Lecture 12. Modeling of Turbulent Combustion
Content

- direct numerical simulation (DNS)

- Statistical approach (RANS)
  - Modeling of turbulent non-premixed flames
  - Modeling of turbulent premixed flames

- Large eddy simulation
Direct Numerical Simulation: DNS

- Solve the entire set of governing equations
  - Down to the smallest flow scales
  - Down to the fine reaction zones

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

\[ \frac{\partial \rho Y_i}{\partial t} + \frac{\partial \rho u_j Y_i}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D_{ij} \frac{\partial Y_i}{\partial x_j} \right) + \omega_i, \quad i = 1, \ldots, N \]

\[ \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \nabla \cdot \left( p \mathbf{I} + \tau \right), \quad (i = 1, 2, 3) \]

\[ p = \rho \frac{1}{W_{\text{mix}}} R_u T, \]

\[ h = \sum_{i=1}^{N} Y_i \left( u_{si} + u_{ci} + \frac{p}{\rho} \right) = \sum_{i=1}^{N} Y_i h_i \]

\[ \nabla X_i = \sum_{j=1}^{N} X_i X_j \left( \nabla \tilde{V}_j - \nabla \tilde{V}_i \right) + (Y_i - X_i) \frac{\nabla p}{p} + \frac{\rho}{p} \sum_{j=1}^{N} Y_i Y_j (f_i - f_j) \]

\[ h_i = u_{si} + u_{ci} + \frac{p}{\rho} = \int_{T_{\text{ref}}}^{T} c_p dT + h^0_{f,i}(T_{\text{ref}}) \]
Principles of DNS

- Governing equations (N+5, N+4)
  - Continuity equation, 1
  - Momentum equations, 3
  - Species transport equations, N (number of species)
  - Enthalpy transport equation, 1
  - Equation of state, 1
  - Calorific equation of state, 1
  - Transport coefficients, N+2
- Independent variables to be simulated (2N+9)
  - Density, pressure, temperature, 3
  - Velocity components, 3
  - Species mass fractions, N
  - Enthalpy, 1
  - Transport coefficients, N+2
Principles of DNS

• Fully resolving all flow scales
  – Kolmogrov scales: length, time, velocity
  – All flame scales: reaction zones
Principles of DNS

• Fully resolving all flow scales
  – Kolmogrov scales: length, time, velocity
  – All flame scales: reaction zones
Cost of DNS to resolve one large eddy

\[
\frac{l_0}{\eta} \propto \text{Re}_{l_0}^{3/4}; \\
\frac{v_0}{v_\eta} \propto \text{Re}_{l_0}^{1/4}; \\
\frac{\tau_0}{\tau_\eta} \propto \text{Re}_{l_0}^{1/2};
\]

Assuming the smallest grid is \( \eta \) and smallest time step is \( \tau_\eta \),

Computational cost for 1-D \( \sim \frac{l_0}{\eta} \frac{\tau_0}{\tau_\eta} \sim \text{Re}_{l_0}^{5/4} \)

Computational cost for 1-D \( \sim \left( \frac{l_0}{\eta} \right)^2 \frac{\tau_0}{\tau_\eta} \sim \text{Re}_{l_0}^2 \)

Computational cost for 1-D \( \sim \left( \frac{l_0}{\eta} \right)^3 \frac{\tau_0}{\tau_\eta} \sim \text{Re}_{l_0}^{11/4} \)
Cost of DNS to resolve one large eddy

Total number of spatial mesh points x time steps needed for resolving one large eddy scales of flames with different spatial dimensions and Reynolds numbers

<table>
<thead>
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<th>$Re_\ell_0$</th>
<th>1-D</th>
<th>2-D</th>
<th>3-D</th>
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- DNS with detailed chemistry for an SI engine takes 30 years
- DNS is used for 2D
- DNS is used for low Reynolds number flames
DNS of hydrogen flame, Mizobuchi et al, 29th symp

H2 Jet flame: 9 species, 17 reactions, 30Dx30D, 22.8 million grids
N.F.I.: normalized flame index – square of concentration gradient
Statistical methods (SM): Ensemble Averages and Modeling

(Reynolds averaged Navier-Stokes equations: RANS)
Principles of ensemble averages

- Turbulent flame is a random process
- Only the statistical mean field is solved
Ensemble average

