Combustion Physics
(Day 2 Lecture)

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Day 2: Generalized Formulations

1. Conservation Equations
   1. Derivation and constitutive relations
   2. Simplified diffusion-controlled system
   3. Conserved scalar formulations

2. Discontinuity Surface Formulations
   1. Generalized reaction-sheet formulation
   2. Reaction-sheet analysis of diffusion flames
   3. Rankine-Hugoniot waves in premixtures
1. Conservation Equations
Control Volume Derivation

• Definitions of velocities
  o \( \mathbf{v}_i \) velocity of species \( i \)
  
  \( \mathbf{v} \) mass weighted velocities \( \sum \rho_i \mathbf{v}_i = \rho \mathbf{v} \)
  
  \( \mathbf{V}_i \) molecular diffusion velocity \( \mathbf{V}_i = \mathbf{v}_i - \mathbf{v} \)
  
  o Consequently: \( \sum \rho_i \mathbf{V}_i = \sum \rho_i \mathbf{v}_i - \rho \mathbf{v} \equiv 0 \)
  
  \( \sum \rho_i / \rho \mathbf{V}_i = \sum Y_i \mathbf{V}_i \equiv 0; \ Y_i \): mass fraction

• General equation of change
  
  o (extensive, intensive) fluid property: \( (\Psi, \psi) \)

  \[
  \frac{\delta \Psi}{\delta t} = \frac{\partial}{\partial t} \int_v \psi \, dV + \int_s \psi \left( \mathbf{v} \cdot \mathbf{n} \right) \, dS
  \]

  o Divergence theorem: \( \int_s \psi \left( \mathbf{v} \cdot \mathbf{n} \right) \, dS = \int_v \left( \nabla \cdot \psi \mathbf{v} \right) \, dV \),

  \[
  \frac{\delta \Psi}{\delta t} = \int_v \left( \frac{\partial \psi}{\partial t} + \nabla \cdot \psi \mathbf{v} \right) \, dV .
  \]

(5.1.5)
Conservation of Total Mass

\[ (\Psi = m, \psi = \rho) \]

\[ \frac{\delta m}{\delta t} = \int_V \left( \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) \right) dV. \]

- Mass conserved in chemical reaction: \[ \frac{\delta m}{\delta t} = 0. \]
- Therefore:\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0. \] (5.1.7)

(Continuity equation)
Conservation of Individual Species

\((m_i, \rho_i)\)

\[
\frac{\delta m_i}{\delta t} = \int_v \left( \frac{\partial \rho_i}{\partial t} + \nabla \cdot \rho_i \mathbf{v} \right) \, dV.
\]

- **Sources and sinks of** \(\frac{\delta m_i}{\delta t} :\)
  - Volumetric (from reaction, \(w_i\)): \(\int_v w_i \, dV\)
  - Surface (from diffusion flux, \(\mathbf{v}_i\)): \(-\int_S (\rho_i \mathbf{v}_i \cdot \mathbf{n}) \, dS\)

  \(\mathbf{v}_i \cdot \mathbf{n} > 0 \Rightarrow \text{loss, hence negative sign}\)

- \(\frac{\partial \rho_i}{\partial t} + \nabla \cdot [\rho_i (\mathbf{v} + \mathbf{v}_i)] = w_i, \quad i = 1, 2, \ldots, N. \) \hspace{1cm} (5.1.10)

- **Since** \(\rho_i = \rho Y_i, \)

  \[
  \frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot [\rho (\mathbf{v} + \mathbf{v}_i) Y_i] = w_i
  \]

  or

  \[
  \rho \frac{DY_i}{Dt} = - \nabla \cdot (\rho \mathbf{v}_i Y_i) + w_i,
  \]

  where

  \[
  \frac{D}{Dt} (\cdot) = \frac{\partial}{\partial t} (\cdot) + \mathbf{v} \cdot \nabla (\cdot)
  \]
Conservation of Momentum

\[ (\mathbf{M}, \rho \mathbf{v}) \]

\[
\frac{\delta \mathbf{M}}{\delta t} = \int_V \left( \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) \right) dV.
\]

- **Sources and sinks of** \( \frac{\delta \mathbf{M}}{\delta t} : \)
  - **Surface source (by stress, \( \mathbf{P} \)):** \(-\int_S (\mathbf{P} \cdot \mathbf{n}) \, dS\)
    \[ \mathbf{P} \cdot \mathbf{n} > 0 \implies \text{system exerting force on surrounding, hence negative sign} \]
  - **Volumetric source (by body force, \( \mathbf{f}_i \)):** \(\sum_{i=1}^{N} \int_V \rho_i \mathbf{f}_i \, dV\)

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla \cdot \mathbf{P} + \rho \sum_{i=1}^{N} Y_i \mathbf{f}_i,
\]

\[
\rho \frac{D \mathbf{v}}{D t} = -\nabla \cdot \mathbf{P} + \rho \sum_{i=1}^{N} Y_i \mathbf{f}_i
\]  
(5.1.17)
Conservation of Energy

\[ (E, \rho e + \rho v^2) \]

\[
\frac{\delta E}{\delta t} = \int_V \left[ \frac{\partial \rho (e + \frac{v^2}{2})}{\partial t} + \nabla \cdot \rho \mathbf{v} (e + \frac{v^2}{2}) \right] dV.
\]

- **Sources and sinks of** \(\frac{\delta E}{\delta t}\):
  - **Surface source (by energy flux \(\mathbf{q}\))**
    \[
    Q = -\int_S (\mathbf{q} \cdot \mathbf{n}) dS = -\int_V \nabla \cdot \mathbf{q} dV.
    \]
  - **Surface source (by surface stress)**:
    \[
    W_s = \int_S \mathbf{v} \cdot d\mathbf{F}_s = -\int_S \mathbf{v} \cdot (\mathbf{P} \cdot \mathbf{n}) dS = -\int_V \nabla \cdot (\mathbf{v} \cdot \mathbf{P}) dV.
    \]
  - **Volumetric source (by body force, \(\mathbf{f}_i\))**:
    \[
    W_v = \sum_{i=1}^N \int_V \mathbf{v}_i \cdot d\mathbf{F}_{V,i} = \sum_{i=1}^N \int_V \mathbf{v}_i \cdot (\rho_i \mathbf{f}_i) dV = \sum_{i=1}^N \int_V (\mathbf{v} + \mathbf{V}_i) \cdot (\rho_i \mathbf{f}_i) dV.
    \]

\[
\rho \frac{D\left(e + \frac{v^2}{2}\right)}{Dt} = -\nabla \cdot \mathbf{q} - \nabla \cdot (\mathbf{v} \cdot \mathbf{P}) + \sum_{i=1}^N (\mathbf{v} + \mathbf{V}_i) \cdot (\rho_i \mathbf{f}_i). \tag{5.1.24}
\]
Summary of Conservation Equations

Continuity:
\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \]

Species:
\[ \rho \frac{D Y_i}{D t} = w_i - \nabla \cdot (\rho Y_i \mathbf{V}_i), \quad i = 1, \ldots, N \]

Momentum:
\[ \rho \frac{D \mathbf{v}}{D t} = -\nabla \cdot \mathbf{P} + \rho \sum_{i=1}^{N} Y_i \mathbf{f}_i \]

Energy:
\[ \rho \frac{D e}{D t} = -\nabla \cdot \mathbf{q} - \mathbf{P} : (\nabla \mathbf{v}) + \rho \sum_{i=1}^{N} Y_i \mathbf{f}_i \cdot \mathbf{v}_i. \]

- The conservation equations are supplemented (i.e. completed) by the specifications of:
  - Diffusion velocity, \( \mathbf{V}_i \)
  - Pressure tensor, \( \mathbf{P} \)
  - Heat flux vector, \( \mathbf{q} \)
  - Reaction rate, \( w_i \)
Constitutive Relations

