi) = \int_0^\xi \frac{d\xi}{|\mu(\xi)|}
\]

\[
\dot{a}_\tau(\tau) = \int_0^\infty \left[ \frac{1}{4\sqrt{f}} \Omega_N'(\xi) + G(\xi) \right] \dot{a}_\tau(\tau - \Delta(\xi)) d\xi
\]
**GENERAL CONCLUSION**

Galloping detonations are due to a **phase shift** in the loop between the lead shock and the heat release, controlled by the **entropy wave** and the **upstream running acoustic wave**.

**Strongly overdriven detonation in the Newtonian limit** (P.C. & L. He 1996)
- quasi-isobaric flow
- dominant mechanism: **entropy wave**

**CJ (or near CJ) conditions close to the instability threshold** (P.C. & F.A. Williams 2002)
- transonic flow
- dominant mechanism: **acoustic wave**

Comparison with DNS

Dynamics of Combustion Waves in Premixed Gases

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Lecture XIII
Stability analysis of shock waves
Lecture 13: Stability analysis of shock waves

13-1. Acoustic waves and entropy-vorticity wave
   - Linearized Euler equations
   - Linearized flow field

13-2. Analyses
   - Dispersion relation for general materials
   - Classification of normal modes
   - Spontaneous emission of sound and instability
   - Stability of shocks in ideal gases
   - Stability of reacting shocks
Acoustic waves and entropy-vorticity wave

Shock wave \approx \text{hydrodynamic discontinuity} + \text{Rankine-Hugoniot conditions}
\quad \text{thickness \approx mean free path}

The flow of shocked gas in a planar wave is uniform

\mathcal{D} > a_u \Rightarrow \text{the upstream flow in a wrinkled shock is not perturbed}
\quad \text{supersonic wave}

Flow velocity \tilde{u}_N \text{ is sufficiently large } \Rightarrow \text{the diffusive fluxes are negligible:}
\quad \text{compressed gas: } \quad Ds/Dt = 0 \iff \partial s/\partial t + u.\nabla s = 0
\quad \text{no entropy production in the compressed gas}

The entropy of shocked gas is modified at the Neumann state of a wrinkled shock

\Rightarrow \nabla s(r, t) \neq 0
\quad \text{entropy production inside the shock thickness: entropy jump}
Linearized Euler equations

(written in 2-D for simplicity. Extension to 2-D is straightforward)

\[ u = \bar{u}_N + \delta u, \quad w = \delta w, \quad \rho = \bar{\rho}_N + \delta \rho, \quad p = \bar{p}_N + \delta p \]

Compressed gas

\[ \frac{1}{\bar{\rho}_N} \frac{D}{Dt} \delta \rho + \frac{\partial}{\partial x} \delta u + \frac{\partial}{\partial y} \delta w = 0, \]

\[ \frac{D}{Dt} = \frac{\partial}{\partial t} + \bar{u}_N \frac{\partial}{\partial x} \]

\[ \bar{\rho}_N \frac{D}{Dt} \delta u = - \frac{\partial}{\partial x} \delta p, \quad \bar{\rho}_N \frac{D}{Dt} \delta w = - \frac{\partial}{\partial y} \delta p, \]

\[ \frac{\partial p}{\partial \rho} \bigg|_{s=cst} \equiv a \]

\[ \frac{D}{Dt} \delta s = 0 \Rightarrow \frac{D}{Dt} \delta p = \bar{a}_N^2 \frac{D}{Dt} \delta \rho, \]

isentropic: no entropy production but propagation of entropy from the shock

Wave equation for the pressure (d’Alembert equation)

eliminating \( \delta \rho \) \Rightarrow \[ \frac{D}{Dt} \delta p + \frac{\partial}{\partial x} \delta u + \frac{\partial}{\partial y} \delta w = 0 \]

eliminating \( \delta u \) and \( \delta w \) \Rightarrow \[ \frac{D^2}{Dt^2} \delta p - \bar{a}_N^2 \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \delta p = 0 \]

the pressure fluctuations are fully propagated by acoustic waves in the shocked gas moving at constant velocity \( \bar{u}_N \)
Linearized flow field

**Flow splitting**

acoustic wave + vorticity wave

\[ \delta p = \delta p^{(a)}, \quad \delta u = \delta u^{(a)} + \delta u^{(i)}, \quad \delta w = \delta w^{(a)} + \delta w^{(i)} \]

\[ \bar{\rho}_N \left[ \frac{\partial}{\partial t} + u_N \cdot \nabla \right] u^{(a)} = -\nabla p \]

the pressure fluctuations are fully propagated by acoustic waves in the shocked gas moving at constant velocity \( \bar{u}_N \)

**Wave equation for the pressure (d’Alembert equation)**

eliminating \( \delta \rho \)

\[ \frac{1}{\bar{\rho}_N a_N^2} \frac{D}{Dt} \delta p + \frac{\partial}{\partial x} \delta u^{(a)} + \frac{\partial}{\partial y} \delta w^{(a)} = 0 \]

eliminating \( \delta u \) and \( \delta w \)

\[ \frac{D^2}{Dt^2} \delta p - a_N^2 \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \delta p = 0 \]

**Entropy-vorticity wave (isobaric)**

\[ \frac{D}{Dt} = \frac{\partial}{\partial t} + \bar{u}_N \frac{\partial}{\partial x} \]

\[ D \delta u^{(i)}/Dt = 0 \quad \Rightarrow \quad \frac{\partial \delta u^{(i)}}{\partial t} + \bar{u}_N \frac{\partial \delta u^{(i)}}{\partial x} = 0 \]

\[ D \delta w^{(i)}/Dt = 0 \quad \Rightarrow \quad \frac{\partial \delta w^{(i)}}{\partial t} + \bar{u}_N \frac{\partial \delta w^{(i)}}{\partial x} = 0 \]

\[ \frac{1}{\bar{\rho}_N a_N^2} \frac{D}{Dt} \delta p + \frac{\partial}{\partial x} \delta u^{(i)} + \frac{\partial}{\partial y} \delta w^{(i)} = 0 \quad \Rightarrow \quad \frac{\partial}{\partial x} \delta u^{(i)} + \frac{\partial}{\partial y} \delta w^{(i)} = 0 \]

\[ \frac{D}{Dt} \delta u^{(i)} = \bar{u}_N \frac{\partial}{\partial y} \delta w^{(i)} \]
**Linearized flow field**

**Normal-mode analysis**

\[ \alpha(y, t) = \tilde{\alpha}e^{iky + \sigma t} \]

\[ \delta p(x, y, t) = \tilde{p}(x)e^{iky + \sigma t} \]

\[ \tilde{p}(x) = \tilde{p}_N e^{i\pm x} \]

\[ \delta p = \tilde{p}_N \exp(i l_\pm x + ik_y + \sigma t) \]

\[ \begin{aligned}
2\text{-nd order algebraic eq.} & \\
\quad l_\pm(\sigma, k) & = (\sigma + il_\pm u_N)^2 + \tilde{a}_N^2(l_\pm^2 + k^2) = 0 \quad \Leftrightarrow \quad \frac{D^2}{Dt^2} \delta p - \tilde{a}_N^2 \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \delta p = 0 \quad \text{wave eq.}
\end{aligned} \]

No length-scale other than \(|k|^{-1}\) in the problem

\[ i \frac{l_\pm}{|k|} = \frac{M_N S \pm \sqrt{1 + S^2}}{\sqrt{1 - M_N^2}} \quad \text{with} \quad S \equiv \frac{\sigma}{\tilde{a}_N |k|} \frac{1}{\sqrt{1 - M_N^2}}, \]

**Incompressibility condition**

\[ \frac{\partial}{\partial x} \delta u^{(i)} = - \frac{\partial}{\partial y} \delta w^{(i)} \Rightarrow \frac{\partial}{\partial t} \delta u^{(i)} = \tilde{u}_N \frac{\partial}{\partial y} \delta w^{(i)} \]

\[ \begin{aligned}
\delta u^{(i)}(y, t - x/\tilde{u}_N) & = 0 \\
\delta w^{(i)}(y, t - x/\tilde{u}_N) & = 0 \quad \text{RH conditions}
\end{aligned} \]

\[ \begin{aligned}
\delta u^{(i)}(y, t - x/\tilde{u}_N) & = \tilde{u}_N \frac{\partial}{\partial y} \delta w^{(i)}(y, t - x/\tilde{u}_N) \\
\delta w^{(i)}(y, t - x/\tilde{u}_N) & = -\tilde{u}_N \frac{\partial}{\partial x} \delta u^{(i)}(y, t - x/\tilde{u}_N)
\end{aligned} \]

\[ \begin{aligned}
\delta u^{(i)}(y, t - x/\tilde{u}_N) & = 0 \\
\delta w^{(i)}(y, t - x/\tilde{u}_N) & = 0 \quad \text{RH conditions}
\end{aligned} \]

\[ \begin{aligned}
\frac{\partial}{\partial x} \delta u^{(i)} = - \frac{\partial}{\partial y} \delta w^{(i)} \\
\frac{\partial}{\partial t} \delta u^{(i)} = \tilde{u}_N \frac{\partial}{\partial y} \delta w^{(i)} \\
\end{aligned} \]
Lecture 13: Stability analysis of shock waves

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   - Spontaneous emission of sound and instability
   - Stability of shocks in ideal gases
   - Stability of reacting shocks
Dispersion relation for general materials

**Rankine Hugoniot relations (general material)**

\[ M = \frac{D}{a} \]

- Initial fluid:
  - \( D > a_u \)
  - \( u_N < a_N \)
  - \( M_u > 1 \)
  - \( (p_u, \rho_u) \)

- Shocked fluid, Neumann state:
  - \( M_N < 1 \)
  - \( (p_N, \rho_N) \)

\[ x = \alpha(t, y) \]

\[ \alpha(t, y) = \hat{\alpha} e^{\sigma t + iky} \]

2 parameters for the material: \( r \) and \( n \)

**Linear rate**

Quadratic equation for \( \frac{\sigma^2}{\bar{a}_N^2 k^2} \)

\[ aS^4 + 2bS^2 + c = 0, \quad S^2 = \frac{\sigma^2}{\bar{a}_N^2 k^2} \left( \frac{1}{1 - M_N^2} \right) \]

\[ a \equiv (1 + r)^2 - 4M_N^2, \quad b \equiv (1 - r^2)n - 2M_N^2, \quad c \equiv (1 - r^2)n^2 > 0. \]

Classification of normal modes

\[ \alpha(t, y) = \hat{\alpha} e^{\sigma t + ik y} \]

\[ aS^4 + 2bS^2 + c = 0, \quad S^2 \equiv \frac{\sigma^2}{\bar{a}_N^2} \frac{1}{k^2 (1 - M_N^2)} \]

\[ a \equiv (1 + r)^2 - 4M_N^2, \quad b \equiv (1 - r^2)n - 2M_N^2, \quad c \equiv (1 - r^2)n^2 > 0. \]

Re(\(\sigma\)) < 0 : stable mode exponentially damped \[ e^{-|\text{Re}(\sigma)|t} \]

Re(\(\sigma\)) > 0 : unstable mode exponentially amplified \[ e^{|\text{Re}(\sigma)|t} \]

S^2 < 0 : Re(\(\sigma\)) = 0, \(\omega \equiv \text{Im}(\sigma) \neq 0\) neutral oscillatory modes

longitudinal component of the velocity (unperturbed shock) of the sound wave:

\[ \mathbf{e}_x \cdot (\bar{u}_N \mathbf{e}_x - \bar{a}_N \mathbf{e}_K) = \bar{u}_N - \bar{a}_N \frac{l}{\sqrt{l^2 + k^2}} \]

Neutral oscillatory modes

Spontaneous generation of sound. Radiating condition: \( \bar{u}_N \sqrt{l^2 + k^2} - \bar{a}_N l > 0 \)

Non-radiating condition: \( \bar{u}_N \sqrt{l^2 + k^2} - \bar{a}_N l < 0 \)

unstable \( t^n \), stable \( 1/t^n \)
Classification of normal modes

2 non-dimensional parameters

\[ r \equiv -\frac{(\rho_u \overline{D})^2}{d\overline{p}_N/d\overline{\rho}_N} > 0, \]

\[ n \equiv \frac{\overline{\rho}_N}{\rho_u} \frac{\overline{M}_N^2}{1 - \overline{M}_N^2} \]

Neutral oscillatory modes

Spontaneous generation of sound. Radiating condition: \( \overline{u}_N \sqrt{l^2 + k^2} - \overline{a}_N l > 0 \)

