Numerical simulation on gas combustion and spray flames

Fang Wang

Beihang University

- It was established in 1952. Last year, it is the 60 anniversary!
- It comprises 27 schools, 17 academician and 3759 faculties. The enrollment is over 27800, including 14428 UG, 4015 Ph.D candidates, 668 oversea.
Ranking and the School

- General ranking: 7-15 in China;
- Aerospace propulsion Theory and Engineering, No.1, Power Engineering and Engineering Thermal Physics, No.7.
- Our school has four departments and one national key laboratory: Department of Aviation propulsion, Department of Fluid Machinery, Department of Engineering Thermophysics, Department of Thermal Engineering, The National Key Laboratory on Aero-Engines.

Content

- Numerical simulation on
  - gas combustion: An algebraic sub-grid scale turbulent combustion model
  - spray flames: An droplet burning model
Gas turbine combustor

- Gas-liquid two phase turbulent combustion
- Droplets tracing, chemical kinetics, turbulent flow in complex geometry, turbulent reaction rate, radiation, ...
Turbulent combustion rate

- RANS, LES, DNS are the three strategies...
- Turbulent combustion rate is a big problem in combustion simulation, because of the exponential part.

\[ w_i = B \rho^2 Y_1 Y_2 \exp\left(-\frac{E}{RT}\right) \]

- The average reaction rate is not the function of the averaged value
- Couple with turbulence...another big problem
- Turbulent combustion models are needed for engineering applications.

Background – about SGS combustion model

- Recently, Large eddy simulation (LES) is becoming used in engineering applications.
- For gas turbine combustion chambers, it is used to solve the flow topology, emission, compressor/turbine interaction, cooling, ...problems
- The sub-grid scale (SGS) combustion model is one of the key aspects of LES method.
- There are various SGS combustion models: the laminar flamelet model (Pitsch et al., Senoner et al. and Mattsson et al.), assumed PDF combustion model (Moin et al, James et al.), linear eddy model (Menon et al.), EBU model (Menon et al.), PDF equation model (James et al.), Dynamically Thickened Flame combustion model (Poinsot et al.) …
- The SGS turbulent combustion model is still in developing
**Background - DNS verification and LES validation**

- As an important tool for fundamental studies, **direct numerical simulation (DNS)** attracted increasing interest in recent years.
- Attention is paid to finding detailed instantaneous flow and flame structures, understanding the turbulence/flame interaction (Poinset et al., Zhang and Rutland) and verifying RANS and LES models (Zhang and Rutland, Luo, Overholt and Pope, Bedat et al., Sreedhara and Huh, Hawkes and Chen, Chong and Heinz).
- **So the SGS model should be better verified by DNS before applying to test cases.** Thus, in this paper:
  - A direct numerical simulation of turbulent reacting channel flows, taking the buoyancy effects account, is performed using a spectral method, and the DNS database is used to verify the SGS combustion model.
  - This SGS combustion model is tested using methane and *methanol-air* jet flame.

**DNS Governing Equations**

\[
\frac{\partial u_i}{\partial x_i} = 0
\]

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ v \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - F_i \right] - F'_i = - \frac{g}{T_w} \frac{T - T_w}{T_w}
\]

\[
\frac{\partial}{\partial t} \left( Y_i \right) + \frac{\partial}{\partial x_j} (u_j Y_i) = \frac{\partial}{\partial x_j} (D \frac{\partial Y_i}{\partial x_j}) - \frac{w_i}{\rho} \quad i = 1, 2
\]

\[
\frac{\partial}{\partial t} (T) + \frac{\partial}{\partial x_j} (u_j T) = \frac{\partial}{\partial x_j} \left( \frac{\lambda}{c_p \rho} \frac{\partial T}{\partial x_j} \right) + w_i Q_i / (c_p \rho)
\]

- The buoyancy effect using Boussinesq approximation.