Reynolds decomposition: $u = \bar{u} + u'$, $\bar{u} = \frac{1}{M} \sum_{m=1}^{M} u_m$

Favre decomposition: $u = \bar{u} + u''$, $\bar{u} = \frac{\rho u}{\bar{\rho}}$
Cost of Statistical Methods to resolve one large eddy

Total number of spatial mesh points x time steps needed for resolving one large eddy scales of flames with different spatial dimensions and Reynolds numbers

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Governing equations for the mean flame

Mass: \[ \frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j}{\partial x_j} = 0 \]

Momentum: \[ \frac{\partial \bar{\rho} \bar{u}_i}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i \bar{u}_j}{\partial x_j} = - \frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \bar{\rho} u_i^\prime u_j^\prime}{\partial x_j} \]

Species: \[ \frac{\partial \bar{\rho} \bar{Y}_i}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i \bar{Y}_i}{\partial x_j} = - \frac{\partial}{\partial x_j} \left( \bar{\rho} u_i^\prime \bar{Y}_i^\prime \right) + \bar{\omega}_i \]

Energy equation: similar as above
Modeling issues

\[ \frac{\partial \rho \tilde{Y}_i}{\partial t} + \frac{\partial \rho \tilde{Y}_i u_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D_i \frac{\partial \tilde{Y}_i}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( -\rho Y_i'' u_j'' \right) + \bar{\omega}_i \]

Turbulent transport flux

Turbulent reaction rate

Turbulence models
  e.g. K-epsilon model

Combustion models

X.S. Bai

Modeling of TC
Modeling of Turbulent Non-premixed flames

- Flame sheet model
- Flamelet models
- Eddy dissipation concept model
- Conditional moment closure models
- Probability density function models
Turbulent Combustion of a fuel jet
Presumed PDF Burke-Schumann model
Burke-Schumann flame sheet model

- In 1970s Bilger advocated - in diffusion flames there is such as ‘magic’ variable called mixture fraction ($Z$). All the species mass fractions, temperature, density etc, are uniquely related to $Z$ …
- Burke-Schumann were the first one found this magic relationship

\[
Y_F = \begin{cases} 
\frac{Z - Z_{st}}{1 - Z_{st}} & Z \geq Z_{st} \\
0 & Z < Z_{st}
\end{cases} \quad 
Y_{O2} = \begin{cases} 
0.233\left(1 - \frac{Z}{Z_{st}}\right) & Z \leq Z_{st} \\
0 & Z > Z_{st}
\end{cases} \\
Y_P = \begin{cases} 
\frac{1 - Z}{1 - Z_{st}} & Z \geq Z_{st} \\
Z / Z_{st} & Z < Z_{st}
\end{cases} \quad 
T = \begin{cases} 
\frac{1 - Z}{1 - Z_{st}}\left(T_{st} - T_{Fu}\right) + T_{Fu} & Z \geq Z_{st} \\
Z / Z_{st}\left(T_{st} - T_{Ou}\right) + T_{Ou} & Z < Z_{st}
\end{cases}
\]
Ensemble average of flame sheet in turbulent flows

\[ Z = \frac{1}{N} \sum_{i=1}^{N} Z(t_i) = \frac{1}{N} \sum_{m=1}^{M} n(Z_m) Z_m = \sum_{m=1}^{M} \frac{n(Z_m)}{N \Delta Z} Z_m \Delta Z = \int_0^1 p(Z) Z dZ \]

\[ \bar{Y} = \frac{1}{N} \sum_{i=1}^{N} Y(Z(t_i)) = \frac{1}{N} \sum_{m=1}^{M} n(Z_m) Y(Z_m) = \sum_{m=1}^{M} \frac{n(Z_m)}{N \Delta Z} Y(Z_m) \Delta Z = \int_0^1 p(Z) Y(Z) dZ \]

Measurement at a flow field point

Probability density function: pdf
Presumed PDF: \[ p(Z) = \frac{Z^a (1-Z)^b}{\int_0^1 Z^a (1-Z)^b \, dZ} \]

\[ \bar{Z} = \int_0^1 Z p(Z) \, dZ, \quad g = (Z - \bar{Z})^2 = \int_0^1 (Z - \bar{Z})^2 \, p(Z) \, dZ \]

\( a, b \leftrightarrow \bar{Z}, g \quad \text{Two equations, two unknowns} \)