Diffusion velocity, $V_i$

$$\nabla X_i = \sum_{k=1}^{K} \left( \frac{X_i X_j}{D_{i,j}} (V_j - V_i) + (Y_i - X_i) \left( \frac{\nabla p}{p} \right) + \left( \frac{\rho}{p} \right) \sum_{j=1}^{N} Y_j Y_j (f_i - f_j) \right)$$

+ $\sum_{k=1}^{K} \left[ \left( \frac{X_i X_j}{\rho D_{i,j}} \right) \left( \frac{D_{T,j}}{Y_j} - \frac{D_{T,i}}{Y_i} \right) \right] \left( \frac{\nabla T}{T} \right)$, $i = 1, \ldots, N$.  
(5.2.5)

Pressure tensor, $P$

$$P = \left[ p \left( \frac{2}{3} \mu - \kappa \right) (\nabla \cdot v) \right] U - \mu [(\nabla v) + (\nabla v)^T],$$

(5.2.6)

Heat flux vector, $q$

$$q = -\lambda \nabla T + \rho \sum_{i=1}^{N} h_i Y_i V_i + R^T \sum_{i=1}^{N} \sum_{j=1}^{N} \left( \frac{X_j D_{T,i}}{W_i D_{i,j}} \right) (V_i - V_j) + q_R,$$

(5.2.7)

Reaction rate, $w_i$

$$w_i = W_i \sum_{k=1}^{K} (v''_{i,k} - v'_{i,k}) B_k T^{\alpha_k} \exp(-E_{a,k}/R^T) \prod_{j=1}^{N} c^v_{j,k}, \quad i = 1, \ldots, N,$$

(5.2.8)
Discussion on Diffusion Velocity, $V_i$

$$\nabla X_i = \sum_{i=1}^{N} \left( \frac{X_i X_j}{D_{i,j}} \right) \left( \mathbf{V}_j - \mathbf{V}_i \right) + \left( Y_i - X_i \right) \left( \frac{\nabla p}{p} \right) + \left( \frac{\rho}{p} \right) \sum_{j=1}^{N} Y_i Y_j \left( \mathbf{f}_i - \mathbf{f}_j \right)$$

$$+ \sum_{j=1}^{N} \left[ \left( \frac{X_i X_j}{\rho D_{i,j}} \right) \left( \frac{D_{T,j}}{Y_j} - \frac{D_{T,i}}{Y_i} \right) \right] \left( \frac{\nabla T}{T} \right), \quad i = 1, \ldots, N. \quad (5.2.5)$$

- Diffusion can be induced through:
  - Concentration gradient (Fickian)
  - Pressure gradient, $\nabla p$
  - Body force, $\mathbf{f}_i$
  - Temperature gradient, $\nabla T$ (Soret diffusion):
    Important for light ($\text{H, H}_2$) and heavy (large HC’s, polymers, soot) species; respectively up & down the $\nabla T$
Discussion on Pressure Tensor, $P$

- $P$ discussed in fluid mechanics texts
  - Controls the fluid motion, both inertia and viscous
  - Temperature and hence density variations inherently important in flames
  - *Constant density is a poor assumption*
  - Buoyancy effect inherently important
  - Role of electromagnetic, body force, is unclear
Discussion on Heat Flux Vector, \( q \)

- Heat flux consists of:
  - Conduction due to temperature gradient
  - \( \rho \sum_{i=1}^{N} h_i Y_i \mathbf{v}_i = 0 \) for \( h_i = h \); heat diffusion for different \( c_{p,i} \)
  - Heat transfer due to concentration gradient (Dufour effect): Generally not important
  - Radiation \( q_R \); reduces flame temperature and hence reaction rate; relevant for large-scale phenomena (e.g. furnace flame, building and wildland fires) and sooty flames
Auxiliary Relations

- **Ideal Gas Equation of State**

  \[ p = \rho R^o T \left/ \sum_{i=1}^{N} X_i W_i \right. = \rho R^o T \sum_{i=1}^{N} \frac{Y_i}{W_i} = \frac{\rho R^o T}{W}, \]

- **Energy–Enthalpy Relation**

  \[ h = \sum_{i=1}^{N} Y_i h_i = e + p / \rho. \]

- **Calorific Equation of State**

  \[ h_i = h_i^0 (T^o) + h_i^s (T ; T^o) \quad h_i^s (T ; T^o) = \int_{T^o}^{T} c_{p,i} dT. \]

- **Mole and Mass Fractions**

  \[ X_i = \frac{Y_i / W_i}{\sum_{j=1}^{N} Y_j / W_j}, \quad Y_i = \frac{X_i W_i}{\sum_{j=1}^{N} X_j W_j}. \]

Important concept: Combustion is a mixed-unit discipline

- Convection is mass based, described by Newtonian mechanics
- Reaction is mole based, describing frequency of collision
- Concentration diffusion is mole based
Assumption on Diffusion Coefficient

• Allow only concentration diffusion

\[ \nabla \ln X_i = \sum_{j=1}^{N} \left( \frac{X_j}{D_{i,j}} \right) (V_j - V_i), \quad i = 1, 2, \ldots, N, \]

• Assume equal diffusivity: \[ D_{i,j} = D \]

\[ V_i = -D \nabla \ln Y_i, \quad \text{(5.2.16)} \]

This is Fick’s law of mass diffusion

• Assume \[ D_{i,j} = D_{i,N} \], \( N \): an abundant species

(e.g. \( N_2 \)) \[ V_i = -D_{i,N} \nabla \ln Y_i \quad \text{(5.2.17)} \]

• \( \rho D = \text{constant} \) (or \( \rho^2 D = \text{constant in boundary layer formulation, to be shown later} \))
Isobaric Assumption

• Relevant for subsonic flows

\[ \rho u \frac{du}{dx} = - \frac{dp}{dx}, \quad \left( \frac{\rho_o u_o^2}{p_o} \right) \left( \hat{\rho} \frac{d\hat{u}}{dx} \right) = - \frac{d\hat{p}}{dx}, \quad \gamma M_o^2 \left( \hat{\rho} \frac{d\hat{u}}{dx} \right) = - \frac{d\hat{p}}{dx} \]

• Let \( \hat{p}(x, t) = \hat{p}_0(x, t) + \hat{p}_1(x, t) \)

\( \hat{p}_o = O(1) \quad \hat{p}_1 = O(M_o^2). \)

\( O(1) : \quad \frac{d\hat{p}_o}{dx} = 0, \quad O(M_o^2) : \quad \gamma M_o^2 \left( \hat{\rho} \frac{d\hat{u}}{dx} \right) = - \frac{d\hat{p}_1}{dx} \)

• Therefore: \( \nabla \hat{p}_o = 0 \quad \text{or} \quad p_o = p_o(t). \) \hspace{0.5cm} (5.2.24)

\[ p_0(t) = \rho RT = \text{thermodynamic pressure} \]

\[ p_1(x, t) = \text{dynamic pressure} \]
A Simplified Diffusion-Controlled System

- Specialize to subsonic flows
- Four (minimum) key processes included:
  - Unsteadiness
  - Diffusion: 2nd order, highest order differential
  - Convection: 1st order, describes fluid mechanics
  - Reaction
- Derivation only involves energy (with separate sensible & chemical terms) and species equations, which explicitly show reaction terms
- Momentum does not explicitly contain reaction term
  - Indirectly chemical heat release $\Rightarrow$ temperature variation $\Rightarrow$ density variation $\Rightarrow$ momentum equation is variable density
Distinct Specific Heat and Diffusivity Formulations

- **Distinct specific heat:** \( c_{p,i} \) distinct, \( D_{i,j} = D \)

  - Energy conservation:
    
    \[
    \frac{\partial}{\partial t} (\rho h^s) + \nabla \cdot \left[ \rho \mathbf{v} h^s - \rho D \nabla h^s + \lambda \left( \frac{1}{Le} - 1 \right) \nabla T \right] = \frac{dp}{dt} - \sum_{i=1}^{N} h_i^o w_i.
    \]

