Combustion Physics
(Day 4 Lecture)

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Day 4: Laminar Premixed Flames

1. The standard premixed flame
   1. Phenomenological and asymptotic analyses
   2. Parametric dependence
   3. Chemical structure

2. Limit phenomena
   1. The S-curve concept
   2. Extinction through volumetric heat loss

3. Aerodynamics of flames
   1. Hydrodynamic stretch
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1. The Standard Premixed Flame
Structure of (Standard) Premixed Flame

1. Hydrodynamic, Rankine-Hugoniot level (strong discontinuity):
   - Flame sheet
   - Uniform upstream and downstream states

2. Reaction-sheet level (weak discontinuity):
   - Additional preheat, diffusion zone of thickness $\ell^o_D$ : reaction frozen due to large $T_a$, diffusion-convection controlling

3. Complete structure
   - Additional reaction zone: $\ell^o_R << \ell^o_D$ for large activation energy
   - Convection negligible relative to diffusion due to small $\ell^o_R$, diffusion-reaction controlling
   - System is conservative

\[ f = \rho u = \rho_u u^o_u = \rho_b u^o_b, \quad c_p (T^o_b - T_u) = q_c Y_u \]
Flame Characteristics (1/5)

- Characteristic temperature change across reaction zone

\[
(\Delta T)_R = [T_b^o - T(x_f^-)] \sim [w/(dw/dT)]_{T_b^o} = (T_b^o)^2/T_a \\
\]

\[
w \sim \exp(-T_a/T) \\
\]

- Continuity of heat flux through preheat and reaction zones

\[
\frac{\ell^o_R}{\ell^o_D} \sim \frac{(\Delta T)_R}{T_b^o - T_u} = \frac{(T_b^o)^2}{(T_b^o - T_u)T_a} = Ze^{-1} \ll 1. 
\]

(7.2.5)
Flame Characteristics (2/5)

- Convection and diffusion balance in preheat zone:

\[
(f^o \frac{d}{dx} \sim \frac{d}{dx}[(\frac{\lambda}{c_p}) \frac{d}{dx}], \quad f^o \sim (\frac{\lambda}{c_p}) \frac{d}{dx})
\]

\[
f^o \sim \frac{\lambda}{c_p} \frac{d}{\ell^o_D}.
\]

(7.2.6)

- Overall mass flux conservation:

Reactant mass flux entering flame \((Y_u f^o)\) =

Reaction flux through reaction zone \((Y_u w_b^o \ell^o_R)\)

\[
\Rightarrow \quad f^o \sim w_b^o \ell^o_R.
\]

(7.2.7)
Flame Characteristics (3/5)

- Solving for $f^o$ and $\ell^o_D$ from (7.2.6) and (7.2.7), using (7.2.5)

\[
(f^o)^2 \sim \frac{(\lambda / c_p)w^o}{Ze}, \quad (\ell^o_D)^2 \sim \frac{(\lambda / c_p)}{w^o}Ze
\]  

(7.2.8, 9)

- Results show three fundamental quantities governing flame response
  - $\lambda/c_p$ : diffusion
  - $w^o_b$ : reaction
  - $Ze$ : activation ($T_a$) and exothermicity ($T_b^o$)
Flame Characteristics (4/5)

- Propagation rate, which is a response of the flame, is the geometric average of the diffusion and reaction rates, which are the driving forces in forming the flame.

  \[ f^o \sim \sqrt{\left(\frac{\lambda}{c_p}\right)w^o_b} \]

- Dependence on transport:
  - Nonpremixed flame: \( f^o \sim \frac{\lambda}{c_p} \); diffusion dominating
  - Premixed flame: \( f^o \sim \sqrt{\frac{\lambda}{c_p}} \); “diluted” by reaction

- (7.2.8) and (7.2.9) can be alternately expressed as
  - \( f^o \ell^o_D \sim \frac{\lambda}{c_p} \): depends only on transport
  - \( \frac{f^o}{\ell^o_p} \sim \frac{w^o_b}{Ze} \): depends only on reaction
Since there are only two controlling processes (diffusion and reaction: $\lambda / c_p, w_b^o$), flame characteristics are described by two independent relations, which can be expressed in three different ways to convey different messages:

- **Balance of processes:**
  
  \[ f^o \sim \frac{\lambda / c_p}{\ell^o_D}, \quad f^o \sim w_b^o \ell^o_R \]

- **Explicit expressions for the responses:**
  
  \[ (f^o)^2 \sim \frac{(\lambda / c_p) w_b^o}{Z e}, \quad (\ell^o_D)^2 \sim \frac{(\lambda / c_p) w_b^o}{Z e} \]

- **Explicit dependence on individual processes:**
  
  \[ f^o \ell^o_D \sim \lambda / c_p, \quad \frac{f^o}{\ell^o_D} \sim \frac{w_b^o}{Z e} \]
Specific Dependence on Pressure

- $w_b^o \sim p^n; \lambda / c_p$ pressure insensitive
- $f^o \sim [(\lambda / c_p)w_b^o]^{1/2} \sim (w_b^o)^{1/2} \sim p^{n/2}$, $s_u^o \sim f^o / \rho_u \sim f^o / p \sim p^{(n-1)/2}$
  
