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Chemical Reaction Engineering IV”
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DNS and LES of
Turbulent Combustion

Luc Vervisch
INSA de Rouen, IUF, CORIA-CNRS
Pascale Domingo, Julien Réveillon
Sandra Payet, Cécile Péra & Raphael Hauguel
Combustion system:

- Turbulent flow
  - Large Scales → Smaller Scales → DNS
  - LES
  - RANS

- Unsteady large scales lead to an imperfect mixing in the system. Those scales are geometry dependent and feature a long lifetime.

- Micro-mixing mechanisms bring reactants in contact within thin reaction zones.
OUTLINE

✓ DNS of turbulent combustion.

✓ Overview of turbulent combustion modeling.

✓ One example of SGS modeling in LES of premixed turbulent combustion.

✓ SGS modeling of partially premixed combustion.
Resolution needed for full simulation:

- **Flow:**

\[ \eta_k \approx \frac{l_t}{Re_\lambda^{3/2}} \]

\[ 10^{-6} \text{ m} < \eta_k < 10^{-4} \text{ m} \]

<table>
<thead>
<tr>
<th>Re_\lambda</th>
<th>Memory</th>
<th>Speed</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>70</td>
<td>50 Gbytes</td>
<td>50 Gflops</td>
<td>1993</td>
</tr>
<tr>
<td>300</td>
<td>50 Tbytes</td>
<td>50 Tflops</td>
<td>2002</td>
</tr>
<tr>
<td>1500</td>
<td>50 Pbytes</td>
<td>50 Pflops</td>
<td>2015?</td>
</tr>
</tbody>
</table>

*J. Jiménez, Eng. Turbulence Modelling and Experiments-5, 2002*

- **Flame (CH4/AIR):**

\[ h \approx 5 \times 10^{-6} \text{ m} \]

\[ \Delta t \approx 1 \times 10^{-6} \text{ s} \]

So far, three types of ‘full solutions’ (DNS):

- DNS of synthetic model problem (freely decaying turbulence).
- DNS of laboratory flame, but at much lower Re.
- DNS of laboratory flame.

**Chemistry:**
- Single-step
- Reduced
- Tabulated
- Detailed

**Transport:**
- Fixed Lewis and Schmidt
- Variable Lewis & Schmidt
- Complex
Premixed Turbulent V-Flame

RANS VIEW

HOT WIRE

DNS

Boukhalfa & Renou, INSA de Rouen
Complex chemistry FPI-FGM:

$u'/S_L = 2.5$

$u'/S_L = 1.25$

$u'/S_L = 3.75$
Overview of turbulent combustion modeling tools
Geometrical analysis

Iso-surface:
Study topology and dynamics of iso-mixture fraction surfaces

Flame normal analysis:
Gather information in the direction normal to the flame surface defined by \( Z = Z_{st} \)

One-point statistical analysis
Collect information at every point of the flow

Flame surface density
\( G \)-Eq or \( c \)-Eq

Flamelet modeling

CMC

PDF transport
Control parameter of molecular mixing?

\[ \rho \left( \frac{\partial Z}{\partial t} + u \cdot \nabla Z \right) = \nabla \cdot (\rho D \nabla Z) \]

\[ f = Z(1 - Z) \]

\[ \rho \left( \frac{\partial f}{\partial t} + u \cdot \nabla f \right) = \nabla \cdot (\rho D \nabla f) + 2\rho D |\nabla Z|^2 \]

\[ V_d = D |\nabla Z| \quad l_d = |\nabla Z|^{-1} \]

\[ \tau^{-1} = V_d / l_d = D |\nabla Z|^2 = \chi Z \]
Micromixing

Conditional scalar dissipation rate

\[
\frac{\overline{P}(c^*; x, t)}{\partial t} = \cdots \cdot \frac{\partial^2}{\partial c^2} \left( \left( \rho \chi \frac{\nabla c}{c^*} \right) \overline{P}(c^*; x, t) \right)
\]

Combustion Tools

Veynante & Vervisch,Prog In Energ Sci, 28:193-266 2002

\[
\overline{P}(c^*; x, t) \rightarrow \Sigma(c^*; x, t) = \left( \left\langle \frac{\nabla c}{c^*} \right\rangle \overline{P}(c^*; x, t) \right) G(c^*; x, t)
\]

Surface or G-field
"Academic" combustion regimes

Prémélange

Fuel + Oxidizer

_products

\[ \Phi(Z_o) \]

Diffusion

\[ Z = 0 \]

Oxi  Fuel  Oxi

\[ Z_s \]

\[ Z = 1 \]
Premixed flame LES filtering

Filtering a stoichiometric premixed Propane/Air Flame

GS fluctuation

 прогрессивный
SGS Probability Density Function in premixed flames:

- The thin flame front has a characteristic scale within the subgrid.
- The thin flame is seen at the grid scale $\Delta$.