    Note role of \( Le \neq 1 \) in energy conservation

  - Species conservation:
    
    \[
    \frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \mathbf{v} Y_i - \rho D \nabla Y_i) = w_i, \quad i = 1, 2, \ldots, N.
    \]

- **Distinct diffusivity:** \( c_{p,i} = c_p; \quad D_{i,j} = D_{i,N} \)
A Set of Final Conservation Equations (with Appropriate Assumptions)

- \[
\frac{\partial \tilde{\rho}}{\partial t} + \nabla \cdot (\tilde{\rho} \tilde{v}) - \nabla^2 \tilde{h}^s = -\tilde{w}_F \tag{5.6.6}
\]

- \[
\frac{\partial \tilde{\rho}}{\partial t} + \nabla \cdot (\tilde{\rho} \tilde{v}) - \frac{1}{Le} \nabla^2 \tilde{Y}_i = \tilde{w}_F \tag{5.6.7}
\]

- \[
\tilde{w}_F = -Da_c \tilde{Y}_o^{v_0} \tilde{Y}_F^{v_F} e^{-E_a/R^oT} \tag{5.6.8}
\]

- Governed by 3 parameters: \(Le, Da_c, E_a\)
Nondimensional Numbers

• **Lewis number**: \( Le = \text{thermal diffusivity/mass diffusivity} \approx 1 \)

• **Collision Damköhler number**: \( Da_c (>>1) \):

\[
Da_c = \frac{\ell^2_o / (\lambda / c_p \rho_o)}{(\rho_o / B_c)} = \frac{\text{Characteristic diffusion time}}{\text{Characteristic collision time}}.
\]

• **Reaction Damköhler number**: \( Da = O(1) \):

\[
Da = Da_c \exp(-Ar) = \frac{\text{Characteristic flow time or diffusion time}}{\text{Characteristic reaction time}}.
\]

\[
\tilde{w}_F = -Da_c \tilde{Y}_o\tilde{Y}_F^e^{-E_o / R^*T} = -Da \tilde{Y}_o\tilde{Y}_F^e \exp \left[ Ar \left(1 - \frac{\tilde{T}}{T_{\text{max}}} \right) \right]
\]

\[
\begin{align*}
\circ\quad Ar(1 - T_{\text{max}} / T) &= O(1) \quad \Rightarrow \quad (T_{\text{max}} - T) = O(T / Ar) \approx O(T_{\text{max}} / Ar) = O(Ze^{-1})
\end{align*}
\]

\[
\circ\quad \text{Zel’dovich number: } Ze >> 1 \quad Ze = \frac{Ar}{T_{\text{max}}} = \frac{T_a}{T^2_{\text{max}}}.
\]
Conserved Scalar Formulations
Conserved Scalar Formulation: Rationale

• Chemical source term \( \omega_i \sim Y_i^{n_i} Y_j^{n_j} \exp \left( - \frac{E_a}{R^o T} \right) \)
  o is nonlinear in both \( Y_i \) and \( T \)
  o couples the conservation equations for \( Y_i \) and \( T \)

• Stoichiometry relates the reaction entities \( \Rightarrow \)
  conserved quantities during a reaction
  e.g. total enthalpy

• Are these quantities still “conserved” (i.e. not affected by reaction) in a convective-diffusive medium?
Coupling Function Formulation (1/5)

- Species conservation (for \( D_{i,j} = D \)):

  \[
  L(Y_i) = w_i, \\
  L(\cdot) = \left[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v} - \rho D \nabla) \right](\cdot)
  \]

- For \( \sum_{i=1}^{N} v_i'M_i \rightarrow \sum_{i=1}^{N} v_i''M_i \).

  \[ \omega = \frac{W_i}{W_i(v''_i - v'_i)} = B T^\alpha \exp\left(-\frac{E_a}{R T}\right)c_j^{v_j} \]

  o Thus

  \[ L(Y_i) = \omega W_i(v''_i - v'_i) \]

  \[ L \left[ \frac{Y_i}{W_i(v''_i - v'_i)} \right] = \omega \] (A)

  o Similarly for j:

  \[ L \left[ \frac{Y_j}{W_j(v''_j - v'_j)} \right] = \omega \] (B)

- Subtracting (B) from (A)

  \[ L \left[ \frac{Y_i}{W_i(v''_i - v'_i)} - \frac{Y_j}{W_j(v''_j - v'_j)} \right] = 0 \] (C)

which does not depend on the reaction rate \( \omega \)!
Coupling Function Formulation (2/5)

• Thus

\[
\frac{Y_i}{W_i(v_i^\prime - v_i^\prime)} - \frac{Y_j}{W_j(v_j^\prime - v_j^\prime)} = \beta_{i,j}
\]

is a conserved scalar for the reacting flow system, with \( L(\beta_{i,j}) = 0 \)

  ○ Consequently, the fundamental variable is not \( Y_i \), but a stoichiometrically-weighted variable \( \frac{Y_i}{W_i(v_i^\prime - v_i^\prime)} \)

• Can also define a nondimensional function

\[
\tilde{Y}_i = \frac{W_n(v_n^\prime - v_n^\prime)}{W_i(v_i^\prime - v_i^\prime)} \frac{Y_i}{Y_{n,B}}
\]

  ○ Then \( \beta_{i,j} = \tilde{Y}_i - \tilde{Y}_j \)

n: a reference species; B: a boundary
Coupling Function Formulation (3/5)

- For energy conservation (with \( Le = 1 \))

\[
L(h^s) = \frac{dp}{dt} - \sum_{i=1}^{N} h_i^o w_i = \frac{dp}{dt} - \left[ \sum_{i=1}^{N} h_i^o W_i (v_i'' - v_i') \right] \omega.
\]

- Define

\[
\tilde{h}^s = \frac{h^s}{Y_{n,B} q_{c,n}}, \quad \tilde{T} = \frac{c_p T}{Y_{n,B} q_{c,n}},
\]

\[
q_{c,n} = \sum_{k=1}^{N} \frac{h_k^o W_k (v_k'' - v_k')}{W_n (v_n'' - v_n')}, \quad \tilde{p} = \rho \tilde{T} \quad L(\tilde{h}^s) = \left( 1 - \frac{1}{\gamma} \right) \frac{d \tilde{p}}{dt} - w_n \quad (D)
\]

- Adding (A) and (D) results

\[
L(\beta_i) = \left( 1 - \frac{1}{\gamma} \right) \frac{d \tilde{p}}{dt}.
\]

- \( L(\beta_i) = 0 \) for \( \frac{d \tilde{p}}{dt} = 0 \).
Coupling Function Formulation (4/5)

- Thus in chemically reacting flows and diffusive system governed by (N+1) equations

\[
L(\tilde{Y}_i) = \omega_n \quad i = 1, 2, 3, \ldots, N \quad \text{(E)}
\]

\[
L(\tilde{h}^s) = -\omega_n \quad \text{(F)}
\]

can be alternatively described by

\[
L(\tilde{\beta}_i = \tilde{Y}_i + \tilde{h}^s) = 0 \quad i = 1, 2, 3, \ldots, N
\]

\[
L(\tilde{h}^s) = -\omega_n
\]

or any other linear combination of (E) and (F)
Coupling Function Formulation (5/5)

• Consequently, $N$ equations can be solved for the conserved scalars $\beta_i$ (or $\beta_{i,j}$).

• Chemical information is contained in the $(N+1)^{th}$ equation, say $L(\tilde{h}^*) = -\omega_n$ which is solved last.