  $\ell_D^o \sim (\lambda / c_p / w_b^o)^{1/2} \sim p^{-n/2}$

- Implications:
  - For $n = 2$: $s_u^o \neq f(p)$; cancellation between density and reaction; this is not a fundamental result
  - For $0 < n < 2$: $f^o$ increases and $s_u^o$ decreases with increasing $p$
  - Dependence of $\ell_D^o$ on $p$ is through reaction, not diffusion
Asymptotic Analysis
Governing Equations \((Le = 1)\) \((1/2)\)

- **Dimensional:**
  \[
  f^o c_p \frac{dT}{dx} - \lambda \frac{d^2 T}{dx^2} = q_c w,
  \]
  \[
  f^o \frac{dY}{dx} - \rho D \frac{d^2 Y}{dx^2} = -w
  \]

- **Nondimensional:**
  \[
  \frac{d^2 \tilde{T}}{d\tilde{x}^2} - \frac{d\tilde{T}}{d\tilde{x}} = -D \alpha^o_c \tilde{Y} e^{-\tilde{T}/\tilde{T}_o},
  \]
  \[
  \frac{d^2 (\tilde{T} + \tilde{Y})}{d\tilde{x}^2} - \frac{d (\tilde{T} + \tilde{Y})}{d\tilde{x}} = 0; \quad Le = 1
  \]
  \[
  Da^o_c = \frac{\lambda / c_p}{\left(f^o\right)^2} B_c, \quad \tilde{x} = \frac{f^o}{\lambda / c_p} x,
  \]

- **B.C.** :
  \[
  \tilde{x} = -\infty: \quad T = T_u, \quad \tilde{Y} = 1,
  \]
  \[
  \tilde{x} = \infty: \quad T = T_b, \quad \tilde{Y} = 0,
  \]
  \[
  \tilde{x} = \pm \infty: \quad \frac{dT}{d\tilde{x}} = \frac{d\tilde{Y}}{d\tilde{x}} = 0.
  \]
Governing Equations (2/2)

- Integrating (7.3.5’) once; with b. c. at $\tilde{x} = -\infty$,

$$\frac{d(T + \tilde{Y})}{dx} = \frac{d(T + \tilde{Y})}{dx} = (T_a + 1). \quad (7.3.10’)$$

  o Evaluating (7.3.10’) at $\tilde{x} = +\infty$ yields $T_{ad}$: $T_b^o = 1 + T_u = \hat{T}_{ad}$

- Integrating (7.3.10’) again:

$$T + \tilde{Y} = T_b^o + c_1 e^{\hat{x}} = T_b^o \quad \text{for boundedness at } \hat{x} = \infty$$

- Substituting $\hat{Y} = \tilde{T}_b^o - \tilde{T}$ into (7.3.4) yields the single equation that needs to be solved:

$$\frac{d^2 \tilde{T}}{dx^2} - \frac{d \tilde{T}}{dx} = -D a_c \left( T_b^o - \tilde{T} \right) e^{-\hat{T}_a/\hat{T}} \quad (7.3.13)$$

  o This is why $\beta = \hat{T} + \hat{Y}$ is called a (de-)coupling function
The Cold Boundary Difficulty

• Evaluating\[\frac{d^2\tilde{T}}{d\tilde{x}^2} - \frac{d\tilde{T}}{d\tilde{x}} = -D a_c^0 \tilde{Y} e^{-\tilde{T}/T_{\infty}},\] (7.3.4)

at the \(\tilde{x} = -\infty\) freestream, where

- \(\frac{d^2\tilde{T}}{d\tilde{x}^2} = 0, \frac{d\tilde{T}}{d\tilde{x}} = 0 \Rightarrow LHS = 0\)
- \(\tilde{Y} = 1, \tilde{T} = \tilde{T}_{-\infty} \Rightarrow RHS \neq 0\)

Thus the governing equation is unbalanced \(\Rightarrow\) ill posed

• Difficulty exists for many steady-state problems with premixture at ambience: reactive ambience has infinite time to react \(\Rightarrow\) all reactants would be reacted before arrival of flame \(\Rightarrow\) unphysical posing of problem

• Recourse
  - Artificial suppression of reaction term at \(\tilde{x} = -\infty\)
  - Asymptotic analysis: Rational freezing of reaction at \(\tilde{x} = -\infty\)
    due to large activation energy.
Distinguished Limit (1/2)

• Asymptotic analysis capitalizes on the largeness of activation energy which localizes reaction to a thin zone.
• Consider reaction rate: \( \tilde{w} \sim Da_c \tilde{Y} e^{-\tilde{T}_a/\tilde{T}} \)
• For \( \tilde{T}_a >> 1 \to \infty \) and \( Da_c \tilde{Y} \) fixed, \( \Rightarrow \tilde{w} \to 0 \) \( \Rightarrow \)
• No reaction in the reaction zone, obviously wrong!
• Thus the limit \( \tilde{T}_a \to \infty \) must be taken rationally
Distinguished Limit (2/2)