**EFFECTS**

1. Thickening by the filter of the thin flame front over the coarse LES grid.
2. Wrinkling of the flame within the subgrid that results from interaction with subgrid vortices.
Flame surface density contains information on the flame characteristic length:

\[ \Sigma(c^*; x, t) = \left( \overline{\nabla c} \right) \tilde{P}(c^*; x, t) \]
Filtered gradient contains two points information

\[
\bar{G}_\Delta(c(x)) = \int_{+\infty}^{\infty} |\nabla c|^{FP_{PI}} G_\Delta(x - x') \, dx'
\]
Get the PDF from the Flame Surface Density inside the flame:

\[
\tilde{P}(c^*; x, t) = \frac{\Sigma(c^*; x, t)}{|\nabla c||c^*|}
\]

\[
\tilde{P}(c^*; x, t) = \alpha(x, t)\delta(c^*) + \beta(x, t)\delta(1 - c^*)
\]

\[
+ \frac{\sigma(x, t)}{G_\Delta(c^*)} H(c^*) H(1 - c^*)
\]

\[
\overline{G}_\Delta(c(x)) = \int_{-\infty}^{+\infty} |\nabla c|^{FP\overline{I}} G_\Delta(x - x') dx' \]
Describing SGS variance of progress variable:

\[ \tilde{C}_v = \tilde{CC} - \tilde{C} \tilde{C} \]

Energy that is not resolved by the coarse LES grid.

• Try to get it from resolved scales:
  - Scale similarity hypothesis.
  - Equilibrium hypothesis.

• Solve a balance equation to get SGS variance:
  - Which balance equation is the best?
  - Close unknown terms.
\[ \tilde{C}_V = \tilde{C}C - \tilde{C}\tilde{C} \]

Scale similarity assumption:

\[ \tilde{C}_V = C_C (\tilde{C}\tilde{C} - \tilde{C}\tilde{C}) \]

\[ \hat{\Delta} > \Delta \]

Filtered DNS
\[ \widetilde{C}_v = \widetilde{C}\tilde{C} - \widetilde{C}\widetilde{C} \]

**Equation for SGS variance:**

\[
\frac{\partial \bar{\rho} \widetilde{c}_v}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u} \widetilde{c}_v) = -\nabla \cdot \overline{\tau}_{cv} + \nabla \cdot (\bar{\rho} D \nabla \widetilde{c}_v) \\
- 2\overline{\tau}_c \cdot \nabla \widetilde{c} + 2\bar{\rho} D |\nabla \widetilde{c}|^2 - 2\bar{\rho} D |\nabla \widetilde{c}|^2 \\
+ 2\bar{\rho} (\widetilde{\omega}_c \bar{c} - \widetilde{\omega}_c \widetilde{c})
\]

**Production - Dissipation and Source**

**Dissipation:**

\[ \bar{\rho} D |\nabla \widetilde{c}|^2 - \rho D |\nabla \widetilde{c}|^2 \approx -\bar{\rho} \widetilde{c}_v / \tau_t \]

\[ \nu_T \approx (C_s \Delta)^2 |\tilde{S}| \quad |\tilde{S}| = (2\tilde{S} \cdot \tilde{S})^{1/2} \]

\[ \tau_t \approx \Delta^2 / (\nu_T / SC_T) \quad \tilde{S} = (1/2)(\nabla \bar{u} + \nabla^T \bar{u}) \]
Equilibrium hypothesis:

\[ \tilde{c}_v = C_v \left( \Delta^2 |\nabla \tilde{c}|^2 + \left( \tilde{\omega}_c c - \tilde{\omega}_c \tilde{c} \right) \frac{\Delta^2}{(\nu_T / S \epsilon_T)} \right) \]

Filtered DNS
Chose the appropriate variable to be transported (the one that minimizes LES numerical problems…)