• Key assumption: Equal diffusivity for all quantities:

$$D_{i,j} = D, \quad Le = \lambda/\rho c_p = 1$$
Other Formulations

- **Coupling function formulation** requires equal diffusivity or unity Lewis number
- Local coupling function formulation: holds only in the reaction region, governed by reaction and diffusion
- Near-equidiffusion formulation: Since $Le \approx 1$ for most gases, expand around $Le = 1$
- Element conservation formulation: an element is a conserved scalar; still requires $Le = 1$ assumption because elements are associated with molecules; insufficient relations because $N >> L$

- **Mixture fraction formulation**: Normalized coupling function; a mixture fraction can be used as a generalized independent variable; useful for non-premixed flame formulation.
- Progress variable formulation: Normalized product concentration; useful for premixed flame formulation

- **Reaction-sheet formulation**
Mixture Fraction Formulation (1/3)

Appropriate for nonpremixed (diffusion) flame analysis

- From coupling function formulation (for $Le_i=1$)
  \[ L(\beta_{i,j}) = 0 \]

- Define mixture fraction for $(F,O)$ as
  \[ Z = \frac{\beta_{F,o} - \beta_{F,o,b^-}}{\beta_{F,o,b^+} - \beta_{F,o,b^-}} \]  \hspace{1cm} (5.4.39)

  - $Z \equiv 0$ and $1$ at boundaries of $F$ and $O$,
  - Then \[ L(Z) = 0 \]  \hspace{1cm} (5.4.40)

- Superficially $Z$ is just a normalized definition of $\beta$
  - Utility of $Z$ is actually rather broad, subjected nevertheless to the $Le_i=1$ assumption

  For any $i$, and using $j = F$, we have
  \[ L(\beta_{i,F}) = 0 \]  \hspace{1cm} (5.4.41)

- Observing (5.4.40) and (5.4.41), a possible solution for $\beta_{i,F}$ is
  \[ \beta_{i,F} = c_{1,i} + c_{2,i} Z \]  \hspace{1cm} (5.4.42)

  - Solution degenerates to that of (5.4.42) and (5.4.40)
Mixture Fraction Formulation (2/3)

• Unique features of $\beta_{i,F}(Z)$
  
  o $Z$ is now an independent variable
  o $\beta_{i,F}$ varies linearly with $Z$
  o $\beta_{i,F}$ is configurationally independent. (e.g., spherical flame, stagnation flame, turbulent flame), hence general.
  o But only for $Le_i \equiv 1$

• Let $i=O$, then applying b.c. on (5.4.42) at $Z=(0,1)$ yields
  
  $\tilde{Y}_O - \tilde{Y}_F = -\tilde{Y}_{F,B^*} + (\tilde{Y}_{F,B^*} + \tilde{Y}_{O,B^*})Z$. \hspace{1cm} (5.4.44)

  Similar operation for $\beta = \tilde{h}^s + \tilde{Y}_i$ yields
  
  $\tilde{h}^s + \tilde{Y}_F = (\tilde{h}_{B^*} + \tilde{Y}_{F,B^*}) + (\tilde{h}_{B^*} - \tilde{h}_{B^*} - \tilde{Y}_{F,B^*})Z$, \hspace{1cm} (5.4.45)

  \[ \tilde{h}^s + \tilde{Y}_O = \tilde{h}_{B^*} + (\tilde{h}_{B^*} - \tilde{h}_{B^*} + \tilde{Y}_{O,B^*})Z. \] \hspace{1cm} (5.4.46)
Mixture Fraction Formulation (3/3)

- To study effects of chemistry in $Z$-space, transform
  \[ \rho \frac{\partial h^s}{\partial t} + \rho \mathbf{v} \cdot \nabla \tilde{h}^s - \nabla \cdot (\rho D \nabla \tilde{h}^s) = -w_n. \]  
  \[ \text{(5.4.49)} \]
  from $(t, x, y, z)$ to $(\tau, X, Y, Z)$

- Designate 2D tangential operator in $X$ and $Y$ as
  \[ \nabla_i = \left( \frac{\partial}{\partial X}, \frac{\partial}{\partial Y}, 0 \right) \]
  \[ \text{(5.4.49)} \] is transformed to
  \[ \rho \frac{\partial h^s}{\partial t} + \rho \mathbf{v}_i \cdot \nabla_i \tilde{h}^s = -w_n + \rho D \left| \nabla Z \right|^2 \frac{\partial^2 \tilde{h}^s}{\partial Z^2} + \nabla_i \cdot (\rho D \nabla_i \tilde{h}^s) \]
  \[ \text{(5.4.53)} \]

- If we identify $Z=$constant surface as that of a flame, and if the flame is very thin such that $\nabla_i \ll \frac{\partial}{\partial Z}$, then (5.4.53) simplifies to
  \[ \rho \frac{\partial h^s}{\partial t} = \rho D \left| \nabla Z \right|^2 \frac{\partial^2 h^s}{\partial Z^2} - w_n \]

- Note that $D \left| \nabla Z \right|^2$ has the dimension of $t^{-1}$

$\Rightarrow$ Inverse of characteristic diffusion time of the flame; called scalar dissipation rate
2. Discontinuity Surface Formulations
2.1 Reaction-Sheet Formulation

Because of large activation energy, reaction region can be approximated as a reaction sheet

- Gradients of properties (e.g., $T$, $Y_i$) change discontinuously across the reaction sheet; values are continuous
- Mathematically this is a weak discontinuity; in contrast a shock is a strong discontinuity across which the property values change
- A reaction sheet is a source and sink for the reaction entities
- Jump relation: change in the slopes across the sheet represents conservation relation.
Jump Relations \((1/4)\)

- A general curved reaction zone can be treated as locally planar
  - Gradient dominates in normal direction
  - Minimum gradient in tangential direction
- Conservation equations in normal \((n)\) direction

\[
\frac{\partial}{\partial t} (\rho \tilde{h}^s) + \frac{\partial}{\partial n} \left( \rho u \tilde{h}^s - \left( \lambda / c_p \right) \frac{\partial \tilde{h}^s}{\partial n} \right) = \left( 1 - \frac{1}{\gamma} \right) \frac{d \tilde{p}}{dt} - w_n \quad (A)
\]

\[
\frac{\partial}{\partial t} (\rho \tilde{Y}_i) + \frac{\partial}{\partial n} \left( \rho u \tilde{Y}_i - \rho D_i \frac{\partial \tilde{Y}_i}{\partial n} \right) = w_n \quad (B)
\]

\[
\frac{\partial}{\partial t} (\rho \tilde{Y}_j) + \frac{\partial}{\partial n} \left( \rho u \tilde{Y}_j - \rho D_j \frac{\partial \tilde{Y}_j}{\partial n} \right) = w_n \quad (C)
\]
Jump Relations \((2/4)\)

- Subtracting (C) from (B) eliminates \(\mathcal{W}_n\)
  \[
  \frac{\partial}{\partial t} \left[ \rho (\tilde{Y}_i - \tilde{Y}_j) \right] + \frac{\partial}{\partial n} \left[ \rho u (\tilde{Y}_i - \tilde{Y}_j) + \left\{ \rho D_i \frac{\partial \tilde{Y}_i}{\partial n} - \rho D_j \frac{\partial \tilde{Y}_j}{\partial n} \right\} \right] = 0
  \]

- Integrate across reaction zone along normal direction, from \(n_f^+ < n < n_f^-\)
  \[
  \int_{n_f^-}^{n_f^+} \frac{\partial}{\partial t} \left[ \rho (\tilde{Y}_i - \tilde{Y}_j) \right] dn + \left[ \rho u (\tilde{Y}_i - \tilde{Y}_j) \right]_{n_f^-}^{n_f^+} - \left[ \rho D_i \frac{\partial \tilde{Y}_i}{\partial n} - \rho D_j \frac{\partial \tilde{Y}_j}{\partial n} \right]_{n_f^-}^{n_f^+} = 0 \quad \text{(D)}
  \]

- Shrink reaction zone to a sheet, \(n_f^+ \rightarrow n_f^-\), assume weak discontinuity such that
  \[
  (\rho u)^+ = (\rho u)^- , \quad Y_i^+ = Y_i^- , \quad T^+ = T^- , \quad \text{etc.}
  \]
Jump Relations (3/4)