Non-radiating condition: \( \overline{p}_N \sqrt{l^2 + k^2} - \overline{a}_N l < 0 \)

Classification of the normal modes in the parameters space

UNSTABLE oscillatory modes

\( Re(\sigma) > 0 \)
\( -(1 + 2M_N) \)

STABLE oscillatory modes

\( Re(\sigma) < 0 \)
\( \frac{n - 1}{n + 1} \)

\( Re(\sigma) = 0 \)
\( r^* \)

oscillatory unstable
\( t^n \)
\( n > 0 \)

oscillatory stable
\( 1/t^n \)
\( n = 0 \)

\( r^* = \frac{n - \sqrt{(1 - \overline{M}_N^2)\left(1 - \frac{\overline{\rho}_u}{\overline{\rho}_N}\right)}}{n + 1} \)

Stability of shocks in ideal gases

polytropic gas, $\gamma = \text{cst.}$

$$\frac{u_N}{D} = \frac{\rho_u}{\rho_N} = \frac{(\gamma - 1)M_u^2 + 2}{(\gamma + 1)M_u^2}, \quad \frac{p_N}{p_u} = \frac{2\gamma M_u^2 - (\gamma - 1)}{(\gamma + 1)}, \quad M_N^2 = \frac{(\gamma - 1)M_u^2 + 2}{2\gamma M_u^2 - (\gamma - 1)}$$

$$r \equiv -\frac{(\rho_u D)^2}{dp_N/d\bar{p}_N^{-1}} = \frac{1}{M_u^2}, \quad n \equiv \frac{\bar{p}_N}{\rho_u} \frac{M_N^2}{(1 - M_N^2)} = \frac{M_u^2}{(M_u^2 - 1)}$$

$$\pm 2M_NS\sqrt{1 + S^2} = (1 + r)S^2 + (1 - r)n, \quad \Rightarrow \quad \pm 2S\sqrt{1 + S^2} = S^2 \left(1 + M_u^{-2}\right) + 1$$

$$M_u > 1, \quad \gamma > 1 \Rightarrow \frac{(n - 1)/(n + 1)}{r < r^*}$$

$$r^* = \frac{n - \sqrt{(1 - M_N^2) \left(1 - \frac{\rho_u}{\rho_N}\right)}}{n + 1} \quad \frac{1}{2M_u^2 - 1} < \frac{1}{M_u^2} < \frac{M_u^2 - (M_u^2 - 1)^2 \sqrt{2M_u^{-2}[2\gamma M_u^2 - (\gamma - 1)]^{-1}}}{2M_u^2 - 1}$$

Shock waves in polytropic gases have neutral modes with non-radiating acoustic waves

They are stable with a relaxation of initial disturbances in power laws $1/t^{3/2}$

OK with experiments K.C. Lapworth (1959) *J.F.M.*, 6, 469-480

Formation of Mach stems (see next lecture)
Stability of reacting shocks


Reacting shocks = detonations considered as an hydrodynamic discontinuity

thickness = 0: no modification of the inner structure

\[
\frac{d}{dp_b} \frac{\varepsilon^2}{\rho_b} = \frac{M_b^2}{1 - M_b^2} \frac{1 + \varepsilon_b}{M_b^2 \varepsilon_b} \quad \varepsilon_b = \frac{M_u^2 - (1 + \chi)}{2} \quad \chi = \sqrt{(1 - M_u^{-2}) - 4QM_u^{-2}} \\
\]

\[
r = \left( \frac{1 - \chi + \frac{1}{M_N^2}}{(1 + \chi) + \frac{1}{M_u^2}} \right) = \left( \frac{n - 1}{n + 1} \right) \left[ \frac{1 + \frac{1}{M_u^2(1+\chi)}}{\frac{1}{M_u^2(1-\chi)}} \right] \\
\]

\[
\left( \frac{n - 1}{n + 1} \right) \leq r \\
\]

Overdriven reacting shocks in polytropic gases have neutral modes with non-radiating acoustic waves

They are stable with a relaxation of initial disturbances in power laws

For the CJ marginal regime the acoustic waves in the burned gas propagate in the direction parallel to the unperturbed planar solution
Details of the calculation
P.Clavin XIII

Rankine Hugoniot relations (general material)

\[ M = \mathcal{D}/a \]

\[ M_u > 1 \quad M_N < 1 \quad (p_u, \rho_u) \]

\[ \mathcal{D} / a > a_u \quad u_N < a_N \]

\[ \mathcal{D} / a = D \quad \text{shocked fluid, Neumann state} \]

\[ x = \alpha(t, p) \]

Jump conditions  \( p.5 \) lecture IV

\[ \rho_N(u_N - \partial \alpha / \partial t - w_N \partial \alpha / \partial y) = \rho_u(D - \partial \alpha / \partial t) \]

\[ \Rightarrow \delta \rho_N \bar{u}_N + \bar{p}_N (\delta u_N - \partial \alpha / \partial t) = -\rho_u \partial \alpha / \partial t \]

\[ \delta m = -\rho_u \partial \alpha / \partial t \]

\[ \frac{\delta \rho_N}{\bar{p}_N} = \frac{1}{r} \frac{(\rho_u D)^2}{\bar{p}_N} \delta \rho_N \]

Jump conditions  \( p.5 \) lecture IV

\[ \frac{\delta \rho_N}{\bar{p}_N} = -2 \left( \frac{1 - \rho_u}{1 - r} \right) \frac{\partial \alpha / \partial t}{D}, \quad \frac{\delta \rho_N}{\bar{p}_N} = \frac{1}{1 - r} \frac{\rho_u - 1}{r} \frac{\partial \alpha / \partial t}{D} \]

\[ \frac{\delta u_N}{\bar{u}_N} = \left( \frac{\bar{p}_N}{\rho_u} - 1 \right) \frac{1 + r}{1 - r} \frac{\partial \alpha / \partial t}{D}, \quad \frac{\delta w_N}{\bar{u}_N} = \left( \frac{\bar{p}_N}{\rho_u} - 1 \right) \frac{\partial \alpha / \partial y}{D} \]

Linear rate

\[ \pm \sqrt{S^2 + 1} \frac{\bar{p}_N}{\bar{p}_N \bar{u}_N \bar{u}_N} = -S \frac{\bar{u}_N}{\bar{u}_N} + \frac{ik \bar{w}_N}{|k| \bar{u}_N} \frac{M_N}{\sqrt{1 - M_N^2}} \]

\[ \alpha(y, t) = \dot{\alpha} e^{iky + \sigma t} \quad \frac{\partial \alpha}{\partial t} = \sigma \alpha \quad \frac{\partial \alpha}{\partial y} = i k \alpha \]

\[ \Rightarrow \]

\[ aS^4 + 2bS^2 + c = 0, \]

\[ a \equiv (1 + r)^2 - 4M_N^2, \quad b \equiv (1 - r^2)n - 2M_N^2, \quad c \equiv (1 - r^2)n^2 > 0. \]

Quadratic equation for \( \sigma^2 / \bar{u}_N^2 k^2 \)

\[ \sigma^2 \equiv \frac{1}{a_N^2 k^2 (1 - M_N^2)} \]

\[ S^2 \equiv \frac{\sigma^2}{a_N^2 k^2 (1 - M_N^2)} \]

\[ S = \frac{\sigma}{a_N |k| \sqrt{1 - M_N^2}} \]

\[ a = (1 + r)^2 - 4M_N^2, \quad b = (1 - r^2)n - 2M_N^2, \quad c = (1 - r^2)n^2 > 0. \]
Dispersion relation for general materials

Compatibility condition

\[
\left( \frac{\partial}{\partial t} + u_N \frac{\partial}{\partial x} \right)^2 \delta p - u_N^2 \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \delta p = 0
\]

\[
\left( \sigma + il \pm u_N \right)^2 + u_N^2 (l^2 \pm k^2) = 0 \Rightarrow \sigma^2 + 2i\sigma l \pm u_N - t^2 \pm u_N^2 + \tilde{u}_N^2 (l^2 \pm k^2) = 0
\]

\[
-(il \pm u_N \sigma + u_N^2 k^2) = \sigma^2 + il \pm u_N - (\tilde{u}_N^2 - u_N^2) (l^2 \pm k^2)
\]

\[
\Rightarrow \quad \sigma = (\sigma + il \pm u_N) \left[ \sigma - \left(1 - 1/M_N^2\right) (\sigma + il \pm u_N) \right]
\]

\[
\Rightarrow \quad -il \pm u_N \sigma + u_N^2 k^2 = -(\sigma + il \pm u_N) \sqrt{1 - M_N^2} \left[ \pm \sqrt{1 + S^2} \right] |k| \tilde{u}_N
\]

\[
\frac{\delta p_N}{\tilde{p}_N} \propto \frac{\alpha_t}{u_N}, \quad \frac{\delta u_N}{u_N} \propto \frac{i \sigma l}{u_N}, \quad \frac{\delta \tilde{u}_N}{\tilde{u}_N} \propto \frac{\alpha_t}{u_N}, \quad \frac{\delta \tilde{w}_N}{\tilde{w}_N} \propto \alpha_y', \quad \frac{\delta \tilde{w}_N}{\tilde{w}_N} \propto il \tilde{\alpha}
\]

Downstream boundary condition

\[ x \to \infty : \quad \text{bounded condition (in the unstable case, \( \text{Re} \sigma > 0 \))} \]

\[ \delta p = \tilde{p}_N \exp (il \pm x + ik y + \sigma t) \]

selection of the the sign in \( l_\pm \) such that \( e^{il \pm x} \) does not diverge
Spontaneous emission of sound and instability

**Oscillatory neutral modes**

\[ \pm 2M_N S \sqrt{1+S^2} = (1+r)S^2 + (1-r)n \]

Neutral oscillatory mode

\[ S = i \Omega, \quad \Omega > 1 \]

\[ \Rightarrow \]

\[ \left\{ \begin{array}{l}
\text{radiating waves: } l/|k| = \left[ M_N \Omega - \sqrt{\Omega^2 - 1} \right] / \sqrt{1-M_N^2}, / \sqrt{1-M_N^2}, \\
2M_N \Omega \sqrt{\Omega^2 - 1} = -\Omega^2 (1+r) + (1-r)n > 0, \\
\text{non-radiating waves: } l/|k| = \left[ M_N \Omega + \sqrt{\Omega^2 - 1} \right] / \sqrt{1-M_N^2}, \\
-2M_N \Omega \sqrt{\Omega^2 - 1} = -\Omega^2 (1+r) + (1-r)n < 0 
\end{array} \right. \]

**Transmitted or reflected sound wave**

\[ D > a_u \rightarrow u_N < a_N \]

\[ \text{incident} \xrightarrow{\sigma} \text{transmitted} \]

\[ D > a_u \rightarrow u_N < a_N \]

\[ \text{incident} \xrightarrow{\sigma} \text{reflected} \]

If a normal mode is radiating the response of the shock diverges when the reflected (or transmitted) waves matched the radiating normal mode

\[ \text{reflected} \rightarrow \tilde{p}_r = \frac{[2M_N \Omega \sqrt{\Omega^2 - 1} - \Omega^2 (1+r) + (1-r)n]}{[-2M_N \Omega \sqrt{\Omega^2 - 1} - \Omega^2 (1+r) + (1-r)n]} \]

\[ \text{incident} \rightarrow \tilde{p}_i = \frac{2M_N \Omega \sqrt{\Omega^2 - 1} + \Omega^2 (1+r) - (1-r)n}{2M_N \Omega \sqrt{\Omega^2 - 1} - \Omega^2 (1+r) + (1-r)n} \]

\[ \text{denominator goes through 0} \]

A neutral oscillatory mode that is radiating is considered as unstable

**Power laws of neutral modes**

Square root in the dispersion relation \[ \pm 2M_N \Omega \sqrt{\Omega^2 - 1} - \Omega^2 (1+r) + (1-r)n = 0 \]

\[ \Rightarrow \text{cut in the complex plane} \]

\[ \Rightarrow \text{power laws} \]

Damping \( n < 0 \) or amplification \( n > 0 \) involving power laws \( t^n \)

\[ \text{can be described by Laplace transform not by Fourier transform} \]

Neutral modes with non-radiating acoustic waves relax following a power law in time \( t^n \)

Neutral modes with a radiating acoustic wave is unstable according a power law in time \( t^n \)
Dynamics of Combustion Waves in Premixed Gases

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Lecture XIV
Nonlinear dynamics of shock waves. Triple point and Mach stem formation.
Lecture 14: Nonlinear dynamics of shock waves
Mach stem formation

14-1. Experimental and DNS results
   What is a Mach stem?
   Mach stems and cellular detonations
   Spontaneous formation of Mach stems

14-2. Multidimensional dynamics of shock fronts
   Linear dynamics
   Weakly nonlinear analysis

14-3. Shock-vortex interaction
   Formulation
   Analysis of the crossover

14-4. Shock-turbulence interaction
   Composite solution
   Model equation
   Comparison with DNS
Introduction.
Recent experimental and DNS results

What is a Mach stem?