- Distinguished limit:
  \[ T_a \to \infty \text{ requires } D a_c \to \infty \text{ such that } \tilde{w} \text{ is fixed.} \]

- Express \( D a_c \sim D a e^{T_a / T_b^o} \)

  Then
  \[ \tilde{w} \sim D a \exp \left[ T_a \left( \frac{1}{T_b^o} - \frac{1}{T} \right) \right] \approx D a \exp \left[ -Z e \left( T_b^o - \tilde{T} \right) \right] \]

- Thus for \( \tilde{w} \) to remain fixed, \( Z e \to \infty \) requires

  \[ \tilde{T} \to \tilde{T}_b^o \Rightarrow \text{thin reaction zone} \]
Procedure for Asymptotic Analysis

• Separately obtain (partial) solutions for the three zones:
  o Broad upstream, convective-diffusive, preheat zone, subject to b. c. at $\tilde{x} = -\infty$ only. No downstream b. c.
  o Thin reactive-diffusive zone, without any b. c.
  o Broad downstream, equilibrium zone.

• Partial solutions determined to leading order of reaction sheet ($Ze \to \infty$) and next order of broaden reaction zone ($Ze >> 1$, but finite)

• Asymptotically match these partial solutions to determine the various boundary conditions, hence completing the solutions
Structure Equation for Inner, Reaction Zone (1/2)

• Define inner “stretched” variable and inner solution for reaction zone as

\[
\chi = \tilde{x} / \varepsilon = O(1) \quad \tilde{T}_{in}(\chi) = \theta_o - \varepsilon \theta_1(\chi) + O(\varepsilon^2)
\]

• Then G.E. becomes

\[
- \frac{d^2 \theta_1}{d \chi^2} + \varepsilon \frac{d \theta_1}{d \chi} = - \left( \varepsilon^2 Le Da^o \right) \theta_1 e^{-\varepsilon Ze \theta_1}.
\]

• Observations:
  o Diffusion term: \(O(1)\); Convection term: \(O(\varepsilon)\)
  o To retain exponential nonlinearity essential to chemical reaction: \(\varepsilon Ze \sim O(1) \Rightarrow \varepsilon \sim Ze^{-1}\) identified
  o For reaction term to be \(O(1)\) in order to balance diffusion term:

\[
\varepsilon^2 Da^o \sim O(1) \Rightarrow Da^0 \sim \varepsilon^{-2}
\]

  o \(\varepsilon^2\): one \(\varepsilon\) from thin zone, one \(\varepsilon\) from reduced concentration
Structure Equation for Inner, Reaction Zone (2/2)

- Final structure equation:
  \[ \frac{d^2 \theta_1}{d \chi^2} = \frac{\Delta^o}{2} \theta_1 e^{-\theta_1}, \quad \Delta^o = \frac{2LeDa^o}{Ze^2}. \]  
  (7.5.44,45)

- Solution:
  \[ \frac{d}{d \theta_1} \left( \frac{d \theta_1}{d \chi} \right)^2 = \Delta^o \theta_1 e^{-\theta_1} \]  
  (7.5.16)

  Integrating with b. c.: \( \theta_1 = d \theta_1 / d \chi = 0 \) at \( \chi \to \infty \)

  \[ \left( \frac{d \theta_1}{d \chi} \right)^2 = \Delta^o \int \theta_1 e^{-\theta_1} d \theta_1 + c_{in} = -\Delta^o (1 + \theta_1) e^{-\theta_1} + c_{in}. \]  
  (7.5.47)

  Evaluating at \( \chi \to \infty \)

  \[ \lim_{\chi \to -\infty} (1 + \theta_1) e^{-\theta_1} = \lim_{\chi \to -\infty} \left[ 1 - (c_1^- + \chi) \right] e^{(c_1^- + \chi)} = 0 \]  
  (7.5.48)

  Final result: \( \Delta^o = 1 \)

  In physical terms:

  \[ (f^o)^2 = \frac{2(\lambda / c_p) B_c}{Ze^2} e^{-T_a / T_b^o} \]

  Phenomenological derivation only missed the term \( 2Le / Ze \)
Dependence on $T_{\text{ad}}$

- Correlates well with $T_{\text{ad}}$ through heat of combustion
  - Equivalence ratio
  - C/H ratio
Dependence on $Le$

- More rigorous derivation shows $(f^o)^2 \sim Le$
  - Concentration effect
  - $T_f \equiv T_{ad}$ is not affected for the standard flame, hence weak effect; exaggerated for hydrogen ($Le_{lean} \approx 0.3$, $Le_{rich} \approx 2.3$)
  - Effects are more significant for stretched flames for which $T_f$ is affected
Dependence on Molecular Structure

- Flame speed increases with ethane ($C_2H_6$), ethylene ($C_2H_4$), and acetylene ($C_2H_2$).