- (D) then yields
\[
\left[ \rho D_i \frac{\partial \tilde{y}_i}{\partial n} \right]_{n_f}^{n_j} = \left[ \rho D_j \frac{\partial \tilde{y}_j}{\partial n} \right]_{n_f}^{n_j}, \quad \text{or} \quad \left[ \rho D_i \frac{\partial Y_i}{\partial n} \right]_{n_f}^{n_j} = \sigma_{i,j} \left[ \rho D_j \frac{\partial Y_j}{\partial n} \right]_{n_f}^{n_j}.
\]
  - (E) shows the stoichiometric relation between the fluxes of the \(i^{th}\) and \(j^{th}\) species

- Similar derivation for (A) and (B) yields energy conservation across interface (for \(dp / dt = 0\))
\[
\left( \frac{q_c}{\sigma_i} \right) \left[ \rho D_i \frac{\partial Y_i}{\partial n} \right]_{n_f}^{n_j} = - \left[ \lambda \frac{\partial T}{\partial n} \right]_{n_f}^{n_j},
\]
  - (E) and (F) are conservation relations for species and energy across the reaction surface
Jump Relations (4/4)

• Premixed flame (e.g., fuel lean, $Y_{F,f}^+ = 0$)

$$- [\rho D_F n \cdot \nabla \tilde{Y}_F]_{n_f} = [\rho D_O n \cdot \nabla \tilde{Y}_O]_{n_f}^+, \quad \text{and} \quad [\rho D_F n \cdot \nabla \tilde{Y}_F]_{n_f} = [(\lambda / c_p) n \cdot \nabla \tilde{h}^s]_{n_f}^+ - [(\lambda / c_p) n \cdot \nabla \tilde{h}^s]_{n_f}^-.$$

• Nonpremixed flame ($Y_{F,f}^+ \equiv 0, Y_{O,f}^- \equiv 0$)

$$[\rho D_F n \cdot \nabla \tilde{Y}_F]_{n_f}^- = -[\rho D_O n \cdot \nabla \tilde{Y}_O]_{n_f}^+, \quad \text{and} \quad [\rho D_F n \cdot \nabla \tilde{Y}_F]_{n_f}^- = [(\lambda / c_p) n \cdot \nabla \tilde{h}^s]_{n_f}^+ - [(\lambda / c_p) n \cdot \nabla \tilde{h}^s]_{n_f}^-.$$
Adiabatic Flame Temperature (1/4)

- General conservation equation

\[
\frac{\partial}{\partial t}(\rho h^s) + \nabla \cdot (\rho \mathbf{v} h^s - (\lambda / c_p) \nabla h^s) = - \sum_{i=1}^{N} h_i^o w_i
\]  

(A)

\[
\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \mathbf{v} Y_i - \rho D_i \nabla Y_i) = w_i, \quad i = 1, 2, \cdots, N,
\]  

(B)

- For reactions confined to a sheet, regions bounded away from it \((x < x_f \text{ and } x > x_f)\) are nonreactive

\[
\frac{\partial}{\partial t}(\rho \tilde{h}^s) + \nabla \cdot (\rho \mathbf{v} \tilde{h}^s - (\lambda / c_p) \nabla \tilde{h}^s) = 0,
\]  

(C)

\[
\frac{\partial}{\partial t}(\rho \tilde{Y}_i) + \nabla \cdot (\rho \mathbf{v} \tilde{Y}_i - \rho D \nabla \tilde{Y}_i) = 0, \quad i = O, F.
\]  

(D)

- A general solution (for \(Le = 1\)) is

\[
\tilde{h}^s = c_{1,i} + c_{2,i} \tilde{Y}_i,
\]
Adiabatic Flame Temperature (2/4)

- Premixed flame
  \[
  (\tilde{h}^s)^- = c_{1,F} + c_{2,F} \tilde{Y}_F.
  \]
  - At upstream boundary: \((\tilde{h}^s)^- = \tilde{h}^s_u; \quad \tilde{Y}_F = \tilde{Y}_{F,u},\)
  - At reaction sheet: \((\tilde{h}^s)^- = \tilde{h}^s_f; \quad \tilde{Y}_F = 0,\)
  - Solving for \(c_{1,F}\) and \(c_{2,F}\) yields
    \[
    (\tilde{h}^s) = \tilde{h}^s_f - \frac{(\tilde{h}^s_f - \tilde{h}^s_u)}{Y_{F,u}} Y_F.
    \]
    \(\text{(E)}\)
  - Substituting (E) into the jump relation just derived, get
    \[
    \tilde{h}^s_f = \tilde{h}^s_u + \tilde{Y}_{F,u}, \quad \text{or} \quad h^s_f = h^s_u + Y_{F,u} q_c,
    \]
  which is the relation for adiabatic flame temperature
Adiabatic Flame Temperature (3/4)

- Nonpremixed flame
  - Fuel side:
    \[(h^s)^- = c_{1,F} + c_{2,F} Y_F^-; \quad (h^s)^- = h_f^s - \frac{(h_f^s - h_B^s)}{Y_{F,B^-}} Y_F^-\]
  - Oxidizer side:
    \[(h^s)^+ = c_{1,O} + c_{2,O} Y_O^+; \quad (h^s)^+ = h_f^s - \frac{(h_f^s - h_B^s)}{Y_{O,B^+}} Y_O^+\]
  - Substituting into the jump relation yields
    \[
    \frac{\tilde{h}_f^s - \tilde{h}_B^s}{Y_{F,B^-}} + \frac{\tilde{h}_f^s - \tilde{h}_B^+}{Y_{O,B^+}} = 1
    \] (F)
Adiabatic Flame Temperature (4/4)

- Nonpremixed flame:
  - In dimensional form
    \[
    (Y_{F,B^-})q_c = (h_f^s - h_{B}^s) + \left( \frac{Y_{F,B^-}}{Y_{O,B^+}} \right) (h_f^s - h_{B_2}^s).
    \]
  - \[
  \phi^* = \frac{Y_{F,B^-}}{Y_{O,B^+}}\sigma_O
  \]
    \[
    \frac{\text{Available fuel/Stoichimetric fuel requirement}}{\text{Available oxidizer/Stoichiometric oxidizer requirement}}
    \]
  - \(\phi^*\) can be interpreted as the equivalence ratio for a nonpremixed flame
2.2. Reaction Sheet Analysis of Diffusion Flames
Structure of Diffusion Flames

• **General structure**: thin reaction zone separating a broad fuel-rich zone from a broad oxidizer-rich zone

• **For infinitely fast reaction**, compared to diffusion, reaction zone shrinks to a sheet ⇒ phenomenon is diffusion controlled ⇒ diffusion flame

• **For finite but large reaction rate**
  o Reaction zone broadened
  o Reactants leak through the flame
  o Excessive leakage leads to extinction
1D Chambered Flame: Coupling Function Formulation

- **Problem definition**
  \[ x = 0: \ Y_F = Y_{F,0}, \ Y_O = 0, \ Y_P = 0, \ T = T_0 \]
  \[ x = \ell: \ Y_F = 0, \ Y_O = Y_{O,\ell}, \ Y_P = 0, \ T = T_\ell \]  \hfill (6.1.1)

- **Coupling function formulation:**
  \[ \frac{d^2 \beta_i}{dx^2} = 0 \ \Rightarrow \ \beta_i = c_{1,i} + c_{2,i} x \]

- **Applying (6.1.1) yields**
  \[ \beta_F = \tilde{T} + \tilde{Y}_F = (\tilde{Y}_{F,0} + \tilde{T}_0) + (\tilde{T}_\ell - \tilde{T}_0 - \tilde{Y}_{F,0}) \tilde{x} \]  \hfill (6.1.5)

  \[ \beta_O = \tilde{T} + \tilde{Y}_O = \tilde{T}_0 + (\tilde{T}_\ell - \tilde{T}_0 + \tilde{Y}_{O,\ell}) \tilde{x} \]  \hfill (6.1.6)

Result is general, not limited to reaction sheet
1D Chambered Flame: Reaction-Sheet Solution