Triple point = 3 shock waves + 1 slip line (degenerescence of shear layer)
called also contact line discontinuity (Courant Friedrichs 1948)

First observed during the reflection of an oblique shock front incident an a wall

Example of a triple point propagating in a uniform flow

Example of stationary triple point
Mach stems and cellular detonations

Experimental observations of the cellular structure of detonations

Transverse structures of gaseous detonations have been observed for a long time

Shchelkin and Troshin (1965) Mono Book Corp.

F. Joubert et al. (2008) Combust. Flame, 152, 482-495

marksings left on soot-coated foils on the walls


visualisation of the cellular structures by optical methods

Underlying linear mechanisms

longitudinal oscillation of the complex shock reaction zone

(Galloping detonation) see lecture XII

+ transverse oscillatory modes (normal modes of the lead shock)

see lecture XIII

Nonlinear mechanisms

singularity of slope of the lead shock \( \Rightarrow \) formation of Mach stems

Theory:


Clavin and Denet (2002) P.R.L 88 (4) 044502


Mach stems propagating in the transverse direction

trajectory of triple points
Spontaneous formation of Mach stems on shock fronts

Schlieren experiments in shock tubes

K.C. Lapworth (1959) *J.F.M*, 6, 469-480

Shock reflection from a wavy wall

M.G. Briscoe and A.A. Kovitz (1968) *J.F.M*, 31(3), 529-546

DNS in 2 dimension geometry

G. Lodato et al. (2016) *J.F.M*, 789, 221-258

Comparison with experiments


quite similar to the markings left by the transverse structure of cellular detonations
Spontaneous formation of Mach stems

G. Lodato et al. (2016) J.F.M, 789, 221-258

The incoming shock wave is not strong, $M_u = 1.5$ and the amplitude of wavy wall is small 1 mm
Immediately after reflection the wrinkled reflected shock has a smooth sinusoidal form
Singularity of slope is formed spontaneously at about 15 $\mu$s leading to triple points clearly observed as early as 20 $\mu$s

Long-lived Mach stems on quasi-planar inert shock front

Sufficiently far from the wall the wall effect becomes negligible

The shock is quasi-planar with Mach stems propagating in the transverse direction crossing each other without deformation as solitons are known to do
Multidimensional analysis of shock fronts

*Analysis for strong shocks in the Newtonian limit*


**Linear dynamics**

In order to simplify the presentation the analysis is performed for strong shock in the Newtonian limit

\[ M_u^2 \gg 1, \quad (\gamma - 1) \ll 1, \]

\[ M_u^2 (\gamma - 1) = O(1), \quad M_N^2 \approx (\gamma - 1)/2 + 1/M_u^2 \ll 1, \]

\[ \epsilon^2 \equiv M_N^2 \ll 1 \quad M_u = O(1/\epsilon), \quad (\gamma - 1) = O(\epsilon^2) \]

\[ \bar{u}_N/D \approx \epsilon^2, \quad \bar{a}_N^2 \approx \bar{u}_N D, \quad \bar{a}_N/a_u = O(1) \]

**Rankine-Hugoniot relations** (see p. 6 & p. 9 lecture XIII)

\[ \frac{\delta p_N}{p_N} \approx -2 \frac{\dot{\alpha}_t}{D}, \quad \frac{\delta \rho_N}{\rho_N} = -2 \left( \frac{\bar{u}_t}{\bar{a}_N} \right)^2 \frac{\dot{\alpha}_t}{D}, \]

\[ (\delta u_N - \dot{\alpha}_t) = - \left[ (\gamma - 1)M_u^2 - 2 \right] \frac{\dot{\alpha}_t}{2M_u^2} \]

\[ \delta w_N \approx D \alpha'_y, \]

where for simplicity some unimportant \( \epsilon^2 \) terms have been omitted in \( \delta p_N \) and \( \delta w_N \)

**Quasi-isobaric approximation of the flow in the shocked gas**

\[ \pm 2SM_N \sqrt{1 + S^2} = S^2 \left( 1 + M_u^2 \right) + 1 \]

\[ S \equiv \frac{\sigma}{\bar{a}_N |k|} \sqrt{\frac{1}{1 - M_N^2}} \Rightarrow \sigma \approx \pm i \bar{a}_N |k| \]

Dispersion relation see p. 10 lecture XIII

\[ \omega \approx \bar{a}_N k, \]

\[ \partial^2 \alpha/\partial t^2 - \bar{a}_N^2 \partial^2 \alpha/\partial y^2 = 0 \]

\[ x = \alpha(y, t) \quad \text{Wave equation} \]
\[\epsilon^2 \equiv M_N^2 \ll 1 \quad \overline{M_u} = O(1/\epsilon), \quad (\gamma - 1) = O(\epsilon^2)\]

\[\overline{u}_N/\overline{D} \approx \epsilon^2, \quad \overline{a}_N^2 \approx \overline{u}_N \overline{D}, \quad \overline{a}_N/a_u = O(1)\]

\[\omega \approx \overline{a}_N k, \quad \frac{\partial^2 \alpha}{\partial t^2} - \overline{a}_N^2 \frac{\partial^2 \alpha}{\partial y^2} = 0\]

**Wave equation**

\[\omega \approx \overline{a}_N |k| \quad \dot{\alpha}_t = O(\overline{a}_N \alpha'_y)\]

\[\delta p = \tilde{p}_N \exp(\text{i} l \pm x + ik y + \sigma t) \quad il = \pm il,\]

(see pp.4-5 lecture XIII)

\[(l/|k|) \sqrt{1 - M_N^2} = M_N \Omega + \sqrt{\Omega^2 - 1} > 0 \quad \Rightarrow \quad l/|k| = O(\epsilon)\]

\[\overline{M}_N = \epsilon \quad \Omega \approx \omega/(\overline{a}_N |k|) \approx 1\]

The acoustic waves propagates in a direction quasi-parallel to the front

\[\tilde{u}^{(a)}(t) = -\frac{il \pm \overline{u}_N}{\sigma + il \pm \overline{u}_N} \frac{\tilde{p}_N}{\tilde{p}_N \overline{u}_N} e^{il \pm x}, \quad \delta u^{(a)} = O(\epsilon \delta p_N/\tilde{p}_N \overline{u}_N) \quad \delta u^{(a)} = O(\epsilon^2 \delta p_N/\tilde{p}_N \overline{u}_N)\]

\[\tilde{w}^{(a)}(t) = -\frac{ik \overline{u}_N}{\sigma + il \pm \overline{u}_N} \frac{\tilde{p}_N}{\tilde{p}_N \overline{u}_N} e^{il \pm x}, \quad \delta w^{(a)} = O(\delta p_N/\tilde{p}_N \overline{u}_N) \quad \delta w^{(a)} = O(\epsilon \delta p_N/\tilde{p}_N \overline{u}_N)\]

(see p. 4 lecture XIII)

\[\delta p_N/\tilde{p}_N \approx -2\dot{\alpha}_t/\overline{D} \Rightarrow \delta p_N/(\tilde{p}_N \overline{u}_N) = O(\dot{\alpha}_t)\]

\[\delta u^{(a)} = O(\epsilon^2 \dot{\alpha}_t) \quad \delta w^{(a)} = O(\epsilon \dot{\alpha}_t)\]

**Weak acoustic wave**

\[\tilde{p}_N/\tilde{p}_N \overline{a}_N^2 \approx \tilde{p}_N \overline{u}_N \frac{\overline{a}_N}{M_N} \quad \frac{\overline{a}_N}{M_N} = \frac{\overline{a}_N/a_u}{M_u M_N} \overline{D} = O(\overline{D})\]
the acoustic waves are negligibly smaller than the vorticity wave

\[ \frac{|\delta u^{(i)} / \delta w^{(i)}|}{\delta w^{(i)}} = O(\epsilon) \]

the vorticity wave is a shear flow quasi-parallel to the front propagating at a subsonic velocity in the normal direction

\[ \left( \frac{\partial}{\partial t} + \frac{\nu_N}{\nu_N} \frac{\partial}{\partial x} \right) u^{(i)} = 0 \Rightarrow \delta u^{(i)} = \dot{\alpha}_t(y, t - x/\nu_N) \]

\[ \frac{\partial u^{(i)} / \partial x}{\delta t} + \frac{\partial w^{(i)} / \partial y}{\delta t} = 0 \Rightarrow -\frac{1}{\nu_N} \frac{\partial^2 \alpha}{\partial t^2} + \overline{\nu_D} \frac{\partial^2 \alpha}{\partial y^2} = 0 \]

\[ \overline{\nu_N} \overline{D} \approx \overline{u}_N^2 \Rightarrow \text{Wave equation} \]

A subsonic wave that is sufficiently tilted yields a trace on the front that is sonic
Weakly nonlinear analysis

Nonlinear Euler equations

\[
\begin{align*}
\frac{\partial u}{\partial t} + \bar{u}_N \frac{\partial u}{\partial x} &= U - \frac{1}{\rho} \frac{\partial p}{\partial x}, \\
\frac{\partial w}{\partial t} + \bar{u}_N \frac{\partial w}{\partial x} &= W - \frac{1}{\rho} \frac{\partial p}{\partial y},
\end{align*}
\]

where \( \delta u \equiv u - \bar{u}_N \approx u^{(i)} \quad \text{and} \quad w \approx w^{(i)} \)

The weakly nonlinear approximation is valid when the nonlinear terms \( U \) and \( V \) are small (compared with the linear terms)

This is the case for small amplitudes of the wrinkles \( |\alpha'| \ll \epsilon \) where \( \epsilon \equiv M_N = \bar{u}_N / \bar{a}_N \) namely for \( \epsilon \ll 1 \)

Perturbation analysis for \( \epsilon \ll 1 \)

\[
U \approx \frac{1}{2} \frac{\partial H}{\partial x}, \quad W \approx -\frac{1}{2} \frac{\partial H}{\bar{u}_N \partial y},
\]

where \( H \equiv [-\alpha'^2(y, t - x/\bar{u}_N) + \bar{a}_N^2 \alpha'_y(y, t - x/\bar{u}_N)] \).

progressive wave: \( \dot{\alpha}_t = \pm \bar{a}_N \alpha'_y \Rightarrow H = 0, \quad U = 0, \quad W = 0 \)

no first order correction term coming from the Reynolds tensor

the shear wave \( u^{(i)} = \dot{\alpha}_t(y, t - x/\bar{u}_N) \quad w^{(i)} = \bar{D} \alpha'_y(y, t - x/\bar{u}_N) \) is an exact solution of the Euler equations for \( p = 0 \)

the first order correction terms should come from the boundary conditions at \( x = \alpha(y, t) \) (Rankine-Hugoniot)
Limiting the attention to the nonlinear corrections of order \( \varepsilon \equiv |\alpha'_y|/\epsilon \) the Rankine-Hugoniot conditions yield

\[
x = \alpha(y, t) : \quad p = p_N, \quad u = u_N, \quad w = w_N
\]

\[
p_N/\overline{p_N} \approx 1 - 2\dot{\alpha}_t/\overline{D}, \quad u_N - \overline{u}_N \approx \dot{\alpha}_t + \overline{D}\alpha'_y^2, \quad w_N \approx \overline{D}\alpha'_y
\]

The only nonlinear term that yields a correction of order \( \varepsilon \equiv |\alpha'_y|/\epsilon \)

\[
|\dot{\alpha}_t| = O(\overline{\pi}_N\alpha'_y), \quad \overline{D}/\overline{a}_N = O(1/\epsilon) \quad \Rightarrow \quad \overline{D}|\alpha'_y^2/\dot{\alpha}_t| = O(|\alpha'_y|/\epsilon)
\]

The shift of the front position also introduces quadratic terms

\[
x = 0 : \quad \delta u \equiv u_f(y, t) \approx \delta u_N - \alpha u'_x, \quad w \equiv w_f(y, t) \approx w_N - \alpha w'_x
\]