Air as oxidizer

Modified air to match $T_{ad}$

![Graphs showing laminar flame speed ($S_f$) vs. equivalence ratio ($\phi$) for different fuels under different air conditions.](image-url)
Dependence on Pressure

- Dependence of flame speed on pressure is through
  - Chemistry
  - Density
- Observed decreasing trend of flame speed with pressure is density effect, not chemistry effect
- $f^o$ is the proper parameter because it is only affected by chemistry
- $f^o$ usually increases with increasing pressure
Dependence on Transport Properties

• Flame speed can be manipulated through inert substitution, while keeping oxygen mole fraction fixed
  o $N_2$ and Ar have similar molecular weights and hence diffusivities, but different $c_p$, which affects the flame temperature.
  o Ar and He have the same $c_p$ but different diffusivities and densities
Extraction of Global $n$ and $E_a$

\[ n = 2 \left( \frac{\partial \ln f^o}{\partial \ln p} \right)_{T_{ad}}. \]

\[ E_a = -2 R^o \left[ \frac{\partial \ln f^o}{\partial (1/T_{ad})} \right]_p. \]

- Results demonstrate the role of pressure on two-body branching (promoting with pressure) and three-body termination (retarding with pressure) reaction
- Note: possible $n < 0$
Chemical Structure of Flames
Asymptotic versus Chemical Structure

- Asymptotic Structure
  - Broad, convective-diffusive, nonreactive zone followed by:
  - Narrow, diffusive-reactive zone at downstream end of flame
  - One-step overall reaction accounts for both activation and heat release
  - Chemical activation is thermal in nature
Asymptotic versus Chemical Structure

• Chemical Structure (with chain mechanism)
  o Termination reaction is temperature insensitive ⇒ can occur in upstream diffusive zone ⇒ reactions take place throughout entire flame structure
  o Termination reactions can be highly exothermic ⇒ substantial heat release in preheat zone
  o Chemical activation through radicals produced at downstream, high-temperature end that back diffuse to the preheat zone
  o In homogeneous system initiating radicals are produced by original fuel-oxidizer species.
Premixed H$_2$-Air Flame: Diffusive Structure

- H$_2$ diffusion layer is thicker than those of O$_2$ and heat (T) because of its high diffusivity.

- Rapid reduction in H$_2$ concentration (due to diffusion, not reaction) causes a bump in mole fraction of O$_2$. This is not physical, just definitional (on mole basis)
Chain Structure

- **Active reaction zone:** 0.04 cm to 0.1 cm; two zone structure

- **Trailing, H production zone**
  - $\text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H}$; $\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$
  - H back diffuses

- **Leading, H consumption zone**
  - Back-diffused H reacts with O$_2$ at low temperature through $\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$.
  - HO$_2$ subsequently forms H$_2$O$_2$,
  - Contrasts with $\text{H}_2 + \text{O}_2 \rightarrow \text{HO}_2 + \text{H}$ in homogeneous system.

- **Maximum consumption rates of** $\text{H}_2:\text{O}_2 = 2:1$; occurring at same location

- **H$_2$O generated through entire reaction zone.**
Thermal Structure

- Major exothermic reactions
  - H consumption layer,
    \[ \text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M} \]
  - H production layer
    \[ \text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H} \]
- Major endothermic reaction
  - H+O\(_2\)→OH+O
    which is the major branching step
- Maximum heat release occurs at 800 K!
- 30% heat released in H consumption layer, at 1000 K
- Chemical activation, indicated by maximum H production rate, occurs around 1400 K.
Summary of Contrasts with Asymptotic Structure

• Important reactions occur throughout flame structure

• H radical needed for initiation at leading edge is produced in the downstream and back diffuses

• Maximum heat release occur at front of the active reaction zone

• Substantial heat evolved in the moderately low temperature region of the flame
2. Limit Phenomena
Concepts of Ignition & Extinction

- **Thermal runaway**: Feedback loop involving nonlinear Arrhenius heat generation and linear heat loss
- **Radical runaway**: Radical proliferation through chain branching
- **Unsteady (ignition) analysis**: Tracking the temporal evolution of a reacting mixture upon application of ignition stimulus
- **Steady, S-curve analysis**: Identify states at which steady solution does not exist for a non-reacting situation, signaling ignition, or a strongly burning situation, signaling extinction
- **Ultimate (extinction) consideration**: system adiabaticity
Principle of Well-Stirred Reactor

- In steady-state operation:

\[
\dot{V} \rho_o c_p (T_f - T_o) = V Q_c B c_F e^{-T_a/T_f} \\
\tilde{T} - \tilde{T}_o = D a_c (T_{ad} - T_f) e^{-\tilde{T}_a/\tilde{T}_f},
\]

\[
D a_c = \frac{B}{V/V} = \frac{\text{Characteristic flow time}}{\text{Characteristic collision time}}
\]

- Using:

\[
\tilde{T} = \tilde{T}_{ad} - \tilde{c}_F
\]

- Solutions:

1: Weakly-reactive state
2: Strong-burning state
I: Ignition state
E: Extinction state
3: Triple solution \(\Rightarrow\) nonmonotonicity and hysteresis
Concept of S-Curve

• Ignition/extinction turning points defined by

\[
\left( \frac{d \ln D a_c}{dT_f} \right)_{cr} = 0
\]

• (8.1.23) yields the two roots

\[
\tilde{T}_{f, cr} = \frac{(\tilde{T}_{ad} + \tilde{T}_o) \pm \{1 - 4(\tilde{T}_o \tilde{T}_{ad} / \tilde{T}_a)\}^{1/2}}{2(1 + 1 / \tilde{T}_a)}
\]  \hspace{1cm} (8.1.29)

• Folding possible when \{\cdot\} > 0 in (8.1.29). Otherwise S-curve is stretched for:
  o Low activation energy reactions
  o High initial temperatures
Premixed Flame Extinction (through Heat Loss) (1/3)

• The standard flame, being adiabatic, does not exhibit any extinction behavior, i.e. finite $f^o$ for finite $Y_u$.