• Now apply reaction-sheet assumption ⇒ no reactant leakage:

\[
\tilde{Y}_F = 0, \quad \tilde{x}_f \leq \tilde{x} \leq 1; \quad \tilde{Y}_O = 0, \quad 0 \leq \tilde{x} \leq \tilde{x}_f
\]  

(6.1.7)

• Apply (6.1.7) to (6.1.5) and (6.1.6) yields

\[
\tilde{T}^- = \tilde{T}_0 + (\tilde{T}_\ell - \tilde{T}_0 + \tilde{Y}_{O,\ell}) \tilde{x}, \quad 0 \leq \tilde{x} \leq \tilde{x}_f
\]  

(6.1.8)

\[
\tilde{T}^+ = (\tilde{T}_0 + \tilde{Y}_{F,0}) + (\tilde{T}_\ell - \tilde{T}_0 - \tilde{Y}_{F,0}) \tilde{x}, \quad \tilde{x}_f \leq \tilde{x} \leq 1
\]  

(6.1.9)

• Apply \( \tilde{T}^- \) to \( \beta_F \) and \( \tilde{T}^+ \) to \( \beta_O \) yields

\[
\tilde{Y}_F = \tilde{Y}_{F,0} - (\tilde{Y}_{F,0} + \tilde{Y}_{O,\ell}) \tilde{x}, \quad 0 \leq \tilde{x} \leq \tilde{x}_f
\]  

(6.1.10)

\[
\tilde{Y}_O = -\tilde{Y}_{F,0} + (\tilde{Y}_{F,0} + \tilde{Y}_{O,\ell}) \tilde{x}, \quad \tilde{x}_f \leq \tilde{x} \leq 1
\]  

(6.1.11)

Problem completely solved – how straightforward!
1D Chambered Flame: Reaction-Sheet Properties

• Flame sheet (i.e. reaction sheet) location:
  o Set $\tilde{Y}_F = 0$, or $\tilde{Y}_0 = 0$ at $\tilde{x} = \tilde{x}_f$ yields

$$\tilde{x}_f = \frac{Y_{F,o}}{Y_{F,o} + Y_{O,\ell}} \equiv \frac{1}{1 + \frac{\phi^*}{1 + \phi^*}} = \Phi^*$$

$\Phi^*$: Normalized equivalence ratio; Flame located closer to deficit reactant

• Flame (-sheet) temperature:
  o Substitute $\tilde{x}_f$ in either (6.1.8) or (6.1.9),

$$\frac{T_f - T_o}{Y_{F,o}} + \frac{T_f - T_\ell}{Y_{O,\ell}} = 1$$

  o Identical to the general expression for flame temperature derived earlier

• Fuel consumption flux:

$$f = -\rho D \left( \frac{dY_F}{dx} \right)_{x_f} = \rho D \left( Y_{F,0} + \frac{Y_{O,\ell}}{\sigma_o} \right)$$
1D Chambered Flame: Reaction-Sheet Formulation (1/2)

- Assume reaction-sheet right from the beginning
  - Separately solve for non-reactive regions
  - Match these solutions by applying jump relations

- Governing equations:

\[
0 \leq \tilde{x} < \tilde{x}_f : \quad \frac{d^2 Y_F}{d\tilde{x}^2} = 0 \quad \frac{d^2 T^-}{d\tilde{x}^2} = 0 ; \quad \tilde{x}_f < \tilde{x} \leq 1 : \quad \frac{d^2 Y_o}{d\tilde{x}^2} = 0 \quad \frac{d^2 T^+}{d\tilde{x}^2} = 0 .
\]

- Solving subject to:

\[
\tilde{T}^- = \tilde{T}^+ = \tilde{T}_f ; \quad \tilde{Y}_F = \tilde{Y}_o = 0 \quad \text{at} \quad \tilde{x} = \tilde{x}_f
\]

Note: $\tilde{x}_f, \tilde{T}_f$ not known; determined through matching
1D Chambered Flame: Reaction-Sheet Formulation (2/2)

- Solution:

\[
0 \leq \tilde{x} \leq \tilde{x}_f: \quad Y_F = Y_{F,o} \left(1 - \frac{\tilde{x}}{\tilde{x}_f}\right); \quad T^- = T_o + (T_f - T_o) \left(\frac{\tilde{x}}{\tilde{x}_f}\right)
\]

\[
\tilde{x}_f \leq \tilde{x} \leq 1: \quad Y_O = Y_{O,f} \left(1 + \frac{\tilde{x} - \tilde{x}_f}{\tilde{x}_f}\right); \quad T^+ = T_f - (T_f - T_o) \left(1 - \frac{\tilde{x}}{\tilde{x}_f}\right)
\]

- Applying matching:

\[
\left(\frac{dY_F}{dx}\right)_{\tilde{x}_f} = -\left(\frac{dY_O}{dx}\right)_{\tilde{x}_f}; \quad \left(\frac{dT_F}{dx}\right)_{\tilde{x}_f} = \left(\frac{dT^+}{dx}\right)_{\tilde{x}_f} - \left(\frac{dT^-}{dx}\right)_{\tilde{x}_f}
\]

yields \(\tilde{x}_f\) and \(T_f\)
2.3. Rankine – Hugoniot Waves in Premixtures
1D Wave Structure in Premixtures

• Nonpremixed (Diffusion) flame is diffusion controlled, through stoichiometry requirement.
  o Diffusion $\Rightarrow$ subsonic flow

• A premixture is ready to react, not controlled by fuel-oxidizer stoichiometry
  o Once ignited, a chemical wave will propagate through the mixture, converting it to product
  o Propagation rate affected by reaction rate
    (vs. infinite reaction rate for nonpremixed combustion)
  o Propagation is a wave phenomena: can be either subsonic or supersonic
Rankine-Hugoniot Relations (1/4)

- Relates the equilibrium states far upstream and downstream of the wave
- Does not consider the nonequilibrium processes of diffusion and reaction within the wave \( \Rightarrow \) problem not completely specified \( \Rightarrow \) wave speed, the most important flame response, is given instead of determined
- Solution shows two branches
  - Subsonic, deflagration wave
  - Supersonic, detonation wave
- Wave speed determined by analyzing the wave structure: material for rest of the course.
Rankine-Hugoniot Relations (2/4)

- **Mass:** \( \rho_u u_u = \rho_b u_b = f \)

- **Momentum:** \( \rho_u u_u^2 + p_u = \rho_b u_b^2 + p_b \)

- **Energy:** \( h_u + \frac{1}{2} u_u^2 = h_b + \frac{1}{2} u_b^2 \)

- **Rayleigh Lines:** mass and momentum conservation:

  \[
  p_b - p_u = -(\rho_u u_u)^2 \left( \frac{1}{\rho_b} - \frac{1}{\rho_u} \right) = -f^2 (\nu_b - \nu_u) 
  \]

  \[
  M_u^2 = -\frac{\hat{p} - 1}{\gamma (\hat{\nu} - 1)}, \quad M_b^2 = -\frac{(\hat{p} - 1)\hat{\nu}}{\gamma (\hat{\nu} - 1) \hat{p}} \quad (7.1.5)
  \]

  - Straight lines passing through \((\hat{p}, \hat{\nu}) = (1, 1)\)
  - Negative slope of \(-\gamma M_u^2\)
  - Solution only for: \((\hat{p} > 1, \hat{\nu} < 1)\) i.e. \((\hat{p} > 1, \hat{\rho} > 1)\)
    \[
    (\hat{p} < 1, \hat{\nu} > 1) \text{ i.e. } (\hat{p} < 1, \hat{\rho} < 1)\]
Rankine-Hugoniot Relations (3/4)