The nonlinear equations for the wrinkles is obtained from the incompressible condition

\[
-H = 0 \quad \Rightarrow \quad \text{the nonlinear terms coming from shift of the front position do not contribute}
\]

\[
-\frac{1}{\overline{u}_N} \frac{\partial u_N}{\partial t} + \frac{\partial w_N}{\partial y} = 0 \quad \Rightarrow \quad \frac{\partial^2 \alpha}{\partial t^2} - \overline{a}_N^2 \frac{\partial^2 \alpha}{\partial y^2} + \overline{D} \frac{\partial}{\partial t} \left( \frac{\partial \alpha}{\partial y} \right)^2 = 0 \quad (\overline{a}_N^2 \approx \overline{D} \overline{u}_N)
\]

nonlinear correction of order \( \varepsilon \), \( \overline{D}\alpha'_y^2/|\dot{\alpha}_t| \approx (\overline{D}/\overline{a}_N)|\alpha'_y| \approx \varepsilon \)
Mach stem formation

\[
\frac{\partial^2 \alpha}{\partial t^2} - \alpha^2_N \frac{\partial^2 \alpha}{\partial y^2} + \mathcal{D} \frac{\partial}{\partial t} \left( \frac{\partial \alpha}{\partial y} \right)^2 = 0
\]

Two timescales problem:
- Short time \( \tau_s \equiv L/\alpha_N \) (period of oscillation)
- Long time \( \tau_l \equiv \tau_s/\varepsilon \) (for the formation of a singularity of slope)

Non-dimensional form \( t \equiv t/\tau_s, \ y \equiv y/L, \ A \equiv \alpha/(\varepsilon L) \)

\[
\frac{\partial^2 A}{\partial t^2} - \frac{\partial^2 A}{\partial y^2} + \varepsilon \frac{\partial}{\partial t} \left( \frac{\partial A}{\partial y} \right)^2 = 0
\]

Small nonlinear correction term producing a singularity at finite (but long) non-dimensional time \( 1/\varepsilon \), \( t = O(1/\varepsilon) \)

so that \( A \) may be considered to depend on two reduced time variables \( t \) and \( t' \equiv \varepsilon t \),

Considering a simple progressive wave \( y' = y \pm t \)

and looking for a solution in the form \( A(y, t) = A(y', t') \) one gets

\[
2\varepsilon \frac{\partial^2 A}{\partial t \partial y} + \varepsilon^2 \frac{\partial^2 A}{\partial y^2} + \frac{\partial A}{\partial t} \left( \frac{\partial A}{\partial y} \right)^2 + \varepsilon^2 \frac{\partial^2}{\partial y^2} \left( \frac{\partial A}{\partial y} \right)^2 = 0
\]

leading order \( \frac{\partial A}{\partial t} + \left( \frac{\partial A}{\partial y} \right)^2 \approx 0 \)

Geometrical construction for the slip line and the secondary shock

Collapse of points \( C \) and \( D \) by a Huygens like construction

\[
\alpha_t \approx \mathcal{D} \alpha_y^2
\]

different only by a numerical factor 1/2


Non-radiative acoustic wave

Secondary shock

Slip line (triple point)

Vorticity wave (shear flow)
Numerical solution of the model equation and comparison with experiments

\[ \frac{\partial^2 \alpha}{\partial t^2} - \tilde{a}_N \frac{\partial^2 \alpha}{\partial y^2} + \tilde{D} \frac{\partial}{\partial t} \left( \frac{\partial \alpha}{\partial y} \right)^2 = 0 \]

Initial condition: sinusoidal shock front of small amplitude

The formation of corners is clearly observed

Good agreement with experiments and DNS

G. Lodato et al. (2016) *J.F.M.*, **789**, 221-258

The trajectory of the corners looks quite similar to the traces left on the wall by a cellular detonation

Consider a cylindrical and very subsonic vortex of diameter $L$ and turnover velocity $v_e$, $v_e/a_u = O(1/M_u)$. Interaction time $\tau_{int} = L/D \ll$ turnover time $L/v_e$, frozen flow $u_e(r) w_e(r) +$ small disturbances of the front.

The disturbances of the front during the crossover can be described by a linear analysis.

Interaction time $\tau_{int} = L/D \ll$ propagation time in the transverse direction of the wrinkles $L/\alpha_N$.

After the interaction time, $t > \tau_{int}$, the wrinkled shock front propagates in a quiescent medium.

2 timescales: short crossover and longer transverse propagation of the wrinkles. The crossover provides the initial conditions.

**Linear analysis of the crossover**

Similar analysis but with an upstream flow

$\delta u_1(r, t), \; \delta w_1(r, t), \; \delta p_1(r, t)$

Rankine-Hugoniot (generalization of the relations p. 6)

(the subscript $f$ denotes the value at the shock front of the upstream flow)

$$\frac{\delta p_N - \delta p_{1f}}{\rho_N} \approx 2 \frac{(\delta u_{1f} - \dot{\alpha}_t)}{D}, \quad \frac{\delta \rho_N - \delta \rho_{1f}}{\rho_N} = 2 \left(\frac{\alpha_u}{\alpha_N}\right)^2 \frac{(\delta u_{1f} - \dot{\alpha}_t)}{D},$$

$$\frac{\delta u_N - \dot{\alpha}_t}{\alpha_N} = \frac{[\gamma - 1][\rho_M^2 - 2]}{2\rho_M^2} (\delta u_{1f} - \dot{\alpha}_t), \quad \delta w_N \approx D \alpha'_y + \delta w_{1f},$$

$$\delta u_{1f}(y, t) = u_e|_{y = -D}, \quad \delta w_{1f}(y, t) = w_e|_{y = -D}, \quad \delta p_{1f}(y, t) = p_e|_{y = -D}$$
**Acoustic burst**

Acoustic in the shocked gases (Doppler neglected for simplicity) \(0 < t < \tau_{\text{int}}\)

\[
\frac{\partial u^{(a)}}{\partial t} \approx -\frac{1}{\bar{p}_N} \frac{\partial p}{\partial x}, \quad \frac{\partial w^{(a)}}{\partial t} \approx -\frac{1}{\bar{p}_N} \frac{\partial p}{\partial y}, \quad \frac{\partial^2 p}{\partial t^2} \approx \frac{\sigma_N^2}{\bar{p}_N} \left( \frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} \right)
\]

\(x = 0, \quad 0 < t < \tau_{\text{int}}: \quad \frac{\partial}{\partial t} = O(\bar{D}/L), \quad \frac{\partial}{\partial y} = O(1/L)\)

A quasi-planar and longitudinal pressure burst of transverse extension \(L\) is generated

\[
\frac{\partial p}{\partial x} \approx \frac{1}{\bar{u}_N} \frac{\partial p}{\partial t} \approx \frac{\bar{D}}{\bar{u}_N} \frac{\partial p}{L} \approx \epsilon^{-1} \left( \frac{\partial p}{\partial y} \right) \Rightarrow \left| \frac{\partial w^{(a)}}{\partial y} \right|/\left| \frac{\partial u^{(a)}}{\partial x} \right| = O(\epsilon)
\]

Rankine-Hugoniot \(\delta p_1/\bar{p}_u\) is negligible

\[
\frac{\delta p_1/\bar{p}_u}{\delta p/\bar{p}_u} \approx \frac{(v_e/\bar{u}_u)^2}{v_e/\bar{D}} \approx \frac{(v_e/\bar{u}_u)}{\epsilon} \ll 1
\]

\[
\delta u^{(a)} \approx \delta p/(\bar{p}_N \bar{u}_N) \quad v_e/\bar{u}_u \ll \epsilon: \quad \delta p_1/\bar{p}_N \approx 2(\delta u_{1f} - \dot{\alpha}_t)/\bar{D}
\]

\[
\delta w^{(a)} \approx \dot{\alpha}_t - 2(\bar{a}_N)/\bar{D} \quad \delta u^{(i)} \bigg|_{x=0} \equiv \delta u^{(a)}_N \approx \frac{2}{(\bar{a}_N/\bar{D})} (\delta u_{1f} - \dot{\alpha}_t)
\]

**Vorticity wave (transmitted vortex)**

\[
\delta u^{(i)} \bigg|_{x=0} \equiv \delta u^{(i)}_N = \delta u_N - \delta u^{(a)}_N \approx \dot{\alpha}_t - 2(\bar{a}_N)/\bar{D} \delta u_{1f}
\]

\[
\delta w^{(i)} \bigg|_{x=0} \equiv \delta w^{(i)}_N = \delta w_N - \delta w^{(a)}_N \approx \bar{D} \alpha'_y + \delta w_{1f} - \delta w^{(a)}_N
\]

Vorticity wave \(\delta u^{(i)} = \delta u^{(i)}(y, t-x/\bar{u}_N), \delta w^{(i)} = \delta w^{(i)}(y, t-x/\bar{u}_N)\)

\[
\frac{\partial \delta u^{(i)}}{\partial x} = -\frac{1}{\bar{u}_N} \frac{\partial \delta u^{(i)}}{\partial t} = O \left( \frac{\bar{D}}{\bar{u}_N} \frac{\delta u^{(i)}}{L} \right) = O \left( \frac{\delta u^{(i)}}{\epsilon^2 L} \right)
\]

Incompressibility \(\partial \delta u^{(i)}/\delta x + \partial \delta w^{(i)}/\delta y = 0\)

\[
|\delta u^{(i)}|/|\delta w^{(i)}| = O(\epsilon^2) \quad \text{The vorticity wave is quasi-parallel to the front}
\]

To leading order

\[
(\bar{a}_N/\bar{D}) \delta u_{1f} = O(\epsilon v_e) \Rightarrow (\bar{a}_N/\bar{D}) \delta u_{1f}/\delta x \approx v_e/(\epsilon L) \gg \frac{\partial \delta w_{1f}}{\partial y} = O(v_e/L)
\]

Wrinkles of very small amplitude are left on the shock front by the vortex

\[
|\alpha| = O(\epsilon^2 L v_e/\bar{u}_u), \quad |\alpha'_y| = O(\epsilon^2 v_e/\bar{u}_u)
\]
Shock-turbulence interaction


Strong shock propagating in a weakly turbulent flow

Composite solution for a single vortex

\[ \frac{v_e}{a_u} \ll \epsilon, \ 0 < t < \tau_{\text{int}} : \ \dot{\alpha}_t \approx 2(\bar{a}_N/\bar{D})\delta u_{1f}, \ \alpha(y, t) = 2\frac{\bar{a}_N}{\bar{D}} \int_{-\bar{D}t}^{0} dx \frac{u_e(x, y)}{\bar{D}} \]

\[ \begin{align*}
&\ \text{beginning of interaction} < t < \text{end of interaction} : \\
&\ \frac{\partial^2 \alpha}{\partial t^2} \approx 2\frac{\bar{a}_N}{\bar{D}} \frac{\partial \delta u_{1f}}{\partial t} \\
&\ \text{valid during a short lapse of time of order } L/\bar{D}
\end{align*} \]

\[ \begin{align*}
&\ \text{After crossover} \\
&\ \frac{\partial^2 \alpha}{\partial t^2} - \bar{a}_N^2 \frac{\partial^2 \alpha}{\partial y^2} + \bar{D} \frac{\partial}{\partial t} \left( \frac{\partial \alpha}{\partial y} \right)^2 \approx 0 \\
&\ \text{involves a time scale of evolution } L/\bar{a}_N \text{ longer than } L/\bar{D} \\
&\ \epsilon = \bar{a}_N/\bar{D} \ll 1
\end{align*} \]

Composite equation

\[ \begin{align*}
&\ \frac{\partial^2 \alpha}{\partial t^2} - \bar{a}_N^2 \frac{\partial^2 \alpha}{\partial y^2} + \bar{D} \frac{\partial}{\partial t} \left( \frac{\partial \alpha}{\partial y} \right)^2 = 2\frac{\bar{a}_N}{\bar{D}} \frac{\partial \delta u_{1f}}{\partial t} \\
&\ \text{taking advantage of the two different time scales}
\end{align*} \]

\[ \delta u_{1f}(y, t) = u_e |_{x = -\bar{D}t} \]

\[ \begin{array}{l}
\text{frozen velocity field} \\
\text{short living forcing term}
\end{array} \]
Model equation