• Heat loss lowers flame temperature from $T_{ad}$, leading to abrupt extinction, at finite $Y_u$. System becomes non-conservative.

• Radiation from flame is an inherent heat loss mechanism.

• Assume loss occurs only in the preheat zone, and with $L$ being a loss coefficient, then amount of loss is

$$ q^- = \int_0^\ell L \, dx \approx \ell D L \approx \frac{\lambda}{c_p} \frac{L}{f} $$
Premixed Flame Extinction (2/3)

- Overall energy conservation

  \[ f c_p (T_{ad} - T_u) = f c_p (T_f - T_u) + \frac{\lambda / c_p}{f} L . \]  
  \[ T_f = T_{ad} (1 - \frac{\lambda / c_p^2}{f^2 T_{ad}} L) = T_{ad} (1 - L' / f^2) \]  

- In analogy to standard flame result

  \[ (f^o)^2 = \frac{(\lambda / c_p) w^o}{Z e} ; \quad w^o = \exp(-E_a / R^0 T_{ad}) \]  

  we can write

  \[ (f)^2 = \frac{(\lambda / c_p) w}{Z e} ; \quad w = \exp(-E_a / R^0 T_f) \]  

- Using (8.4.4’) in \( w \)

  \[ \dot{w} \sim \exp[(-(E_a / R^0) / (1 - L' / f^2))] = \exp(-E_a / R^0) \exp(-\dot{L} / f^2) \]  
  \[ \dot{L} = (E_a / R^0) L' \]
Premixed Flame Extinction (3/3)

- C/B using D:
  \[ \tilde{f}^2 = \left( \frac{f}{f^0} \right)^2 = w / w^0 = \exp\left(-\tilde{L} / \tilde{f}^2\right), \]

  from which \[ \tilde{f}^2 \ln \tilde{f}^2 = -\tilde{L}. \] (8.4.9)

- (8.4.9) is the generalized equation governing flame propagation with loss.

  - For \( \tilde{L} = 0, \tilde{f} = 1, f = f^0 \)

  - Extinction, turning point:
    \[ \left( \frac{dL}{df^2} \right)_x = 0 \]

  - Solving:
    \[ \tilde{L}_E = e^{-1}, \tilde{f}_E = e^{-1/2} \]
Other Limit Phenomena

- Flammability Limits:
  - For given mixture temperature and pressure, the leanest and richest concentrations beyond which flame propagation is absolutely not possible
  - Set the ultimate boundaries for extinction

- Blowoff and Flashback
  - Consequence of lack of dynamic balance between flame speed and flow speed
  - Has nothing to do with extinction and ignition
Flammability Limit

- Simulation for methane/air mixtures shows
  - Extinction $\phi = 0.493$
    - empirical: $\phi = 0.48$
  - $f/f^o = e^{-1/2} \approx 0.6$
  - $(T_f)_{ext} \approx 1,450$ K

- Extinction temperature result corroborates with the concept of limit temperature for hydrocarbon fuels
Stabilization Mechanism of Premixed Flame at Burner Rim

- Gas stream
- Profile of gas velocity $u_v$
- $s_u < u_u$
- Combustion wave
- $s_u = u_u$
- $s_u > u_u$
- Solid rim
- Open atmosphere
Triple-Flame Stabilization Mechanism of Nonpremixed Flame at Burner Rim
3. Aerodynamics of Laminar Flames
Standard Flame vs. Real Flame (1/2)

Hydrodynamic Limit

Reaction-Sheet Limit
Standard Flame vs. Real Flame (2/2)

• Standard 1D Planar Flame
  - \( f^o = f^o(q_c, Le_{i,j}, w_k) \)
  - System is conservative, \( T_b^o = T_b^o(q_c) \)
  - \( f^o \sim \sqrt{Le_{i,j}} \)

• General Stretched Flame
  - \( f = f(q_c, Le_{i,j}, w_k; Ka, L) \)
    - \( Ka \): Karlovitz number, representing aerodynamic effects of flow nonuniformity, flame curvature, flame/flow unsteadiness
    - \( L \): Generalized loss parameter
  - System could become locally or globally nonconservative
    - \( T_b = T_b(q_c, Le_{i,j}, w_k; Ka, L) \)
  - \( O(\varepsilon) \) modification of flame temperature leads to \( O(1) \) change in flame speed \( \Rightarrow \) locally intensified burning or extinction
The Stretch Rate