**One-step Arrhenius chemical kinetics**

\[
w_i = B \rho^2 \alpha \beta \gamma \exp \left(- \frac{E}{RT} \right)
\]
Numerical Methods

- **Galerkin-Tau spectral** expansion method: Fourier transform is used in x and z directions and the Chebyshev transform is used in the y direction;
- **Uniform grid** distribution is used in x and z directions and the Gauss-Lobatto nonuniform grid distribution is used in the y direction. $128 \times 128 \times 129$ results in a total of 2.11 million nodes. The time step used is $0.01H/U_m$ with a third-order scheme.
- For all cases the mass fraction of species 1 (fuel) is given as 1.0 at the top wall and 0.0 at the bottom wall, whereas the mass fraction of species 2 (oxidizer) is given as 0.0 at the top wall and 1.0 at the bottom wall. The wall temperature is given as 900K.
- Periodic boundary conditions are used in the longitudinal and span-wise directions and solid-wall boundary conditions are used on the top and bottom boundaries.

Parameters for DNS Cases

<table>
<thead>
<tr>
<th>Case</th>
<th>B</th>
<th>E/R (K)</th>
<th>Q  (kJ/kg)</th>
<th>$F_y$ (m/s²)</th>
</tr>
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<td>0</td>
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<td>8</td>
<td>$10^8$</td>
<td>15000</td>
<td>100</td>
<td>$F_y$</td>
</tr>
<tr>
<td>9</td>
<td>$10^8$</td>
<td>20000</td>
<td>100</td>
<td>$F_y$</td>
</tr>
</tbody>
</table>

\[
\frac{\partial}{\partial t} T + \sum_j \frac{\partial}{\partial x_j} (u_j T) = \sum_j \left( \frac{\lambda}{c_p \rho} \frac{\partial T}{\partial x_j} + w_i Q_i / (c_p \rho) \right) + w_i Y_i \exp\left(-\frac{E}{RT}\right) = \rho^2 KY_i Y_z
\]
**LES Governing Equations**

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho \tilde{u}_j) = 0
\]

\[
\frac{\partial}{\partial t} (\rho \tilde{u}_i) + \frac{\partial}{\partial x_j} (\rho \tilde{u}_i \tilde{u}_j) = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial P}{\partial x_i} - \rho \frac{\partial \tau_{ij}}{\partial x_j} \right)
\]

Smagorinsky-Lilly's eddy viscosity model

\[
\tau_{ij} = -2 \mu_i \tilde{S}_{iy} + \frac{1}{3} \tau_{kk} \delta_{ij}
\]

\[
\frac{\partial \rho \tilde{Y}_s}{\partial t} + \frac{\partial}{\partial x_j} (\rho \tilde{u}_j \tilde{Y}_s) = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \tilde{Y}_s}{\partial x_j} - \frac{\partial g_{sj,i}}{\partial x_j} \right) - \frac{\partial q_{sj}}{\partial x_j}
\]

The filtered reaction rate and the SGS reaction rate

\[
g_{sj,i} = \frac{\mu_i}{Sc_{s,i}} \frac{\partial \tilde{Y}_s}{\partial x_j}
\]

\[
q_{sj} = \frac{\mu_i}{Pr} \frac{\partial \tilde{T}}{\partial x_j}
\]

**ASSCM SGS Combustion Model**

\[
\frac{\partial \rho \tilde{Y}_s}{\partial t} + \frac{\partial}{\partial x_j} (\rho \tilde{u}_j \tilde{Y}_s) = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \tilde{Y}_s}{\partial x_j} - \frac{\partial g_{sj,i}}{\partial x_j} \right) - \frac{\partial q_{sj}}{\partial x_j}
\]

The filtered reaction rate The SGS reaction rate

\[
\tilde{W}_s = \rho^2 K \tilde{Y}_{ox} \tilde{Y}_{fu}
\]

\[
w_{s,i} = \rho^2 \left[ K (\tilde{Y}_{ox} \tilde{Y}_{fu} - \tilde{Y}_{ax} \tilde{Y}_{fu}) + Y_{ox} (K \tilde{Y}_{fu} - K \tilde{Y}_{ox}) + Y_{fu} (K \tilde{Y}_{ox} - K \tilde{Y}_{ax}) \right]
\]

\[
(K \tilde{Y}_{ox} - K \tilde{Y}_{ax}) = C_{K,\omega} \frac{\partial K}{\partial x_j} \frac{\partial \tilde{Y}_{ox}}{\partial x_j}
\]

The constant \( C \) is 0.005
The DNS Instantaneous Results (1)