Extension to 3 dimensions

\[ \times \left( \frac{LD}{\alpha_N^3} \right) \frac{\partial^2 \alpha}{\partial t^2} - \ddot{a}_N \Delta \alpha + \frac{\nabla |\nabla \alpha|^2}{D} \right) = 2 \frac{\ddot{a}_N}{D} \frac{\partial \delta u_{1f}}{\partial t} \]

where \( \delta u_{1f}(y, z, t) = u_e(x, y, z, t)|_{x=-D/\overline{D}} \)

forcing term varying on the on the length scale \( L \) and on time scale \( L/\overline{D} \)

non-dimensional form

\[ \eta \equiv y/L, \quad \xi \equiv z/L, \quad \tau \equiv \ddot{a}_N t/L, \quad \phi \equiv \alpha/(\epsilon L) \quad \epsilon \equiv \ddot{a}_N/\overline{D} \]

\[ \frac{\partial^2 \phi}{\partial \tau^2} - \Delta \phi + \frac{\partial |\nabla \phi|^2}{\partial \tau} = \frac{\partial \psi(\eta, \xi, \tau/\epsilon)}{\partial \tau} \]

where \( \psi \equiv 2 \left( \frac{\delta u_{1f}}{\ddot{a}_N} \right) \quad |\psi| = O(v_e/\ddot{a}_N) \)

\( \psi \) is a small term varying on the short (reduced) time scale \( \epsilon \) and on the (reduced) length scale unity

\( \partial \psi/\partial \tau \) is a small (reduced) forcing term fluctuating rapidly \( |\partial \psi/\partial \tau| = O(v_e/(\epsilon \ddot{a}_u)) \quad (v_e/\ddot{a}_u \ll \epsilon) \)

Numerical results


The characteristic cell size of the patterns at the shock front is much larger than the integral scale of the turbulence

The size of the patterns looks to grow with time Saturation by the box size ?

length scale of the turbulence at the shock front

wrinkles of the shock front at time \( \tau = 4 \) after starting the interaction
Numerical analysis of the model equation

Spectral analysis of the pattern size
Evolution of the spectra of the wrinkles of the front shock
The size of the pattern increases with time

Comparison with DNS


DNS shock-vortex interaction B. Denet et al. (2015)

Model equation: B. Denet et al. (2015)

\[ \frac{D}{a_u} = 2, \quad \frac{v_e}{a_u} = 0.8, \quad \gamma = 1.4 \]

Two Mach stems are observed as in the model equation
Dynamics of Combustion Waves in Premixed Gases

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Lecture XV
Cellular detonations
Lecture 15: Cellular detonations

15-1. Cellular detonations at strong overdrive
   - Order of magnitude. Scaling
   - Formulation
   - Outer flow in the burnt gas
   - Inner structure
   - Matching
   - Linear growth rate
   - Weakly nonlinear analysis

15-2. Cellular instability near the CJ condition
   - Formulation
   - Scaling
   - Model for CJ or near CJ regimes
   - Multidimensional stability analysis
Cellular detonations

Underlying mechanisms

Longitudinal oscillation of the complex shock reaction zone
+ Transverse oscillatory mode of the lead shock

Pulsation $\approx 2\pi/\bar{t}_N$

Trajectory of triple points
Trajectory of Mach stems = makings

Mach stems propagating in the transverse direction

Longitudinal oscillation
Cellular detonations

**Underlying linear mechanisms**

longitudinal oscillation of the complex shock reaction zone +
transverse oscillatory mode of the lead shock

**Cellular detonations at strong overdrive**


Order of magnitude and scaling

Overdriven detonations in the Newtonian approximation $M_u \gg 1, M_N \ll 1$

$\overline{M}_N = \overline{u}_N / \overline{a}_N$

$\epsilon^2 \equiv \overline{M}_N^2 \ll 1, \quad \Leftrightarrow \quad \overline{M}_u = O(1/\epsilon^2), \quad (\gamma - 1) = O(\epsilon^2)$

period of oscillation: $\bar{t}_N \equiv \tau_r(\overline{T}_N)$

transverse velocity of the shock disturbances: $\overline{a}_N$

$\Rightarrow$

wavelength of unstable disturbance $\overline{a}_N \bar{t}_N = d_N / \epsilon$

detonation thickness $d_N = \overline{u}_N \bar{t}_N$ \quad $\bar{t}_N \equiv \tau_r(\overline{T}_N)$

The unstable wavelengths are much larger than the detonation thickness by an order $1/\epsilon$
Weakly unstable detonations at strong overdrive

Overdriven detonations in the Newtonian approximation

\[ \overline{M}_N = \frac{\overline{u}_N}{\overline{a}_N} \]

\[ \epsilon^2 \equiv \frac{\overline{M}_N^2}{M_u} \ll 1, \quad \Leftrightarrow \quad \frac{\overline{M}_N^2}{M_u} = O(1/\epsilon^2), \quad (\gamma - 1) = O(\epsilon^2) \]

Stability limit

\[ q_N = O(\epsilon^2) \]

\[ q_N \equiv \frac{Q}{c_p \overline{T}_N} \]

The detonation is stable against the longitudinal disturbances

The unstable wavelengths are much larger than the detonation thickness by an order \(1/\epsilon\)

Non-dimensional variables of order unity

\[ u \equiv \frac{\hat{u}}{\overline{u}_N}, \quad v \equiv \frac{\epsilon \hat{v}}{\overline{u}_N}, \quad p \equiv \frac{\hat{p}}{\overline{p}_N}, \quad \alpha \equiv \frac{\hat{\alpha}}{d_N} \]

\[ x \equiv \frac{1}{\overline{\rho}_N d_N} \int_{\hat{\alpha}}^{\hat{x}} \rho(\hat{x}', \hat{y}, \hat{t}) d\hat{x}', \quad t \equiv \frac{\hat{t}}{t_N}, \quad y \equiv \frac{\epsilon \hat{y}}{d_N} \]

mass weighted coordinate

\[ \overline{t}_N \frac{D}{Dt} = \frac{\partial}{\partial t} + [m(t) - v(x, y, t)] \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} \]

\[ m(t) \equiv 1 - \epsilon^2 \frac{\partial \alpha}{\partial t} = 1 + O(\epsilon^2) \quad v(x, y, t) \equiv \int_0^x (\partial v/\partial y) dx' = O(1) \]
Linearization

\[ q_N = \varepsilon^2 q_2 \quad u = 1 + \varepsilon^2 \bar{u}_2(x) + \delta u \quad T = 1 + \varepsilon^2 \bar{T}_2(x) + \delta T \quad p = 1 + \varepsilon^4 \bar{p}_4 + \delta p \]

\[ v = \delta v_0^{(i)} + O(\varepsilon^2) \quad \delta u = \delta u_0^{(i)} + O(\varepsilon^2) \quad \delta T = O(\varepsilon^2) \quad \delta p = O(\varepsilon^2) \]

Linear equations valid up to \( \varepsilon^4 \)

\[
\varepsilon^2 \left[ \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) \delta u - v \frac{d\bar{u}}{dx} \right] = -\frac{\partial \delta p}{\partial x}
\]

Euler eq.

\[
\left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) \frac{\partial v}{\partial y} = \bar{u} \frac{\partial^2 \delta p}{\partial y^2}
\]

Energy eq.

\[
\frac{1}{\gamma p} \frac{Dp}{Dt} + \nabla \cdot u = \frac{q}{c_p T} \bar{W}
\]

\[
\frac{1}{\gamma \bar{p}} \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) \delta p + \frac{\partial}{\partial x} \delta u + \bar{u} \frac{\partial}{\partial y} v = q \delta w
\]

divergence

rate of heat release

Boundary conditions

Rankine-Hugoniot

\(| x = 0 : \delta u = \left[1 + (1/\bar{M}_u^2) - (\gamma - 1)/2\right] \partial \alpha / \partial t, \quad v = \left[1 - (1/\bar{M}_u^2)\right] \partial \alpha / \partial y \]

\[ \delta p = -2\varepsilon^2 \partial \alpha / \partial t, \quad \delta T_N / \bar{T}_N \approx - (\gamma - 1) \partial \alpha / \partial t \]

\(| x \to \infty : \) boundedness condition
Linear analysis in normal modes

\[ x = \alpha(y, t) \]

wrinkled front of the lead shock

\[ \alpha = \tilde{\alpha} \exp(\sigma t + i\kappa y) \quad \delta f(x, y, t) = \tilde{f}(x)\tilde{\alpha} \exp(\sigma t + i\kappa y) \]

\[ \sigma \equiv \hat{\sigma} \bar{t}_N, \quad \kappa \equiv \frac{\hat{k} |\bar{u}_N \bar{t}_N|}{\epsilon}, \quad \sigma(\kappa) = s(\kappa) \pm i\omega(\kappa) \]

Expansion in powers of \( \epsilon \)

\[ v = \delta v_0^{(i)} + O(\epsilon^2) \quad \delta u = \delta u_0^{(i)} + O(\epsilon^2) \]

\[ \sigma(\kappa) = \sigma_0(\kappa) + \epsilon^2 \sigma_2(\kappa) + \ldots \quad ? \]

Zeroth-order of the vorticity wave \( \delta p^{(i)} = 0 \)

\[ \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) \delta u_0^{(i)} = 0, \quad \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) \delta v_0^{(i)} = 0 \]

length and time scales of order unity

**Rankine-Hugoniot**

\[ x = 0: \quad \delta u_0^{(i)} = \partial \alpha / \partial t, \quad \delta v_0^{(i)} = \partial \alpha / \partial y \quad \Rightarrow \quad \delta u_0^{(i)} = \frac{\partial}{\partial t} \alpha(t - x, y), \quad \delta v_0^{(i)} = \frac{\partial}{\partial y} \alpha(t - x, y) \]

**continuity**

\[ \partial \delta u_0^{(i)} / \partial t + \partial \delta v_0^{(i)} / \partial y = 0 \quad \Rightarrow \quad \partial^2 \alpha / \partial t^2 - \partial^2 \alpha / \partial y^2 = 0 \]

\[ \sigma_0 = \pm i\kappa \]

transverse travelling waves

the growth or damping rate is of a smaller order
Linear analysis at strong overdrive: acoustics + entropy-vorticity waves

R. Daou and P. Clavin (2003), J. Fluid Mech., 482, 181-206

\[
\delta u = \delta u_0^{(i)}(x, t) + \varepsilon^2 \left[ \delta u_2^{(i)}(x, t) + \delta u_2^{(a)} \right] + \ldots \quad \delta p^{(i)} = 0
\]
\[
\delta v = \delta v_0^{(i)}(x, t) + \varepsilon^2 \left[ \delta v_2^{(i)}(x, t) + \delta v_2^{(a)} \right] + \ldots \quad \delta p = \varepsilon^2 \delta p_2^{(a)} + \ldots
\]

**Two zones:**

Thin quasi-isobaric inner layer where the heat is released \( x = O(1) \)

Outer inert zone

**Acoustic waves in the outer zone**

\[
\frac{D^2}{Dt^2} \delta p - \bar{a}_N \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \delta p = 0 \quad \Rightarrow \quad \left\{ \frac{1}{\gamma \bar{p}_b} \left( \frac{d}{dx} + \sigma \right)^2 - \frac{1}{\varepsilon^2 \frac{d^2}{dx^2} + \bar{u}_b^2 \kappa^2} \right\} \bar{p}(x) = 0
\]

\[
\delta p = \bar{p}(x)e^{\sigma t + i\kappa y}
\]

\[
\sigma = \sigma_0 + \varepsilon^2 \sigma_2(\kappa)
\]

\[
\sigma_0(\kappa) = \pm i\kappa
\]

\[
\sigma^2 + \kappa^2 = O(\varepsilon^2)
\]

\[
\Rightarrow \quad il = O(\varepsilon^2), \quad il = \varepsilon^2 l_2, \quad l_2 = O(1)
\]

the sound waves propagate in the burnt gas in a direction quasi-parallel to the front

Rankine-Hugoniot

\[
x = 0 : \quad \delta p = -2\varepsilon^2 \dot{\alpha}_t \quad \Rightarrow \quad \bar{p}(\varepsilon^2 x) = -2\varepsilon^2 \sigma \exp(i\varepsilon^2 l_2 x) + O(\varepsilon^4)
\]

the sound waves are smaller than the entropy-vorticity wave by a factor \( \varepsilon^2 \)
Outer inert zone

\[ \sigma_0 = \pm i \kappa \]

\[ il_2 = \sigma_0 - \sqrt{2\sigma_0 \sigma_2 + (h + q_2 - 1) \kappa^2} \]

where \( q_N \equiv \epsilon^2 q_2 \) \((\gamma - 1) \equiv \epsilon^2 h \)

\[ u* = \text{constant of integration} \]

\[ u^* \text{ and } \sigma_2 \text{ are obtained by matching with the inner solution} \]