- Definition: Lagrangian time derivative of the logarithm of area $A$ of a surface

$$\kappa = \frac{1}{A} \frac{dA}{dt}$$

$$A(p,q,t) = (e_p dp) \times (e_q dq) = (dp dq)n$$

- Letting

$$v_{f,t} = v_{s,t}$$

$$\kappa = \nabla_t \cdot v_{s,t} + (V_f \cdot n)(\nabla \cdot n)$$

$$v_{s,t} = n \times (v_s \times n)$$

- Sources of stretch:
  - Flow nonuniformity: $v_s$
  - Flame curvature: $n$
  - Flame oblique to flow: $v_s \times n \neq 0$.
  - Flame unsteadiness ($V_f \neq 0$), with curvature $\nabla \cdot n \neq 0$
Examples of Stretched Flames

- **Stagnation Flame:** \( v = \left\{ \frac{a}{(k+1)} x, -a y, 0 \right\}, \kappa = a > 0 \)

- **Expanding Spherical Flame:** \( \kappa = \frac{2}{R_f} \frac{dR_f}{dt} > 0 \)

- **Bunsen Flame:** \( \kappa = \frac{w \sin 2a}{2R_f} < 0 \)

- Each of above has its opposite analog
Effects of Stretch (1/2)

• Hydrodynamic stretch: Flame-sheet limit
  o **Tangential velocity gradient**: changes flame surface area and hence total burning rate, $\int f \, dA$
  o **Normal velocity**: Balances flame speed
  o **Net effect**:
    Distortion of flame geometry
    Modifies total burning rate (e.g. higher burning rate in turbulent flame through surface wrinkling)
Effects of Stretch (2/2)

- Flame stretch: reaction-sheet limit
  - Tangential velocity affects normal mass flux $f_b$ entering reaction zone
  - For $Le\neq 1$, modifies temperature and concentration profiles differently $\Rightarrow$ modifies total enthalpy and flame temperature
    $\Rightarrow$ locally non-conservative

- Hydrodynamic stretch and flame stretch strongly coupled

- Stretch (i.e. convection) in thin reaction zone is unimportant
Example of Hydrodynamic Stretch: Corner Formation in Landau Propagation

- Landau propagation: \( s_u = s_u^o \)
- Concave segment develops into a corner; convex segment flattens
- Positive curvature and hence stretch dominate
- Mathematically described by Burgers equation, similar to that for shock formation

Flame Evolution with \( f_\theta(\hat{x}) = -\cos \hat{x} \)
Flame Stretch due to Flow Straining: The Stagnation Flame (1/2)

- Stretch is positive, $\kappa > 0$; situation reversed for $\kappa < 0$
- Consider total energy conservation in control volume
  - Diffusion: normal to reaction sheet
  - Convection: along (divergent, $\kappa > 0$) streamline
- $Le > 1$: More heat loss than reactant mass gain $\Rightarrow$ system sub-adiabatic
- With increasing $\kappa$:
  - Flame temperature decreases, until extinction
  - Flame at finite distance from stagnation surface at extinction
  - Complete reactant consumption at extinction
The Stagnation Flame (2/2)

- $Le < 1$: More reactant mass gain than heat loss $\Rightarrow$ system super-adiabatic

- With increasing $\kappa$:
  - Flame temperature increases, extinction not possible as long as the flame is away from surface
  - Eventually flame is pushed to the stagnation surface, leading to incomplete reaction and eventually extinction
Flame Stretch due to Flame Curvature: The Bunsen Flame

- For the concave flame curvature, $\kappa < 0$; expect opposite response from the $\kappa > 0$ stagnation flame
- (Negative) flame curvature focuses heat and defocuses mass in the diffusion zone
  - $Le > 1$: Super-adiabatic, burning at flame tip intensified relative to shoulder
  - $Le < 1$: Sub-adiabatic, burning at tip weakens, lead to extinction (i.e. tip opening)
Flame Stretch due to Flame Motion: the Unsteady Spherical Flame

- For the expanding flame, $\kappa > 0$; expect similar behavior as the stagnation flame.

- An increase in flame radius $R_f$ by $\delta R_f$ leads to an increased amount $(4\pi R_T^2 \delta R_f)$ of heat transferred to the preheat zone, and $(4\pi R_M^2 \delta R_f)$ of mass transferred.
  - $Le > 1$: Sub-adiabatic, more heat transferred away
  - $Le < 1$: Super-adiabatic, less heat transferred away

- Stretch rate, $\kappa = \left(\frac{2}{R_f}\right)(dR_f/dt)$
  continuously decreases
  with increasing $R_f$
  approaching the planar limit
Analysis (1/2)
(Based on Stagnation Flame Analogy)

• Energy loss/gain in control volume

\[ f_u c_p (T_{ad} - T_f) = (\lambda \frac{T_f - T_u}{\ell_T}) - (q_c \rho D \frac{Y_u}{\ell_M}) \frac{\kappa}{s_u / \ell_T} \]

- Normal heat flux; loss
- Normal chemical energy flux; gain
- Fraction of flux diverted out of control volume due to stretch