- In cases without scalar-velocity interaction, the velocity is rather independent of the scalar, and the scalar transportation does not affect the velocity field. Typically the velocity/scalar field is full of the strip structures.
- In the interaction cases (case 8), The buoyancy term is a moderate two-way coupling between the velocity and the scalar transportation. The buoyancy force is in the y direction, but the transportation induced by it can be seen in the longitudinal (z) direction.
The DNS Verification (1)

The ASSCM model is generally given as:

$$R_{\Phi \Psi} = \Phi \overline{\Psi} - \Phi \overline{\Psi} = C_{\Phi, \Psi} \frac{\partial \overline{\Phi}}{\partial x_i} \frac{\partial \overline{\Psi}}{\partial x_j}$$

Directly from instantaneous DNS database

From the filter-averaged DNS database

DNS Verification (2)

- The model results has the same trend as the exact solution. For all 3 cases, the $R_{VV}$ value remains in the same range, while the $R_{KV}$ value changes significantly.
- There are maximum errors of about 30%, 50% and even over 100%...
- Though these cases are not ideal examples for real reaction flow, they give a theoretical understanding of the model. In some regions, the ASSCM combustion model is close to the exact solution, so further validation should be carried out.
LES Validation - Gas Jet Flame (Flame D)

Jet flame structure and the simulation mesh

Central section of the simulation mesh

- The methane-air reaction kinetics:

\[ w_{fu} = 2.119 \times 10^{11} Y_{O_2}^{1.3} Y_{H_2}^{0.2} \exp(-2.027 \times 10^8 / RT) \]

Instantaneous Contours for Flame D

- Velocity
- Mean Temperature
- RMS of Temperature
The Average Temperature

The error is less than 5%

ASSCM SGS model validation

- We have proposed the algebraic sub-grid turbulent combustion model (ASSCM) and used it in premixed combustion and a partly-diffusion flame. The statistical results were close to measurements.
- Here, we applied it for two-phase combustion cases.

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  - spray flames: An droplet burning model

Full Status two phase combustion model

There is single droplet burning in combustion chamber and spray flames
Need to be modeling

H H Chiu, AIAA 95-2427, A new droplet model for spray combustion, 1995

The full status droplet combustion model (1)

The upper one is the general treatment of droplet, while the lower one is our new model;

The critical point B is from the droplet ignition studies; and the correlation of the droplet combustion with evaporation state is from single droplet combustion studies.

The full status droplet combustion model (2)

• For the criterion for point B, three judgments are used:
  1. The droplet diameter is bigger than 0.001mm;
  2. The ambient temperature is higher than 1200 K;
  3. The evaporation time is longer than the ignition time.

• The ignition delay time function is:
  \[ \tau_i = A \exp \left( \frac{E}{RT_w} \right) C_{oxygen}^{-0.5} C_{methanol}^{-0.1} \]

• The evaporation time is defined as:
  \[ \tau_e = \frac{d_i^2}{k_e} \]

• As for the burning correlation, the traditional \( D^2 \) law is taken, here the \( k_e \) is 0.7 \( \text{mm}^2/\text{s} \).
  \[ k_e = -d \left( \frac{d_i^2}{dt} \right) \]
\[ \frac{dT_d}{dt} = \frac{NuC_p g}{3 Pr_g C_p l} \left( \frac{T_g - T_d}{\tau_d} \right) + h_{fg} m_d \frac{m_d}{C_p l m_d} \]

\[ m_d = \frac{dm_d}{dt} = -\frac{m_d}{3 Sc g \tau_d} (Sh + Sh^w) \ln(1 + B) \]

After burning:

\[ \frac{d(d_p)}{dt} = \frac{4k_{\infty}}{\rho_p C_{p,\infty} d_p} (1 + 0.23 \sqrt{Re_d}) \ln[1 + \frac{C_{p,\infty} (T_\infty - T_p)}{h_{fg}}] \]

More air, more gas mixture combustion preferential

LES in gas phase; ASSCM turbulent combustion model;

\[ w_{fu} = 1.799 \times 10^{10} \rho^2 Y_{CH_2OH}^{0.25} Y_{O_2}^{1.5} \exp \left( \frac{-1.256 \times 10^8}{RT} \right) \]

Contours of static temperature (K)

Temperature profiles (case 1)

FSDCM - new model; Original – traditional model; □ - experimental data
Temperature profiles (case 2)

FSDCM - new model; □ - experimental data

Temperature profiles (case 3)

FSDCM - new model; □ - experimental data
Thank you!