Inner structure of the detonation

\[ \tilde{u} \equiv \tilde{U}^{(i)}(x) + \tilde{u}^{(a)}(\epsilon^2 x) \quad \tilde{v} \equiv \tilde{V}^{(i)}(x) + \tilde{v}^{(a)}(\epsilon^2 x) \]

method similar to that used for galloping detonations

\[ \nabla \cdot \tilde{V}^{(i)} \approx \left[ -1 + \epsilon^2 \left( 2 + \frac{1}{\epsilon^2 M_U^2} \right) \right] \kappa^2 e^{-\sigma x} \]

\[ \tilde{U}^{(i)}(x) - \left[ 1 + \frac{1}{M_U^2} - \frac{\gamma - 1}{2} \right] \sigma + 2\epsilon^2 il_2 + \tilde{u}(x) \int_0^x \nabla \cdot \tilde{V}^{(i)}dx' \approx q_N \int_0^x \left( \tilde{w} + \tilde{v}_0^{(i)} \tilde{w} \right) dx' \]
Matching

P.Clavin (2002), *Nonlinear PDE’s in condensed matter and active flows*, 49-97, Kluwer
See also the review by Clavin (2017) *Combust. Sci. Technol.* 189 (5) pp 747-775

\[
\lim_{x \to 1} \tilde{U}^{(i)}(x) = \tilde{u}^{(i)}(x)
\]

\[
\tilde{u}^{(i)} = (\pm i\kappa + \epsilon^2 u^*) \exp(\pm i\kappa x - \epsilon^2 \sigma_2 x)
\]

fast oscillation \( x = O(1) \)
slowly damped \( x = O(1/\epsilon) \)

constant terms of \( \lim_{x \to 1} \tilde{U}^{(i)}(x) = 0 \)

\[
\frac{\sigma_0}{\kappa} \sqrt{2\frac{\sigma_0 \sigma_2}{\kappa^2} + h + q_2 - 1 - \frac{\sigma_0 \sigma_2}{\kappa^2} + 1 - \frac{3}{4} h} = \frac{q_2}{2} S^{(i)}(\kappa)
\]

Algebraic equation of second degree for \( \sigma_2 \)

where

\[
\sigma_0 = \pm i\kappa, \quad \frac{q_m}{(c_p T_N)} = \epsilon^2 q_2 \quad (\gamma - 1) \equiv \epsilon^2 h
\]

\[
S^{(i)}(\kappa) \equiv \beta_N (\gamma - 1) s_{\beta N}^{(i)}(\kappa) + s_q^{(i)}(\kappa)
\]

\[
s_{\beta N}^{(i)}(\kappa) \equiv \int_0^\infty \Omega_N'(x) e^{-i\kappa x} dx, \quad s_q^{(i)}(\kappa) \equiv \int_0^\infty (1 + i\kappa x) \Omega(x) e^{-i\kappa x} dx
\]

\( \Omega(x) \) is the distribution of the non-dimensional rate of heat release in the steady state
\( \Omega_N'(x) \) is its derivative with respect to the Neumann temperature, denoting its sensitivity to the overdriven regime
Linear growth rate

R. Daou and P. Clavin (2003), J. Fluid Mech., 482, 181-206

\[
\frac{2 \text{Re}(\sigma)/\kappa}{q_N} = -\text{Im} \left[ S^{(i)}(\kappa) \right] - \frac{M_N}{\sqrt{q_N}} S^{(a)}(\kappa)
\]

quasi-isobaric instability mechanism

\[
S^{(i)}(\kappa) \equiv \beta_N (\gamma - 1) s^{(i)}_\beta(\kappa) + s^{(i)}_q(\kappa)
\]

sensitivity to \( T_N \)

\[
s^{(i)}_\beta(\kappa) = \int_0^\infty \Omega'_N(x)e^{-ix\kappa} \, dx
\]

\[
s^{(i)}_q(\kappa) = \int_0^\infty (1 + ix\kappa) \Omega(x)e^{-ix\kappa} \, dx
\]

strong instability due to wrinkling

\[
\text{stabilizing effect due to compressibility}
\]

\[
S^{(a)}(\kappa) \equiv 2 \left[ \text{Im} \sqrt{\frac{(\gamma - 1)}{2q_N} + S^{(i)}(\kappa) - 1} \right] > 0
\]

\[
q_N \Rightarrow \{ \text{stabilisation}, \text{instability} \}
\]

Threshold of linear instability for \( \beta_N = 0 \)

\[
\gamma = 1.05, \quad M_u^2 = 20 \quad (M_N = 0.267)
\]

good agreement between theory and numeric
Weakly nonlinear analysis of cellular detonations

Near to the instability threshold the dominant nonlinear effects are those responsible for singularity formation on the inert shock front (representative of Mach stem), see p.12 of lecture XIV

Model equation
A weakly nonlinear analysis leads to a combination of the linear equation for the multidimensional instability of an overdriven detonation and the nonlinear equation for the lead shock

equation of the detonation front  \( x = \alpha(y,t) \)

\[
\frac{\partial^2 \alpha}{\partial t^2} - c^2 \nabla^2 \alpha + \frac{\partial |\nabla \alpha|^2}{\partial t} = q_N L^{(i)}(\alpha) - 2M N \sqrt{q_N} \frac{\partial}{\partial t} L^{(a)}(\alpha) \tag{1}
\]

\( c^2 = 1 + 3(\gamma - 1)/2 \)

\( L^{(i)}(\phi) = \beta_N(\gamma - 1) l_{\beta N}^{(i)}(\alpha) + l_q^{(i)}(\alpha) \)

\( L^{(a)}(\alpha) \approx \kappa \alpha /2 \) in Fourier space

\[
l_{\beta N}^{(i)}(\alpha) = \frac{\partial^2}{\partial \alpha^2} \int_0^\infty \Omega_N(x) \alpha(t-x) dx, \quad l_q^{(i)}(\alpha) = \nabla^2 \int_0^\infty \Psi(x) \alpha(t-x) dx
\]

where \( \Psi(x) = \Omega(x) + d(x) / dx \)

Good qualitative agreement with the experimental observation
Conclusion for large overdrives

\[
\begin{align*}
\frac{\partial^2 \alpha}{\partial t^2} - \frac{\partial^2 \alpha}{\partial y^2} + \frac{\partial}{\partial t} \left( \frac{\partial \alpha}{\partial y} \right)^2 &= \left[ q_N G(\alpha) - M_N \sqrt{q_N} D(\alpha) \right] \\
\text{NL term} & \quad \text{linear growth} & \text{linear damping} \\
(\text{quasi-isobaric mechanism}) & \quad (\text{compressible effect}) \\
\end{align*}
\]

Quasi-isobaric instability mechanism

\[
\begin{align*}
G(\alpha) &= \beta_N (\gamma - 1) \frac{\partial^2}{\partial x^2} G_p(\alpha) + \frac{\partial^2}{\partial y^2} G_w(\alpha) \\
G_p(\alpha) &= \int_0^\infty \Omega_N'(x) \alpha(t - x, y) dx \\
G_w(\alpha) &= \int_0^\infty \Psi(x) \alpha(t - x, y) dx \\
\text{thermal sensitivity of the} \\
\text{distribution of heat release rate} \\
\Omega_N'(x) &\equiv \partial \Omega / \partial \Omega_N \\
\Psi(x) &\equiv \Omega(x) + d(x \Omega) / dx
\end{align*}
\]

1-D galloping mechanism 

modification due to wrinkling

Multidim instability before 1-D instability

Superposition of two mechanisms

Nonlinear dynamics of the lead shock + linear oscillation due to the heat release

Oscillatory frequency \( \omega \tilde{t}_N = O(1) \)  
where \( \tilde{t}_N \equiv \tau_{\text{reac}}(\overline{T}_N) \)

Nonlinear wavelength selection \( \Lambda \approx a \overline{u}_N \tilde{t}_N / M_N \quad a \in [2 - 5] \)
Dynamics of the detonation waves near the CJ regime

Analytical solutions have been obtained in two limiting cases (opposite conditions):

**Strongly overdriven detonation in the Newtonian limit**


quasi-isobaric flow
dominant mechanism: entropy wave

**CJ (or near CJ) close to the instability threshold**


Transonic flow

Slowest (dominant) mechanism in the loops: Upwards propagating acoustic wave

Two different coupling mechanisms: \[
\begin{align*}
\text{acoustic waves} & \leftrightarrow \\
\text{entropy wave} & \quad \text{(double arrows indicate bidirectional coupling)}
\end{align*}
\]
Cellular instability near the CJ regime
(basic approximation: small heat release)

Fast: quasi-instantaneous

- Entropy wave
- Downstream running acoustic wave
- Shock wave
- Direct influence
- Feedback loop
- Upstream running acoustic wave

Slow

\[ \alpha = 0 \]
\[ \alpha(t) \]
oscillations

\[ \overline{D} \]
heat release

Distinguished limit

Near the CJ regime the instability threshold concerns transonic conditions associated with small heat release.

Same distinguished limit as in pp 9-10 lecture XII

**\[ \epsilon^2 \equiv \frac{(\gamma + 1)}{2} \frac{q_m}{c_p T_u} \ll 1 \quad (\gamma - 1) = O(\epsilon) \]**

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Cellular CJ detonation (small heat release)

Formulation of the free boundary problem

Reactive Euler equations in 2-D geometry

\[
\begin{align*}
\frac{D}{Dt} & \equiv \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} + w \frac{\partial}{\partial y} \\
\frac{1}{\gamma P} \frac{D^\pm p}{Dt} & \pm \frac{1}{a} \frac{D^\pm u}{Dt} = \frac{q_m}{c_p T} \frac{\dot{w}}{\tilde{t}_N} - \frac{\partial w}{\partial y} \\
\frac{1}{\gamma} \frac{DT}{Dt} & - \frac{(\gamma - 1)}{p} \frac{DP}{Dt} = \frac{q_m}{c_p T_u} \frac{\dot{w}}{\tilde{t}_N}
\end{align*}
\]

Boundary conditions

On the lead shock \( x = \alpha(y, t) \): Neumann conditions
At infty in the burned gas: boundedness condition

Distinguished limit

Transonic flow \( M \equiv a_u^{-1} \partial \alpha / \partial t \)
High thermal sensitivity of the inductio

\[
\epsilon^2 \equiv \frac{(\gamma + 1)}{2} \frac{q_m}{c_p T_u} \ll 1, \quad M_{CJ} - 1 \approx \epsilon, \quad (\gamma - 1)/\epsilon < 1, \quad \epsilon (\gamma - 1) \frac{E}{k_B T_u} = O(1)
\]

\( T_u ! \)

Scaling laws

\[
\begin{align*}
t/\tilde{t}_N & = \epsilon \tau, \quad x/a_u \tilde{t}_N = \xi, \quad y/a_u \tilde{t}_N = \eta/\epsilon^{1/2} \\
u/a_u & = 1 + \epsilon \mu, \quad v/a_u = \epsilon^{3/2} \nu, \quad \ln(p/p_u) = \epsilon \pi, \quad (T - T_u)/T_u = \epsilon^2 \theta
\end{align*}
\]
Cellular CJ detonation (small heat release)

\[ \epsilon^2 \equiv (\gamma + 1) \frac{q_m}{c_p T_u} \ll 1 \]

**Normal mode analysis**

Equation for the front of the lead shock

\[ \xi = \alpha(\eta, \tau) = e^{\sigma \tau + i \kappa \eta} \]

\[ \frac{t}{\bar{t}_N} = \epsilon \tau, \quad \frac{x}{a_u \bar{t}_N} = \xi, \quad \frac{y}{a_u \bar{t}_N} = \eta / \epsilon^{1/2} \]

**Analytical result**

Model for the distribution of heat release rate of the CJ wave

\[ \Omega(\xi) = \xi^n e^{-\xi} / n!, \quad \xi \geq 0, \quad n \geq 1 \]

Algebraic equation for \( \sigma(\kappa) \) with a single parameter

\[ H = (n+1)(\gamma-1) \frac{q_m}{c_p T_N} \frac{E}{k_b T_N} \]

\[ 4 \left( 1 + \frac{\sigma + \sqrt{\sigma^2 + 2\kappa^2}}{2} \right)^{n+2} = H \sigma + \left( 1 + \frac{\sigma + \sqrt{\sigma^2 + 2\kappa^2}}{2} \right) \]

Bifurcation scenario similar to that of the strongly overdriven regimes
Generic character of the results:

The bifurcation scenario of CJ waves is similar to that at large overdrive
The integral equations are of the same type

Increasing the thermal sensitivity of the induction length
or stiffening the distribution of heat release promote the instability.