• In nondimensional form

\[ \tilde{T}_{ad} - \tilde{T}_f = -Ka^0 \frac{Le^{-1} - 1}{f^2} = -S^0 / \tilde{f}^2 \]  

(A)

- \[ S^0 = Ka^0 (Le^{-1} - 1) \]
- Karlovitz number, \[ Ka^0 = \kappa / (s_u^0 / \ell^0_T) \]; nondimensional stretch rate
Analysis (2/2)

- Following same analysis as that for premixed flame with heat loss, yields

\[ \frac{f_u^2}{\tilde{f}_u^2} \ln \frac{f_u^2}{\tilde{f}_u^2} = \sigma^o, \quad \sigma^o = Ze^o S^o = Ze (Le^{-1} - 1) Ka^o \]

- \(-\sigma^o\) has the same role as \(L\) in (8.4.9), showing extinction for \(\sigma < 0\) (i.e. loss due to stretch)

- Further define **Markstein number** as

\[ Ma^o = Ze^o (Le^{-1} - 1) \]

- Then: \(\sigma^o = Ma^o Ka^o\)
Response of Stretched Flame

- From (A): $T_f(>,<) T_{ad}$ for $S^o(,<,>)0$
  Since $S^o=(Le^{-1}-1)Ka^o$, influence is lumped for nonequidiffusion and stretch.
  
  $T_f > T_{ad}$ for $(Ka^o > 0, Le < 1)$ or $(Ka < 0, Le > 1)$
  $T_f < T_{ad}$ for $(Ka^o > 0, Le > 1)$ or $(Ka < 0, Le < 1)$
  $T_f \equiv T_{ad}$ for either $Ka^o = 0$ ($Le \neq 1$) or $Le = 1$ ($Ka \neq 0$)

- Super-lumped parameter for flame speed:
  
  $\sigma^o = Ze^o(Le^{-1}-1)Ka^o$:
  Reactivity $\times$ nonequidiffusivity $\times$ stretch

- Markstein number, $Ma^o=Ze^o(Le^{-1}-1)$:
  Reactivity $\times$ nonequidiffusivity; a property of the mixture.
Results on Stretched Equidiffusive Flame

- Stretched flame ($\kappa \neq 0$) for equidiffusive mixture ($Le = 1$) is not affected by stretch:

$$S^0 = (Le^{-1} - 1)\kappa \equiv 0$$
## Nonequidiffusive Mixtures

<table>
<thead>
<tr>
<th>Mixture for Simulation</th>
<th>$Le \neq 1$ Interpretation</th>
<th>$D_i \neq D_j$ Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lean hydrogen–air</td>
<td>$Le_{H_2} &lt; 1$</td>
<td></td>
</tr>
<tr>
<td>Lean methane–air</td>
<td>$Le_{CH_4} &lt; 1$</td>
<td></td>
</tr>
<tr>
<td>Rich propane–air</td>
<td>$Le_{O_2} &lt; 1$</td>
<td>$D_{H_2} &gt; D_{CH_4} &gt; D_{O_2} &gt; D_{C_3H_8}$</td>
</tr>
<tr>
<td>Rich hydrogen–air</td>
<td>$Le_{O_2} &gt; 1$</td>
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<td></td>
</tr>
</tbody>
</table>
Results on Stretched Nonequidiffusive Flame

(a) Counterflow flame
(b) Outwardly propagating flame
(c) Inwardly propagating flame
Flame Images

\[ \kappa > 0 \]

(a) Lean methane-air: \( Le < 1, S^o > 0 \)

(b) Rich methane-air: \( Le > 1, S^o < 0 \)

(c) Lean propane-air: \( Le > 1, S^o < 0 \)

(d) Rich propane-air: \( Le < 1, S^o > 0 \)

\[ \kappa < 0 \]
Further Implications of Stretched Flame Phenomena

- Determination of laminar flame speeds
- Concentration and temperature modifications in flame chemistry
- Flame stabilization and blowoff
Flame Front Instabilities (1/2)

Diffusional Thermal Instability

Hydrodynamic Instability (Flame sheet, constant flame speed; density jump)
Flame Front Instabilities (2/2)

Diffusional-Thermal
Le<1 Le>1

DL Diffusional-Thermal Le>1 Le<1

DL
Le>1
Closing Remarks of Day 4 Lecture (1/2)

• The standard premixed flame
  o **Concepts introduced**: asymptotic analysis; cold boundary difficulty; distinguished limit; flame structure based on one-step and detailed chemistry; extraction of global kinetic parameters

• Further studies:
  o Need chemical structure of hydrocarbon flames
  o Explain the lack of influence on laminar flame speed by: (a) low-temperature chemistry, and (b) molecular size for large n-alkanes
  o Is it possible to derive a semi-empirical expression for the laminar flame speed based on $T_{ad}$ and extracted global kinetic parameters?
Closing Remarks of Day 4 Lecture (2/2)