Mixture fraction variance:
\[ \frac{\partial \bar{\rho} g}{\partial t} + \frac{\partial \bar{\rho} u_j g}{\partial x_j} = - \frac{\partial}{\partial x_j} \left( \bar{\rho} u_j Z^2 \right) + P - \bar{\rho} \chi \]
Numerical implementation (flame sheet model)

Mass: \[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0
\]

Momentum: \[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} - \frac{\partial \rho u_i u_j}{\partial x_j}
\]

Mixture fraction: \[
\frac{\partial \rho \bar{Z}}{\partial t} + \frac{\partial \rho u_j \bar{Z}}{\partial x_j} = -\frac{\partial}{\partial x_j} \left( \rho u_j \bar{Z}^\prime \right), \quad g - \text{equation}
\]

Flame sheet relation: \[
\bar{T} = \int_{0}^{1} T(Z)p(Z)dZ, \ldots
\]
Presumed PDF flamelet model
Influence of finite rate chemistry on flamelet structure

- Chemical kinetics does not affect the flame shape and flame height very much !!!
- Chemical reaction does affect the species and temperature distribution a lot !!!

CH4/air diffusion flame, p=1 bar, Tu=300 K

\[ \delta_Z \]
Influence of the finite rate chemistry on maximum species mole fraction and $T$

- CH4/air diffusion flame, $p=1$ bar, $Tu=300$ K
The flamelet library

- The flamelet equation can be derived using Crocco transformation

$$\frac{1}{2} \chi \frac{d^2 Y_i}{dZ^2} = w_i$$

- Flamelet library

$$Y_i = f_i(Z, \chi), T = f_T(Z, \chi), \rho = f_\rho(Z, \chi)$$

- How to get?

Solve the above flamelet equation using detailed chemical kinetic mechanisms!!
Numerical implementation

• Ensemble average

$$\bar{Y}_i = \frac{1}{\rho} \left( \int_0^1 \int_0^\infty \varphi(Z, \chi) f_\rho(Z, \chi) f_i(Z, \chi) d\chi dZ \right)$$

$$\bar{\rho} = \left( \int_0^1 \int_0^\infty \varphi(Z, \chi) f_\rho(Z, \chi) d\chi dZ \right)$$

• Presumed PDF

– How to get?

$$\varphi(Z, \chi)$$

Similar to flame sheet model. But here there are four unknown parameters. One needs 4 transport equations.
Continuity + momentum $\rightarrow$ k-epsilon equations $\rightarrow$ Transport equations for the mean and variance of mixture fraction, and scalar dissipation rate

Ensemble averages

$$\bar{\rho} = \int_0^1 \int_0^\infty \phi(Z, \chi) f_{\rho}(Z, \chi) d\chi dZ$$

$$\tilde{Y}_i, \ldots$$
Other modeling approaches
Direct modeling of mean reaction rates: Eddy dissipation concept model

Species:
\[
\frac{\partial \tilde{\rho} \tilde{Y}_i}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_j \tilde{Y}_i}{\partial x_j} = - \frac{\partial}{\partial x_j} \left( \tilde{\rho} \tilde{u}_j \tilde{Y}_i'''' \right) + \bar{\omega}_i
\]

\[
\bar{\omega}_i = C_{EDC} \frac{1}{t_0} \min \left( Y_F, \frac{Y_O}{\gamma} \right)
\]

‘Mixed is burned’ model
Modeling of turbulent premixed flames
Vo=0.45 m/s, phi=1.17; Vin=120 m/s, phi=1.0
Modeling of turbulent premixed flames

- Desirable Models
  - taking into account the basic features of turbulent premixed flames
    - wrinkling
    - stretch
    - local extinction, re-ignition
    - local flame structure
    - ...
  - Computationally inexpensive
  - Valid for wide parameter range

with reasonably detailed chemistry
Modeling of turbulent premixed flames

*a unified model does not exist*

- Examples of models
  - $k-\varepsilon$ model
  - global chemistry + EDC/EBU ...
  - detailed chemistry + G-equation + presumed PDF + flamelet library
  - BML ...
  - Flame surface density models

- Resolved issues
  - Mean flame position
  - Mean major species
    - CO2, O2, UHC, ...
  - Mean temperature

- Unresolved issues
  - intermediate species
    - CO
    - NOx
    - soot
  - flame dynamics
Direct modeling of mean reaction rates: flame surface density model