Detonations are unstable against the transverse disturbances before the longitudinal ones

Unstable wavelengths are larger than the detonation thickness
Thank you for your attention
Details of the calculation (strong overdrive)
Non-dimensional variables of order unity
denoting \( \hat{w} \) the original dimensional quantities and \( w \) the dimensionless quantity

\[
u \equiv \hat{u} / \bar{u}_N, \quad \mathbf{v} \equiv \hat{\mathbf{v}} / \bar{u}_N, \quad p \equiv \hat{p} / \bar{p}_N, \quad T \equiv \hat{T} / \bar{T}_N \quad \text{and} \quad \alpha \equiv \hat{\alpha} / d_N, \quad d_N \equiv \bar{u}_N \bar{T}_N
\]
where the scaling of the transverse velocity \( \hat{v} \) comes from the Rankine-Hugoniot condition

\[
\hat{v}_N / \bar{u}_N \propto (\partial \hat{\alpha} / \partial y, \, \partial \hat{\alpha} / \partial z)
\]
and the scaling of the transverse coordinates \( \partial / \partial y = \epsilon d_N^{-1} \partial / \partial y, \quad \partial / \partial z = \epsilon d_N^{-1} \partial / \partial z \)

Formulation (Clavin et al. 1997, Clavin 2002)

\[
\begin{array}{c}
x = \frac{1}{\bar{p}_N \bar{u}_N \bar{T}_N} \int_{\alpha(y,z,t)}^{x} \rho(\mathbf{x}, y, z, t) dx' \\
y \equiv (\epsilon y / d_N, \epsilon z / d_N) \quad t \equiv \frac{t}{\bar{T}_N}
\end{array}
\Rightarrow
\frac{D}{Dt} = \frac{\partial}{\partial t} + \left[ m(t) - \nu(x, y, t) \right] \frac{\partial}{\partial x} + \mathbf{v} \cdot \nabla \mathbf{y}
\]

\[
m(t) \equiv 1 - (\partial \hat{\alpha} / \partial \hat{t}) / \bar{T} \quad \text{and} \quad \nu(x, y, t) \equiv \int_{0}^{x} \nabla_y \mathbf{v} \, dx' = O(1)
\]

continuity (in the linear approximation) \( \Rightarrow \)
\[
\frac{\partial r}{\partial t} + m(t) \frac{\partial r}{\partial x} = \frac{\partial}{\partial x} \left[ \nu(x, y, t) \right] \quad \text{where} \quad r(x, y, t) \equiv \bar{p}_N / \hat{p}
\]

\[
\textbf{Stability limit} \quad q_N = \frac{q_m}{c_p \bar{T}_N}
\]
\[
q_N = O(\epsilon^2)
\]
\[
\bar{u}_N / \bar{T} = O(\epsilon^2) \Rightarrow m(t) = 1 + O(\epsilon^2)
\]


\[
\text{Expansion in powers of} \ \epsilon^2
\]
\[
q_N = \epsilon^2 q_2 \quad u = 1 + \epsilon^2 \bar{u}_2(x) + \delta u \quad T = 1 + \epsilon^2 \bar{T}_2(x) + \delta T \quad p = 1 + \epsilon^4 \bar{p}_4 + \delta p
\]

Linear equations
\[
\epsilon^2 \left[ \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) \delta u - \nu \frac{du}{dx} \right] = - \frac{\partial \delta p}{\partial x} \quad \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) (\nabla \cdot \mathbf{v}) = - \bar{u} \nabla^2 \delta p
\]
\[
\bar{p}_N \bar{u}_N^2 / \bar{p}_N = \epsilon^2
\]
\[
\frac{1}{\gamma \bar{p}} \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) \delta p + \frac{\partial}{\partial x} (\delta u + \bar{u} \nu) = q_N (\delta \bar{w} + \nu \bar{w}), \quad q_N = \epsilon^2 q_2
\]

Rankine-Hugoniot conditions
\[
\dot{\alpha}_t \equiv (\bar{T}_N / d_N) \partial \bar{\alpha} / \partial t = \bar{u}_N^{-1} \partial \bar{\alpha} / \partial t = O(1) \quad \nabla \alpha \equiv \epsilon d_N^{-1} \left( \frac{\partial \bar{\alpha}}{\partial y} \frac{\partial \bar{\alpha}}{\partial z} \right) = O(1)
\]
\[
x = 0: \quad \delta u \approx \left[ 1 + \frac{1}{M_u^2} - \frac{(\gamma - 1)}{2} \right] \dot{\alpha}_t, \quad \nu \approx \left[ 1 - \frac{1}{M_u^2} \right] \nabla \alpha, \quad \delta p \approx - 2 \epsilon^2 \dot{\alpha}_t, \quad \delta T_N \approx - (\gamma - 1) \dot{\alpha}_t
\]
\[
\alpha(y, t) = \tilde{\alpha} e^{\sigma t + ik_y}, \quad \delta u = \tilde{u}(x) \tilde{\alpha} e^{\sigma t + ik_y}, \quad \delta v = \tilde{v}(x) \tilde{\alpha} e^{\sigma t + ik_y}, \quad \tilde{\rho}(x) \tilde{\alpha} e^{\sigma t + ik_y}
\]

**Outer flow (burnt gas)**

\[
\left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) \delta u^{(i)} = 0, \quad \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) v^{(i)} = 0 \quad \text{valid up to } \epsilon^2 \text{ in the burnt gas}
\]

\[
\tilde{u}^{(i)} = \left[ \sigma_0 + \epsilon^2 \tilde{u}^{(i)}_{b2} \right] e^{-\sigma x} \quad \nabla \tilde{v}^{(i)} = \left[ -\kappa^2 - \epsilon^2 \nabla \tilde{v}^{(i)}_{b2} \right] e^{-\sigma x}
\]

\[
\tilde{p}(\epsilon^2 x) = -2\epsilon^2 \sigma e^{i\epsilon^2 l_2 x} \quad \Rightarrow \quad \tilde{u}^{(a)} = 2\epsilon^2 l_2 e^{i\epsilon^2 l_2 x} \quad \nabla \tilde{v}^{(a)} = -2\epsilon^2 \kappa^2 e^{i\epsilon^2 l_2 x}
\]

The acoustic flow is of order \( \epsilon^2 \), the acoustic flow is small, of order \( \epsilon^2 \), and varies on a long length scale.

**Inner flow (reacting gas)**

**Inner detonation structure (inner zone)**

\[
\frac{1}{\gamma \bar{p}} \left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} (\delta u + \bar{u}v) = q_N (\delta \tilde{w} + \bar{v} \tilde{w}), \quad \Rightarrow \quad \frac{d}{dx} \left[ \tilde{U}^{(i)}(x) + \tilde{u}(x) \tilde{v}^{(i)}(x) \right] \approx q_N \left( \tilde{w} + \tilde{v}^{(i)}_0 \tilde{\bar{w}} \right)
\]

\[
\frac{d\bar{u}}{dx} = q_N \bar{w} \quad \Rightarrow \quad d\tilde{U}^{(i)} / dx + \bar{u} \nabla \tilde{V}^{(i)} \approx q_N \tilde{w}
\]

\[
\left( \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) (\nabla \cdot v) = -\pi \nabla^2 \delta p \quad \Rightarrow \quad (\partial / \partial t + \partial / \partial x) \nabla \tilde{V}^{(i)} \approx 0 \quad \text{valid up to } \epsilon^2
\]

\[
x = 0: \quad v \approx \left[ 1 - \frac{1}{M_u^2} \right] \nabla \alpha \quad \nabla \tilde{V}^{(a)} = -2\epsilon^2 \kappa^2
\]

Rankine-Hugoniot see p.6 lecture X and p.6 lecture XIII

\[
x = 0: \quad \delta u \approx \left[ 1 + \frac{1}{M_u^2} - \frac{(\gamma - 1)}{2} \right] \alpha_t \quad \tilde{u}^{(a)} = 2\epsilon^2 l_2
\]

\[
\tilde{U}^{(i)}(x) = O(1) \quad \tilde{V}^{(i)}(x) = O(1)
\]
internal solution
\[ \ddot{U}^{(i)}(x) - \left[ 1 + \frac{1}{M_{U}^2} - \frac{\gamma - 1}{2} \right] \sigma + 2 \varepsilon^2 \omega_2 + \pi(x) \int_{0}^{x} \nabla . \dot{V}^{(i)}(x') dx' \approx q_{N} \int_{0}^{x} \left( \dot{\bar{w}} + \dot{\bar{v}}^{(i)}(x') \right) dx' \rightarrow q_{N} = \varepsilon^2 q_{2} \]
\[ \nabla . \dot{V}^{(i)} \approx \left[ -1 + \varepsilon^2 \left( 2 + \frac{1}{\epsilon^2 M_{U}^2} \right) \right] \kappa^2 e^{-\sigma x} \Rightarrow \int_{0}^{x} \nabla . \dot{V}^{(i)} dx' = \left[ -1 + \varepsilon^2 \left( 2 + \frac{1}{\epsilon^2 M_{U}^2} \right) \right] \frac{\kappa^2}{\sigma} \left( 1 - e^{-\sigma x} \right) \]

at the end of the reaction \( \bar{w} = 0, \tilde{w} = 0 : \ddot{U}^{(i)}(x) \rightarrow \) constant term + oscillatory term

constant term
\[ \left[ 1 + \frac{1}{M_{U}^2} - \frac{\gamma - 1}{2} \right] \sigma - 2 \varepsilon^2 \omega_2 - \bar{u}_b \left[ -1 + \varepsilon^2 \left( 2 + \frac{1}{\epsilon^2 M_{U}^2} \right) \right] \frac{\kappa^2}{\sigma} + q_{N} \int_{0}^{\infty} \left( \dot{\bar{w}} + \dot{\bar{v}}^{(i)}(x') \right) dx' = 0 \]

\[ \omega_2 \approx \sigma_0 - \sqrt{2 \sigma_0 \sigma_2 + (h + \sigma_2 - 1) \kappa^2} \]

oscillatory term with an amplitude varying on a long length scale, \( \text{Re}(\sigma) = O(\varepsilon^2) \)

matching \( \Rightarrow \) the constant term of the internal solution should be zero \( \Rightarrow \) equation for \( \sigma \) when \( \bar{w} \) is known

**Reaction rate and dispersion relation** \( \sigma_2(\kappa) \)
\[ \frac{\partial T}{\partial t} + \frac{\partial T}{\partial x} = q_{N}(1 + \dot{v}_0^{(i)}(x)) \tilde{w} \quad \frac{\partial \psi}{\partial t} + \frac{\partial \psi}{\partial x} = (1 + \dot{v}_0^{(i)}(x)) \tilde{w} \quad \dot{v}_0^{(i)}(x) = -\frac{\kappa^2}{\sigma_0} (1 - e^{-\sigma_0 x}) \]

\( x = 0 : T = T_N(y, t), \quad \psi = 0 \)

method similar to that used for galloping detonations \( \text{see p.7-8 lecture XII} \)

\[ \sigma_2(\kappa) \equiv \beta_N(\gamma - 1) s_{\beta_N}^{(i)}(\kappa) + s_{q}^{(i)}(\kappa) \]

\( s_{\beta_N}^{(i)}(\kappa) \equiv \int_{0}^{\infty} \Omega_N(x)e^{-i\kappa x} dx \quad s_{q}^{(i)}(\kappa) \equiv \int_{0}^{\infty} (1 + i\kappa x)\Pi(x)e^{-i\kappa x} dx \)

Details of the calculation (CJ wave)
Cellular instability near the CJ condition
*(small heat release)*

Clavin Williams 2009, 2012

**Formulation**

Extension of the analysis of galloping detonations (planar case) pp 9-13 lecture XII

