Numerical simulation study of turbulent combustion phenomena
-INTEGRATE Advanced Study Group (ASG)

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Introduction

- Some combustion related keywords
  - Energy, heat and power, transportation.
  - Emission, clean combustion, global warming.
  - Fossil fuel, Hydrogen, biomass
  - Combustion efficiency, combustion instability
  - Turbulence combustion
Introduction

- To understand turbulent reacting system, a challenge
- Turbulence + Chemistry → Wide range of scales
Research methodology

- Mathematical equations describing turbulent reacting flow
  - Flow turbulence
    - Navier-Stokes equations (Conservation of mass, momentum, energy), assuming low-Mach number.
      \[
      \frac{1}{\rho} \left( \frac{\partial \rho}{\partial t} + u_i \frac{\partial \rho}{\partial x_i} \right) = - \frac{\partial u_i}{\partial x_i} \\
      \rho \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) = \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \right) \\
      \rho C_p \left( \frac{\partial T}{\partial t} + u_i \frac{\partial T}{\partial x_i} \right) = - \sum_{k=1}^{N} \tilde{\omega}_k \tilde{Y}_k - \left( \rho \sum_{k=1}^{N} C_{p,k} \tilde{Y}_k \tilde{V}_{kj} \right) \frac{\partial T}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \lambda \frac{\partial T}{\partial x_j} \right)
      \]
  - Chemistry reaction
    - Conservation of \( N \) species mass
      \[
      \rho \left( \frac{\partial Y_k}{\partial t} + u_j \frac{\partial Y_k}{\partial x_j} \right) = - \frac{\partial \rho Y_k V_{kj}}{\partial x_j} + \tilde{\omega}_k
      \]
      \[
      -Y_k V_{kj} = D_k \frac{\partial Y_k}{\partial x_j} - Y_k \sum_{i=1}^{N} D_i \frac{\partial Y_i}{\partial x_j},
      \]
    - Reaction rates \( \omega_k \) is given by \( M \) elementary chemical reactions

Reactions for CH4/Air

- CH4 + O2 → CO + H2O + 2H
- CH4 + 2O2 → CO2 + 2H2O
- CH3OH + O2 → 2CO + 3H2O
- CH3OH + H2 → CH4 + 2H2
- CH3OH + OH → H2O + CH3
- CH3OH + HO2 → H2O2 + CH3
- CH3OH + H + M → CH3 + H2 + M
- CH3OH + O + M → CH3 + H2O + M
- CH3OH + H2O2 → CH4 + HO2
- CH3OH + OH2 → CH4 + H2O
- CH3OH + H2 → CH4 + H
- CH3OH + O2 → CH4 + O
- CH3OH + HO2 → CH4 + O2
- CH3OH + H2O2 → CH4 + O3
- CH3OH + OH2 → CH4 + H2O
- CH3OH + HO2 → CH4 + O2
- CH3OH + H2O2 → CH4 + HO2
- CH3OH + H2O2 → CH4 + O3
- CH3OH + H2O2 → CH4 + O2
- CH3OH + H2O2 → CH4 + HO2
- CH3OH + H2O2 → CH4 + O3
- CH3OH + H2O2 → CH4 + O2
- CH3OH + H2O2 → CH4 + HO2
Research methodology

- Numerical simulations of P.D.E governing turbulent reacting flow
  - Partial-resolution methods (filtered P.D.E., need models)
    - Reynolds Averaged Navier-Stokes (RANS)
      - Cheap; favored by industrial; Applied approach.
    - Large Eddy simulations (LES)
      - more accurate, capturing dynamic features
  - Full-resolution method (no model)
    - Direct (Detailed) numerical simulations (DNS)
      - Computational expensive, limited to very small size

\[
\begin{align*}
\text{log}(E(k)) \\
\text{resolved LES} & \quad \text{modeled LES} \\
\text{integral} & \quad 2\pi/\eta \\
\text{Kolmogorov} & \quad 2\pi/\delta
\end{align*}
\]
Data analysis: three case studies

1: DNS studies of homogenously charged compression ignition (HCCI) engine combustion.

2: DNS of turbulent premixed flame propagation

3: Fractal flame front structures due to flame (Landau-Darrieus) instability
Case 1: Internal combustion (IC) engine

- Four strokes
  - Intake
  - Compression
  - Expansion
  - Exhalation

- HCCI engine
  - Low NOx emission and high efficiency
  - Control problem

- Types of IC engine
  - Diesel engine
  - Spark ignition (SI) engine
Case 1: How does in-cylinder flow looks like?