- **Limit phenomena**: Extinction is due to insufficient reaction time while flame blowoff/out is due to imbalance between flame and flow speeds
- Extinction is in general caused by enthalpy loss in the preheat zone, leading to $O(\varepsilon)$ reduction in flame temperature and $O(1)$ reduction in flame speed
- Need to distinguish flame stabilization by auto-ignition or flame holding
- **What is the fate of a freely-propagating flame to increasing strength of imposed strain rate?**
- Need detailed study of the chemical structure of stretched flames
! Daily Specials !
1. Low-temperature, NTC flames
2. Pulsations in premixed and diffusion flames:
   a. Extinction
   b. Spiral patterns
3. Pulsation in self-propagating high-temperature synthesis
1. Low-temperature, NTC Flames
The Issue

- NTC behavior observed for homogeneous mixtures in low- to intermediate-temperature range

- NTC behavior not observed in extensive counterflow experiments & simulations
  - Finite residence time shifts ignition temperature to >1000K, hence moves ignition chemistry out of the NTC regime
  - Can NTC behavior be manifested for:
    - Low strain rate flows?
    - High pressures?
NTC Behavior Predicted at Low Strain Rates!

Pressure: 1 Atm.

1 atm, \( k = 200/s \)

1 atm, \( k = 100/s \)
NTC Behavior Exaggerated with Increasing Pressure

At lower pressures, ignition occurs in two stages, final ignition controlled by high-temperature chemistry.

At higher pressures, ignition occurs in one stage, controlled by low-temperature chemistry.
Experimental Observation of Nonpremixed LTC Flame

Infrared Images at Ignition
(1 atm, strain rate: 60/s)

A: Air vs DME
B: N₂ vs DME
C: Ignition (Air vs DME)
D: Ignition (N₂ vs DME)

- Detailed chemical structure study shows that such flames are governed by LTC
Experimental Observation of Premixed LTC Flame

- Different behavior from hot flames
- Insensitive of flame location, implying small variation in flame speed with $\Phi$ variation
- Stronger chemiluminescence for richer cases
2a. Pulsating Extinction of Premixed and Diffusion Flames
The Issue: Heightened Sensitivity Near Extinction

- S-curve analysis is based on steady-state considerations, showing on-off states.
- Near state of extinction, the burning intensity of flame is reduced, implying larger effective activation energies.
- Flamefront pulsating instabilities are also promoted with increasing activation energy.
- Could extinction occur in a pulsating manner, especially for $Le > 1$ flames?
The Issue: Intrinsic Chemical Influence Near Diffusion Flame Extinction

- Finite-rate chemistry plays no role in the reaction-sheet limit of diffusion flames
- Flamefront (pulsating) instability intrinsically requires consideration of finite-rate chemistry
- Since finite-rate chemistry is responsible for extinction, then could extinction occur in a pulsating manner even for diffusion flames, if \( Le > 1 \) for one of the reactants?
Oscillatory Extinction of $Le > 1$

Premixed Flame

Calculated $S$-curve, showing earlier extinction due to pulsation

Calculated extinction dynamics; extinction controlled by steady-state extinction temperature

Experimental observation of oscillatory luminosity
Oscillatory Extinction of Diffusion Flames: Computation

Calculated S-curve, showing earlier extinction due to pulsation

Calculated extinction dynamics; extinction controlled by steady-state extinction temperature
Oscillatory Extinction of Diffusion Flames: Experiment

Steady and oscillatory extinction of diffusion flames experimentally observed
2b. Observations of Spirals over Flame Surfaces
Target Patterns ($Le > 1$)

Experimental conditions:
• Lean butane-air, $\phi = 0.59$
• 30 atm. pressure
• Consecutive frames at framing rate of 15000 fps
• Frame dimension: $2.73\text{cm} \times 5.46\text{cm}$
• Rich hydrogen-air flame ($\phi = 4.30$) at 20 atm.
• Spirals confined within hydrodynamic cells
• Spiral can be either clockwise or counter-clockwise
Magnified View of the Spirals
Disordered Spirals

- Hydrogen-oxygen flame at 30 atm. and $\phi = 6.00$
- Disordered spirals
3. Pulsation in Self-propagating High-temperature Synthesis
Pulsation in Condensed-Phase Flames

- A curious result:
  - Propagation of solid flames exhibit temperature-sensitive Arrhenius behavior, e.g. pulsation
  - But reaction for individual particles is in diffusion flame-sheet limit ⇒ no finite rate chemistry

Laminated product structure due to pulsation
Pulsation in Condensed-Phase Flame

- Explanation: Arrhenius behavior from temperature-sensitive solid-phase diffusivity

- Gas-phase flame speed: \( f_{\text{gas}}^2 \sim (\rho D)_g \omega \sim (\rho D)_g e^{-T_a/T_{ad}} \sim e^{-T_a/T_{ad}} \)

- Condensed-phase flame speed:

\[
f_{\text{SHS}}^2 \sim (\rho D)_s \omega_{\text{SHS}} \sim (\rho D)_s K_c
\]

Since \( K_c = (2 \rho_B D / \rho_A)_s \ln(1 + Y_B / \sigma_O) \sim D_s \) \( \Rightarrow f_{\text{SHS}}^2 \sim D_s^2 \)

But \( D_s \sim e^{-T_d/T} \), therefore: \( f_{\text{SHS}} \sim e^{-T_d/T_{ad}} \)