- Hugoniot Lines
  - Using mass, momentum and energy conservation:
    \[ h_b - h_u = \frac{1}{2} (\nu_b + \nu_u) (p_b - p_u) \quad (7.1.8) \]
  - From chemical heat release:
    \[ h_b - h_u = -q_c + c_p (T_b - T_u) \]
    and \[ c_p/R = c_p/(c_p - c_v) = \gamma/((\gamma-1)) \]
    \[ h_b - h_u = -q_c + \frac{\gamma}{\gamma - 1} \left( \frac{p_b - p_u}{\rho_b} \right) \quad (7.1.10) \]
  - Equating (7.1.8) and (7.1.10)
    \[ \left( \hat{p} + \frac{\gamma - 1}{\gamma + 1} \right) \left( \hat{v} - \frac{\gamma - 1}{\gamma + 1} \right) = \frac{4\gamma}{(\gamma + 1)^2} + 2\hat{q}_c \left( \frac{\gamma - 1}{\gamma + 1} \right), \quad (7.1.11) \]
  - Hyperbolas with asymptotes
    - \( \hat{p} \to - (\gamma - 1) / (\gamma + 1) \)
    - \( \hat{v} \to (\gamma - 1) / (\gamma + 1) \)
    - \( \hat{q}_c = 0 \) line passes through (1,1)
Rankine-Hugoniot Relations (4/4)

- Strong detonation
- Upper CJ point
- Weak detonation
- Weak deflagration
- Lower CJ point
- Strong deflagration

\[ \hat{p} = \frac{\gamma - 1}{\gamma + 1} \]

\[ \hat{v} = \frac{\gamma - 1}{\gamma + 1} \]

- Inaccessible regions, \( f < 0 \)
- Rayleigh lines
- Hugoniot lines

\[ \hat{q}_c > 0 \]

\[ \hat{q}_c \equiv 0 \]
Detonation and Deflagration Waves (1/2)

• Intersection of Rayleigh (7.15) and Hugoniot (7.1.11) lines yields solution

\[
\hat{p}_\pm - 1 = - \frac{(1 - M_u^2)\gamma}{(\gamma + 1)} \left\{ 1 \pm \left[ 1 - \frac{2(\gamma^2 - 1)}{\gamma} \frac{M_u^2}{(1 - M_u^2)^2} \hat{q}_c \right]^{1/2} \right\}. \tag{7.1.13}
\]

• Solution characterized by three parameters:
  o \(\gamma\): compressibility; \(\hat{q}_c\): exothermicity
  o \(M_u\): wave speed that needs to be given

• (7.1.13) shows two solution branches
  o Since \(0 < [\cdot]^{1/2} < 1\), \{\cdot\} > 0, character of solution depends on \(M_u \geq 1\)
    o Detonation: \(M_u > 1\), \(\hat{p} > 1\), \(\hat{v} < 1\), \(\hat{\rho} > 1\)
    o Deflagration: \(M_u < 1\), \(\hat{p} < 1\), \(\hat{v} > 1\), \(\hat{\rho} < 1\)
Detonation and Deflagration Waves (2/2)

- Detonation waves
  - Pressure and density increase across wave
  - Two solutions: strong and weak detonations
  - Tangency point: Chapman-Jouguet (CJ) wave
  - Consideration of wave structure
    - Rules out weak detonation
    - CJ wave prevalent

- Deflagration waves
  - Pressure and density decrease across wave
  - Two solutions: strong and weak deflagrations
  - Strong deflagration ruled out: entropy decreasing
  - Weak deflagration prevalent: near isobaric
Chapman-Jouguet Waves

- Tangency point for the Rayleigh and Hugoniot lines

- Additional tangency condition closes problem ⇒ complete solution for given \( (\gamma, \hat{q}_c) \)

\[
(M_{u,cJ})^2_{\pm} = 1 + \frac{(\gamma^2 - 1) \hat{q}_c}{\gamma} \left\{ 1 \pm \left[ 1 + \frac{2\gamma}{(\gamma^2 - 1) \hat{q}_c} \right]^{1/2} \right\},
\]

\[M_b = 1\]

- (Strong, weak) detonation: \( M_b < 1, > 1 \)

- (Strong, weak) deflagration: \( M_b > 1, < 1 \)
Closing Remarks of Day 2 Lecture (1/2)

• A simplified set of conservation equations were derived for subsonic flows allowing for: unsteadiness, diffusion, convection & reaction

• Controlling nondimensional parameters:
  o Diffusive-reactive: $Le$, $Da$, $Ze$ ($Ar$)
  o Fluid mechanics and transport parameters of interest (e.g. $Re$, $Gr$, $Pe$…)

• Two major classes of rational analysis:
  o Conserved scalar (i.e. coupling function)
  o Reaction/flame sheet
  o Caution: $Le = 1$ assumption frequently embedded
Closing Remarks of Day 2 Lecture (2/2)

• Premixed “flames” are wave phenomena
  o Subsonic, deflagration waves
  o Supersonic, detonation waves
    • Chapman-Jouguet wave dominates (subsonic downstream)

• “Equivalence ratio” defined for diffusion flames

• Discussion focused on heat and mass transport; inclusion of fluid flow through the momentum equation will greatly enrich potential phenomena of interest
! Daily Specials !
Day 2 Special

Liñán’s Unified Formulation of Diffusion and Premixed Flames
A General Analysis of Diffusion Flame Structure

• Use chambered flame as example, with \( Le=1 \)

• Equation system:

\[
\frac{d^2 T}{dx^2} = -D a_c Y_o Y_F e^{-\frac{T_i}{T}}, \tag{9.2.2}
\]

\[
\tilde{T} + \tilde{Y}_o = \tilde{T}_i + (\beta + \tilde{Y}_{o,o})(1 - \tilde{x}), \tag{9.2.4}
\]

\[
\tilde{T} + \tilde{Y}_F = \tilde{T}_o + (1 - \beta) \tilde{x}, \tag{9.2.5}
\]

\[
\beta = \frac{\tilde{T}_o - \tilde{T}_i}{\tilde{T}_o - \tilde{T}_i}, \tag{9.2.6}
\]

\[
\tilde{T}(0) = \tilde{T}_o, \quad \tilde{T}(1) = \tilde{T}_i, \tag{9.2.7, 9.2.8}
\]
Classification of (Nonreactive) Flows Bounded from Reaction Sheets

Consider vanishing of the reaction term in:

\[
\frac{d^2 \tilde{T}}{d\tilde{x}^2} = -D a_c \tilde{Y}_O \tilde{Y}_F e^{-\tilde{T}_a / \tilde{T}},
\]

- Frozen flow \((D a_c \equiv 0)\)
  \[
  \tilde{T} = c_1 + c_2 \tilde{x},
  \]
  \(\text{(9.2.9)}\)

- Equilibrium flow \((\tilde{Y}_O \equiv 0)\)
  \[
  \tilde{T} = (\tilde{T}_o + \tilde{Y}_{o.o}) - (\beta + \tilde{Y}_{o.o}) \tilde{x}.
  \]
  \(\text{(9.2.10)}\)

- Equilibrium flow \((\tilde{Y}_F \equiv 0)\)
  \[
  \tilde{T} = \tilde{T}_o + (1 - \beta) \tilde{x}.
  \]
  \(\text{(9.2.11)}\)
Classification of Flames

• A general analysis of diffusion flame structure based on various combinations of frozen and equilibrium flows separated by reaction sheets (*Acta Astro.*, 1974):
  o Identified four types of flames
    ▪ Near equilibrium, diffusion flame
    ▪ Premixed flame
    ▪ Partial burning
    ▪ Weakly burning, ignition
  o Reduced structure equations to canonical forms
  o Obtained general semi-empirical solutions for structure equations and ignition-extinction criteria and expressions

• Subsequent studies show analysis applicable to wide range of situations
  o Quasi-1D flows; Le≠1; loss
Near Equilibrium Regime

- Flame sheet separates two near-equilibrium flow regions.
- To leading order, fuel and oxidizer respectively vanishes in each region

\[
\tilde{x} < \tilde{x}_f : \quad Y_{F,0}^- = 0, \quad T_0^- = T_o + (1 - \beta) \tilde{x} \quad (9.2.12)
\]

\[
\tilde{x} > \tilde{x}_f : \quad Y_{O,0}^+ = 0, \quad T_0^+ = T_\ell + (\beta + Y_{O,o}) (1 - \tilde{x}) \quad (9.2.13)
\]

- Flame temperature and location can be readily evaluated as

\[
\tilde{T}_f = \tilde{T}_o + (1 - \beta) \frac{Y_{O,o}}{1 + Y_{O,o}} = \tilde{T}_\ell + \left( \beta + Y_{O,o} \right) \quad (9.2.14)
\]

\[
\tilde{x}_f = \frac{Y_{O,o}}{1 + Y_{O,o}} \quad (9.2.15)
\]

- This is just the diffusion flame solution. All flame properties are determined at this level.
- With decreasing Da_c, reactant leakage occurs and will eventually lead to extinction.