- Full cycle LES of turbulent flow inside a typical diesel engine with curved-bowl shaped piston
Case 1: In-cylinder turbulent flow and \( T \) field

Piston with a squared bowl

\[
V = V_m + V_R
\]
Case 1: Some ways of engine-combustion

Engine combustion inside engine starts from an inhomogeneity in Temperature field and fuel/air concentration.

No spark
- Homogenously charged compression ignition (HCCI)
- Sensitive to T fluctuation

Add spark
- (combining flame propagation + ignition)
- Strong turbulence
- Weak turbulence
Case 1: What is HCCI combustion?

2D-DNS of H₂/Air **auto-ignition** in a small square (periodic) domain

**Initial condition:**
- Averaged T: 1070K
- T rms fluctuation: 50K
- Pressure: 41 bar
Case 1: What is HCCI combustion?

3D-DNS of Lean H2/Air auto-ignition in a small cubic (periodic) domain

Observations
- Multiple ignition kernels (initial hot spots)
- Two combustion modes
  - Slow deflagration wave
  - Rapid auto-ignition mode
- Complicate topological surface for the reaction front
  - Saddle surfaces
  - Spherical surfaces

Domain size: $5^3$ mm; Result plotting durations: 2 - 3 ms.
Initial condition: Averaged T: 1070K; T r.m.s. fluctuation: 50K Pressure: 41 bar
Case 1: Data analysis (Displacement speed: $S_d$)

$$S_d = - \frac{\text{Diffusion}(c) + \text{Reaction}(c)}{|\nabla c|}$$

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$$S_d = -\frac{\text{Diffusion}(c) + \text{Reaction}(c)}{|\nabla c|} \bigg|_{c^*}$$

![Graphs showing data analysis results with two sets of data for different L values: L=4.1mm and L=0.75mm.](image)
Case 1: Data analysis
Surface topology and its contribution to combustion process

1: Both strong saddle and spherical fronts occupy small fraction of total flame area, however they contributes more to the flame stretch, due to the associated larger $S_d$.
2: In early stage small spherical fronts contribute to a large fraction of total flame stretch, saddles surfaces changes from convex to concave quite early, they are reasonable for reduction of flame front area in late stage of combustion process.
Case 2: DNS of turbulent, statistical planar, premixed flame
Case 2: More distributed layer of radical species with increased turbulence intensity
Case 2: DNS of turbulent premixed combustion

At Intensive turbulence (Ka = 3350), two different fuel/air reactants

Case 2: Data analysis

Observations: High heat release rate at low temperature region

Non-conventional chemical pathway!
Caused by turbulent transport of the most-diffusive H radical!
Elementary reaction $R(9)$ is greatly enhanced:

$$H + O_2 + M \rightarrow HO_2 + M$$

Heat release contributed from $R(9)$ conditioned at $T<700K$
Case 3: Intrinsic flame instability
Darrieus-Landau (DL) instability (caused by density difference)

V-shaped flame in a weakly turbulent stream

Cusp shapes or cellular flames shapes, developed with no (or weak) turbulence

(From Fox and Weinberg 1963)
Case 3: Simulations of LD instability in periodic channel

Increasing channel width:
- Curved flame, but stationary.
- Non-stationary flame cusp formation.
- Fractal flame structure.
Case 3: Data analysis

- Fractal flame

Fractal cascading structures:

(1) 4-6 (intermediate) cells on a (largest) cell

(2) 4-7 (minor) cells on a (intermedia) cell
Case 3: Data analysis
The Fractal flame cascading concept

Gostintsev, et al. 1988

Koch snowflake
Case 3: Data analysis: Fractal dimension (1+d)

Power-law fitting of the velocity amplification ($U_w$)

Power law fitting of $U_w$
(Propagation speed after reaching statistical stationary)

$$
\frac{U_w}{S_L} \sim C \left( \frac{\lambda}{\lambda_c} \right)^d
$$

$C \approx 0.65 - 0.75$

$d \approx 0.2 - 0.3$

No analytical theory available for large channel width
Case 3: Data analysis: Fractal dimensions ($1 + d'$)
Box-counting of fractal images

Box counting
$d' \approx 0.07 \pm 0.124$
Thanks for your attention