**Reactive Euler equations in 2-D geometry**

Same as in p.9 lecture XII but with \( \frac{D}{Dt} \equiv \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} + w \frac{\partial}{\partial y} \)

\[
\begin{align*}
\frac{1}{\gamma p} \frac{D^+ p}{Dt} + \frac{1}{a} \frac{D^+ u}{Dt} &= \frac{q_m}{c_p T} \dot{w} - \frac{\partial w}{\partial y} \\
\frac{D^+ x}{Dt} &= \frac{\partial}{\partial t} \pm (a \pm u) \frac{\partial}{\partial x} + w \frac{\partial}{\partial y} \\
\frac{Dw}{Dt} &= -\frac{1}{\rho} \frac{\partial p}{\partial y}
\end{align*}
\]

**Distinguished limit**

Near the CJ regime the instability threshold concerns *transonic conditions* associated with *small heat release*

Same distinguished limit as in pp 9-10 lecture XII

\[
\epsilon^2 \equiv \frac{(\gamma + 1)}{2} \frac{q_m}{c_p T_u} \ll 1 \quad (\gamma - 1) = O(\epsilon)
\]

With the notations of p.10 lecture XII \( t = \frac{x}{t_N}, \quad x = \frac{x}{a u t_N}, \quad \tilde{u} = \frac{u}{a u}, \quad \tilde{\pi} = \frac{1}{\gamma} \ln \left( \frac{p}{p_u} \right), \quad \tilde{\theta} = \frac{(T - T_u)}{T_u} \) one introduces \( \tilde{\nu} \equiv \frac{\dot{w}}{a u} \) and \( \frac{x}{a u t_N} \)

Anticipating that the *transverse convection* \( w \partial / \partial y \) introduces negligible corrections, the reduced equations take the form

- **acoustic wave**
  \[
  \left[ \frac{\partial}{\partial t} \pm (1 \pm \tilde{u}) \frac{\partial}{\partial x} \right] (\tilde{\pi} \pm \tilde{u}) = \epsilon^2 \dot{w} - \frac{\partial \dot{\nu}}{\partial y} \]

- **vorticity wave**
  \[
  \left[ \frac{\partial}{\partial t} + \tilde{u} \frac{\partial}{\partial x} \right] \psi = \dot{w} \quad \left[ \frac{\partial}{\partial t} + \tilde{u} \frac{\partial}{\partial x} \right] \tilde{\nu} = -\frac{\partial \tilde{\pi}}{\partial y} \]

- **entropy wave**
  \[
  \left[ \frac{\partial}{\partial t} + \tilde{u} \frac{\partial}{\partial x} \right] [\tilde{\theta} - (\gamma - 1) \tilde{\pi}] = \epsilon^2 \dot{w} \]

Boundary conditions: Rankine-Hugoniot at the shock front and boundedness condition in the burnt gas \( x \to \infty \)
**Scalings**

*Time scale*

As in p. 11 lecture XII the slow time scale is controlled by the upstream-running acoustic wave in the feedback loop between the shock and the reacting gas

\[ \tau \equiv \frac{t}{t_N/\epsilon} = \epsilon t \quad t \equiv t/\tilde{t}_N \quad \tau = O(1) \quad \partial/\partial t = \epsilon \partial/\partial \tau \]

the downstream propagating acoustic wave and the voracity wave are quasi instantaneous

**Longitudinal variations**

\[ q_m \ll c_p T_u \implies \text{the variation across the detonation thickness are small} \]

\[ \ddot{u} \equiv \frac{u}{a_u} = 1 + \epsilon \mu, \quad \ddot{\pi} \equiv \frac{1}{\gamma} \ln \left( \frac{p}{p_u} \right) = \epsilon \pi, \quad \ddot{\theta} \equiv \frac{(T - T_u)}{T_u} = \epsilon^2 \theta \]

**Transverse scaling** (obtained by the linear approximation of the Rankine-Hugoniot relations)

Rankine-Hugoniot

\[ w_N = (D - u_N)\alpha'_y \implies \xi = 0 : \quad \ddot{\nu} = 2\epsilon \sqrt{f} \frac{\partial a}{\partial y}, \quad \partial \ddot{\nu}/\partial y = 2\epsilon \sqrt{f} \partial^2 a/\partial y^2 \quad \text{where} \quad x = a(\epsilon t, x) \]

\[ \frac{\partial}{\partial t} \pm (1 \pm \ddot{u}) \frac{\partial}{\partial x} (\ddot{\pi} \pm \ddot{u}) = \epsilon^2 \ddot{w} - \frac{\partial \ddot{\nu}}{\partial y} \implies \partial \ddot{\nu}/\partial y = O(\epsilon^2) \implies \partial^2 a/\partial y^2 = O(\epsilon) \implies \eta \equiv y/\sqrt{\epsilon} = O(1) \quad \ddot{\nu} = \epsilon^{3/2} \nu \quad \nu = O(1) \]

**Leading order relations**

downstream propagating acoustic wave

\[ \frac{\partial}{\partial t} \left( 1 + \ddot{u} \right) \frac{\partial}{\partial x} (\ddot{\pi} + \ddot{u}) = \epsilon^2 \ddot{w} - \frac{\partial \ddot{\nu}}{\partial y} \]

\[ \Rightarrow \quad \frac{\partial}{\partial x} (\pi + \mu) = 0 \]

transverse convection \( w \frac{\partial}{\partial y} = \frac{\epsilon^2 \nu}{\tilde{t}_N} \frac{\partial}{\partial \eta} \)

is negligible in front of the unsteady term \( \frac{\partial}{\partial t} = \epsilon \frac{\partial}{\partial \tau} \)

same relations as in the planar case see p.11 lecture XII

*Entropy-vorticity wave*

\[ (\gamma - 1) \equiv \epsilon h \]

\[ \frac{\partial}{\partial \xi} [\theta - h\pi - \psi] = 0 \]

\[ \Rightarrow \quad \frac{\partial \nu}{\partial x} = -\frac{\partial \pi}{\partial y} \]

additional relation in the transverse direction (vorticity wave)
In the moving frame \( x = a(\eta, \tau) \)
\[
\tau = \epsilon t, \quad \eta = \sqrt{\epsilon} y, \quad \xi \equiv x - a(\eta, \tau), \quad \frac{\partial}{\partial \xi} - \frac{\partial}{\partial \eta} \to \sqrt{\epsilon} \left( \frac{\partial}{\partial \eta} - a_\eta' \frac{\partial}{\partial \xi} \right), \quad \frac{\partial}{\partial t} \to \epsilon \left( \frac{\partial}{\partial \tau} - \dot{a}_\tau \frac{\partial}{\partial \xi} \right)
\]
the equations for the downstream running acoustic mode and the entropy-vorticity wave yield
\[
\frac{\partial}{\partial \xi} (\pi + \mu) = 0 \quad \frac{\partial}{\partial \xi} [\theta - h\pi - \psi] \approx 0 \quad \frac{\partial \psi}{\partial \xi} = \dot{w}(\theta, \psi) \quad \frac{\partial \nu}{\partial \xi} \approx -\frac{\partial \pi}{\partial \eta} + a_\eta' \frac{\partial \pi}{\partial \xi}
\]

The boundary conditions at \( \xi = 0 \) (Neumann state) for \( \pi \) and \( \theta \) are given by the Rankine-Hugoniot conditions in p.7 of lecture X where \( M_u \)
is replaced by \( \frac{(D - \partial a/\partial t)}{a_u [1 + (\partial a/\partial y)^2]^{1/2}} \) that is, to leading order,
\[
M_u \to 1 + \epsilon \left[ \sqrt{\hat{f}} - \dot{a}_\tau - (1/2)(a_\eta')^2 \right] + ..
\]
the first nonlinear correction is purely geometrical

Up to first order, the boundary conditions at \( \xi = 0 \) for \( \theta, \mu \) and \( \pi \) are the same as in the planar case p 12 lecture XII where \( \dot{\hat{a}}_\tau \to \dot{a}_\tau + (1/2)(a_\eta')^2 \)

\[
\begin{align*}
\xi = 0 : & \quad \mu + \pi = \sqrt{\hat{f}}, \quad \mu = -\sqrt{\hat{f}} + 2[\dot{a}_\tau + (1/2)(a_\eta')^2], \quad \theta = 2h[\sqrt{\hat{f}} - \dot{a}_\tau - (1/2)(a_\eta')^2] \quad \psi = 0 \\
\forall \xi > 0 : & \quad \pi = -\mu + \sqrt{\hat{f}}, \quad \theta = h\sqrt{\hat{f}} - h\mu + \psi \end{align*}
\]
same relations as in the planar case see p. 13 lecture XII

**Upstream-running acoustic wave**
\[
\left[ \frac{\partial}{\partial t} - (1 - \dot{u}) \frac{\partial}{\partial x} \right] (\pi - \dot{u}) = \epsilon^2 \dot{w} - \frac{\partial \dot{w}}{\partial y} \quad \Rightarrow \quad 2 \left[ \frac{\partial}{\partial \tau} + (\mu - \dot{a}_\tau) \frac{\partial}{\partial \xi} \right] \mu = -\dot{w}(\theta, \psi) + \frac{\partial \nu}{\partial \eta} - a_\eta' \frac{\partial \nu}{\partial \xi}
\]
where \( \nu \) is solution to
\[
\frac{\partial \nu}{\partial \xi} = \frac{\partial \mu}{\partial \eta} - a_\eta' \frac{\partial \mu}{\partial \xi}
\]
with the boundary condition \( \xi = 0: \quad \nu = 2\sqrt{\hat{f}}a_\eta' - 2[\dot{a}_\tau + (1/2)(a_\eta')^2]a_\eta' \)
\( x = \alpha : \quad w = (D - u)a_\eta' \quad (p.5 \text{ lecture IV}) \)

3 first order PDEs for \( \nu, \mu \) and \( \psi \) with 3 boundary conditions at \( \xi = 0 \)

An integral equation for \( a(\eta, \tau) \) is obtained when applying the downstream boundary condition
\[
\xi \to \infty : \quad \psi = 1, \quad \dot{w} = 0, \quad \mu = \tilde{\mu}_b = -\sqrt{\hat{f}} - 1 \quad \text{see Clavin-Williams 2009 for a more general condition: radiation condition}
\]
Multidimensional stability analysis (analytical expressions)

Analytical expressions for the linear growth rate vs the wave number, written $\sigma(\kappa)$ in non-dimensional form, can be obtained for a simplified reaction rate, assuming that it depends on temperature only at the Neumann state

$$\dot{w}(\theta, \psi) \approx \dot{w}(\theta_N, \psi) \quad \text{with} \quad (E/k_B T_N)(T_b - T_u)/T_b = O(1)$$

This approximation is well verified for the main mechanism of instability that is associated with the variation of the induction length

**Model equation**

Then the linear problem is reduced to solve a single ODE of second order (with variable coefficients)

$$\frac{d^2 Y}{d\zeta^2} - \sigma \frac{dY}{d\zeta} - \frac{\kappa^2}{2} |\vec{\mu}| Y = \frac{1}{2} \frac{d\Omega}{d\zeta} + \frac{\sigma}{2} \frac{h|\vec{\mu}|}{\Omega'}$$

where $d\zeta = d\xi/|\vec{\mu}(\xi)|$, $\Omega(\xi)$ is the distribution of heat release rate in the steady state and $\Omega'_N(\xi)$ is the distribution denoting the thermal sensitivity (see p.8 lecture XII)

The dispersion relation is obtained by applying the 3 boundary conditions:

$$\zeta = 0 : Y = -2\sqrt{f}, \quad dY/d\zeta = -2\sigma \sqrt{f}, \quad \zeta \rightarrow \infty : Y = 0$$

**Analytical result**

The equation for $\sigma$ becomes polynomial for a particular example $\Omega(\xi) = \frac{\xi^n}{n!} e^{-\xi}$, $\Omega'_N(\xi) = \frac{d(\xi \Omega)}{d\xi}$ and $|\vec{\mu}| \approx 1$

$$\frac{4}{H} \left(1 + \frac{\sigma + \sqrt{\sigma^2 + 2\kappa^2}}{2}\right)^{n+2} = H\sigma + \left(1 + \frac{\sigma + \sqrt{\sigma^2 + 2\kappa^2}}{2}\right)$$

The multidimensional instability develops at a finite wave length (larger than the detonation thickness by a factor $(M_u^2 - 1)^{-1/2}$) when increasing the thermal sensitivity $\beta_N$ or the induction length $n$. The Poincaré-Andronov (Hopf) bifurcation occurs before the planar instability with a pulsating frequency larger than the transit time by a factor $(M_u^2 - 1)^{-1}$

Bifurcation scenario similar to that of the strongly overdriven regimes

see the scaling of length and time p.11