Equation (9.2.12)

Equation (9.2.13)

Equation (9.2.14)

Equation (9.2.15)
Premixed Flame Regime

- Substantial leakage of one reactant is possible, even to the leading order. Leaked reactant freezes after crossing the flame.
- Thus flame separates a frozen flow region from an equilibrium flow region.
- For fuel being the leaked reactant, \( Y_{O,o} + 2\beta < 1 \)
  \[ \tilde{x} < \tilde{x}_f : \quad T_0^- = T_o + (T_f - T_o) \frac{\tilde{x}}{\tilde{x}_f}, \]  \[ (9.2.16) \]
  \[ \tilde{x} > \tilde{x}_f : \quad Y_{O,o}^+ = 0, \quad T_0^+ = T_\ell + (\beta + Y_{O,o})(1 - \tilde{x}), \]  \[ (9.2.17) \]
- Evaluating at reaction sheet yields
  \[ \tilde{T}_f = T_\ell + (\beta + Y_{O,o})(1 - \tilde{x}_f). \]  \[ (9.2.18) \]
  - Flame-sheet solution determined to one unknown;
  - Needs analysis at next order to determine the extra unknown.
Unified Interpretation of Premixed and Diffusion Flames: Leading-Order Structure

**Leading-order Structure of Premixed Flame**

**Limiting species**: Deficient species completely consumed at reaction sheet  
**Abundant species**: Concentration remains $O(1)$ throughout, hence unaffected

**Leading-order Structure of Premixed Flame Regime in Diffusion Flame Analysis**

**Limiting species**: oxidizer (or fuel); completely consumed at reaction sheet  
**Abundant species**: Fuel (or oxidizer) concentration remains $O(1)$ throughout, hence unaffected
Unified Interpretation of Premixed and Diffusion Flames: Reaction Zone Structure

Premixed Flame

\[ w \sim [k(T)Y_{\text{abundant}}]Y_{\text{deficient}} \]
\[ \sim k'(T)Y_{\text{deficient}} \]

Premixed Flame Regime in Diffusion Flame Analysis

\[ w \sim [k(T)Y_{\text{fuel}}]Y_{\text{oxidizer}} \]
\[ \sim k'(T)Y_{\text{oxidizer}} \]

Hence complete physical & mathematical correspondence
Partial Burning Regime

- Excessive leakage occurs for both reactants
- To leading order, flame sheet separates two frozen regions

\[ \tilde{x} < \tilde{x}_f : \quad \tilde{T}_0^- = \tilde{T}_o + (\tilde{T}_f - \tilde{T}_o) \frac{\tilde{x}}{\tilde{x}_f}, \]  
\[ (9.2.19) \]

\[ \tilde{x} > \tilde{x}_f : \quad \tilde{T}_0^+ = \tilde{T}_e + (\tilde{T}_f - \tilde{T}_e) \frac{1 - \tilde{x}}{1 - \tilde{x}_f}, \]  
\[ (9.2.20) \]

- Flame-sheet solution determined to two unknowns
Nearly-Frozen Regime

- Reaction is frozen throughout flow field
- Leading order solutions completely determined
  \[ \tilde{T}_0 = \tilde{T}_o - \beta \tilde{x}. \]  
  \[ \tilde{Y}_{F,0} = \tilde{x}. \]  
  \[ \tilde{Y}_{O,0} = (1 - \tilde{x})\tilde{Y}_{O,o}. \]
- Ignition occurs with finite reaction rates

\[ \tilde{Y}_{F,\ell} (=1) \]

(d) Nearly Frozen Regime
Regime Classifications Based on Energy Levels

\[ \beta < \frac{1}{2} \]
\[ \tilde{Y}_{O,0} + 2\beta < 1 \]
Flame Response with Finite $Da_C$ for Different Regimes

- Near-Equilibrium Regime
- Premixed Flame Regime
- Partial Burning Regime
- Nearly Frozen Regime
Analysis of Nearly-Frozen Regime

• Ignition occurs next to hot boundary, \( x=0 \)
• Similar to hot surface ignition, except \( Y_F=O(\varepsilon) \) in reaction zone
• Structure equation

\[
\frac{d^2 \theta}{d \chi^2} = -\Delta (\chi - \theta) e^{(\theta - \beta x)} \\
\theta(0) = 0 \\
\left( \frac{d \theta}{d \chi} \right)_{x \to \infty} = 0. \\
\Delta = \varepsilon^2 D a c \tilde{Y}_{O,o} \exp(-\tilde{T}_0/T_o) \\
\beta = \tilde{T}_o - \tilde{T} \\
\]

(9.3.2) \hspace{2cm} (9.3.3) \hspace{2cm} (9.3.6)

• Ignition occurs if

\[
\Delta > \Delta_i(\beta) = \frac{\beta^2/2}{1 + 2.17(1 - \beta)/\beta}, \\
\]

(9.3.7)
Analysis of Partial Burning Regime

- Reactant concentrations are $O(1)$ in reaction zone
- Structure equation:
  \[
  \frac{d^2 \theta}{d \chi^2} = -\Delta e^\theta, \quad \Delta = \varepsilon D a_c Y_{o, f} \tilde{Y}_{f, f} \exp(-\tilde{T}_a / \tilde{T}_f)
  \]
- Solution
  \[
  \theta(\chi) = \theta_m - \ln \left\{ \cosh^2 \left( \frac{\Delta}{2} e^{\theta_m} \right)^{1/2} (\chi - \chi_m) \right\}, \quad (9.3.8)
  \]
  determined to two unknowns, $\theta_m$ and $\chi_m$
- Need to go to second-order analysis to solve the problem, using delta function closure
- Existence of such a flame has yet to be confirmed!
Analysis of Premixed Flame Regime

- Same analysis as that conducted previously
- Concentration of one reactant is O ($\varepsilon$) in reaction zone
- With appropriate definitions, obtained identical structure equation, as previously

$$\Delta = 2 \varepsilon^2 D a_c \exp\left(-\frac{\tilde{T}_a}{\tilde{T}_f}\right)$$
Analysis of Near-Equilibrium Regime

- Concentration of both reactants O (ε) in reaction zone
- Structure equation

\[ \frac{d^2 \tilde{\theta}}{d\eta^2} = \delta (\theta - \eta) (\theta + \eta) e^{-(\tilde{\theta} \eta)}, \quad (9.3.23) \]

\[ \left( \frac{d \tilde{\theta}}{d \eta} \right)_{-\infty} = -1, \quad \left( \frac{d \tilde{\theta}}{d \eta} \right)_{\infty} = 1 \quad (9.3.24), (9.3.25) \]

\[ \delta = \frac{4 \Delta}{1 + Y_{\sigma,o}^2}, \quad \Delta = \varepsilon^3 D a_c \exp(-\tilde{T}_a / \tilde{T}_f) \]

- Extinction occurs for:

\[ \delta < \delta_E \]

\[ = \{ (1 - | \gamma |) - (1 - | \gamma |)^2 + 0.26 (1 - | \gamma |)^3 + 0.055 (1 - | \gamma |)^4 \} \varepsilon. \]

\[ \gamma = 1 - \frac{2(1 - \beta)}{1 + Y_{\sigma,o}} = \frac{2(Y_{\sigma,o} + \beta)}{1 + Y_{\sigma,o}} - 1 \]

76