Species:
\[
\frac{\partial \rho \tilde{Y}_i}{\partial t} + \frac{\partial \rho \tilde{u}_j \tilde{Y}_i}{\partial x_j} = - \frac{\partial}{\partial x_j} \left( \rho u_j \tilde{Y}_i \right) + \omega_i
\]

\[
\bar{\omega}_F \approx \frac{\rho_u A_L S_L Y_{F,u}}{V}
\]

\[
= \rho_u S_L Y_{F,u} \left( \frac{A_L}{V} \right)
\]

\[
= \rho_u S_L Y_{F,u} \Sigma
\]
- Mean flame brush
  - ensemble of laminar flamelets

- Global structure
  - Wrinkling and fluctuating laminar flamelets

- Local structure
  - stretched local laminar flamelet
Stretched laminar flamelet library

![Graph showing the mole fraction of oxygen (O₂) and carbon monoxide (CO) with different stretch rates (K). The graph plots mole fraction against the dimensionless stretch parameter (G/mm). The stretch rates are 0 s⁻¹, 500 s⁻¹, 1000 s⁻¹, and 2200 s⁻¹.]
Influence of flame stretch on Laminar flames

- 1-D geometry
  - Counterflow fresh-to-burned configuration
  - Counterflow fresh-to-fresh twin-flame configuration

- Detailed chemical kinetic mechanisms (up to C3)
  - Peters’ group (Lecture notes in physics m15)

- Numerical code
  - Chemkin
  - Cantera
Level-set Based Flamelet Library Approach

Counterflow DNM with detailed chemistry

Structures of laminar flamelet (quenching & species distributions)

Level-set G formulation

Statistics of flamelets (fluctuations and wrinkling)

Ensemble average based on presumed PDF

Mean Turbulent Flame
Mean Flame Position – Level-set G-equation

\[ \tilde{G}(x_i, t) = \tilde{G}_0 = 0 \quad \Rightarrow \quad \frac{\partial \tilde{G}}{\partial t} + \frac{\partial \tilde{G}}{\partial x_i} \frac{\partial x_i}{\partial t} = 0 \quad (1) \]

\[ n_i = -\sqrt{\frac{\partial \tilde{G}}{\partial x_j} \frac{\partial \tilde{G}}{\partial x_j}} \quad (2) \]

\[ \frac{dx_i}{dt} = \tilde{u}_i + n_i s_T \quad (3) \]

*Insert (3) in (1)* \[ \Rightarrow \quad \frac{\partial \tilde{G}}{\partial t} + \tilde{u}_i \frac{\partial \tilde{G}}{\partial x_i} = -s_T n_i \frac{\partial \tilde{G}}{\partial x_i} \]

*Use (2)* \[ \Rightarrow \quad \frac{\partial \tilde{G}}{\partial t} + \tilde{u}_i \frac{\partial \tilde{G}}{\partial x_i} = s_T \sqrt{\frac{\partial \tilde{G}}{\partial x_j} \frac{\partial \tilde{G}}{\partial x_j}} \]
VR-1 LDA data: $u/S_L = 10 - 14; \ l/\delta_L = 40 - 200$

*Thin reaction & flamelet regime (Peters)*!
Previous RANS: CO Simulation

Exp. data
- high $S_T$, high $G_{var}$
- low $S_T$, high $G_{var}$
- low $S_T$, low $G_{var}$

EDC

CO mole fraction

$y$ [m]
RANS with new FLA: profiles at $x=150$ mm

(1) no stretch & wrinkling; (2) with stretch, no wrinkling; (3) with stretch & wrinkling

Nilsson & Bai 29th symp
RANS with new FLA: profiles at $x=350$ mm

(1) no stretch & wrinkling; (2) with stretch, no wrinkling; (3) with stretch & wrinkling

Nilsson & Bai 29th symp
Large eddy simulations: LES

- Filter away the small scales
- Retain the large eddies (larger than Taylor micro scales)
- Large scale unsteady motion is resolved
- Eddies smaller than the filter size need to be modeled
- Flame thickness is typically thinner than the LES grid size
- Models are needed to account for the unresolved scales
- Models are similar to the RANS models
- Computational cheaper than DNS, but more expensive than RANS
Large Eddy Simulation of bluff-body flame

Streamwise vorticity 500 1/s

Flame surface G=0

Flame fluctuations, large scale wrinkling are captured!
LES of HCCI engine