- Solve for the departure from maximum variance:

\[
\tilde{c}_v = \tilde{c}\tilde{c} - \tilde{c}\tilde{c} = \tilde{c}(1 - \tilde{c}) - \tilde{\varphi}_c
\]

\[
\bar{\rho}\tilde{\varphi}_c = \bar{\rho}c(1 - c) = \bar{\rho}\tilde{c}(1 - \tilde{c}) (1 - S)
\]

Unmixedness:

\[
S = \frac{\tilde{c}_v}{\tilde{c}(1 - \tilde{c})}
\]
The modeled balance equations to be solved for presuming the PDF then reads:

\[
\frac{\partial \rho \tilde{c}}{\partial t} + \nabla \cdot (\rho \tilde{u} \tilde{c}) = \nabla \cdot (\rho (D + (\nu_T / S c_T)) \nabla \tilde{c}) + \rho \tilde{\omega}_c
\]

\[
\frac{\partial \rho \tilde{\varphi}_c}{\partial t} + \nabla \cdot (\rho \tilde{u} \tilde{\varphi}_c) = \nabla \cdot (\rho (D + (\nu_T / S c_T)) \nabla \tilde{\varphi}_c)
\]

**Scalar dissipation rate**

\[
+ \quad 2\rho \left( D |\nabla \tilde{c}|^2 + C_D \frac{\nu_T}{S c_T} \frac{\tilde{c}_v}{\Delta^2} \right)
\]

**Chemical source**

\[
+ \quad \rho \left( \tilde{\omega}_c - 2\tilde{\omega}_c \tilde{c} \right)
\]
LES CHEMICAL TABLES

Averaging FGM or FPI

SGE:

✓ Fully Compressible Flow.

✓ 4th ordre in space, 2nd in time.

✓ Dynamic Lagrangian Modeling.
  Meneveau et al, JFM, 353-386, 1996.

✓ Structure Function.
  M. Lesieur Team.
Test premixed SGS modeling on ORACLES (Nguyen and Bruel, AIAA-2003-0958.)
Time averaged streamwise velocity frozen flow mixing:
Progress variable:

Time averaged streamwise velocity:
Time averaged spanwise velocity:
Time averaged spanwise velocity:
Time averaged RMS velocity:
OUTLINE

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Industrial combustion

Nox emission control
Nonpremixed turbulent flame base:

Zone 1: Premixed properties
- Thin reaction zones
- Interface fresh/burnt
- Propagation
- Stabilization

Zone 2: Diffusion properties
- Mixing controlled
- Pollution
- Flame length

Muniz & Mungal, Combust. Flame 111(1/2), 1997
Chemistry is faster

Diffusion is faster

Flux in Z

Diffusion flame

Premixed Combustion

Equilibrium

Methane-air

Takeno’s flame index to determine combustion regime:

\[ G_{FO} = \nabla Y_F \cdot \nabla Y_O \]

<table>
<thead>
<tr>
<th>Premixed</th>
<th>Diffusion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel + Oxidizer → Products</td>
<td>Fuel → Oxidizer</td>
</tr>
</tbody>
</table>

\( G_{FO} > 0 \) \quad \text{Premixed} \\

\( G_{FO} < 0 \) \quad \text{Diffusion}
DNS of lifted flames:

Mixture fraction

Progress variable

Conditional flame index

Premixed Diffusion

Hot air 900K \( St = 0.4 \)

Sixth order PADE, Third order time stepping, NSCBC Boundary conditions

\[
\xi_p = \frac{1}{2} \left( 1 + \vec{n}_F \cdot \vec{n}_O \right),
\]
DNS of weakly turbulent flame bases:

Gaseous

Spray

Marley et al.
FTaC 72(1), 29-47, 2004
Turbulent flame base structure (gaseous case):


Amplitude of the burning rate in premixed mode:

\[ \xi_p = \frac{1}{2} \left( 1 + \frac{\nabla Y_F}{|\nabla Y_F|} \cdot \frac{\nabla Y_O}{|\nabla Y_O|} \right) = 1 \text{ Premixed} \]

\[ = 0 \text{ Diffusion} \]

\[ W_p(x) = \frac{\int_y \xi_p \dot{\omega} dy}{\int_y \dot{\omega} dy} \]
Fraction of premixed burning:

\[ W_p(x) = \frac{\int \xi_p \omega_F \, dy}{\int \omega_F \, dy} \]

![Graphs showing comparison between Gaseous and Spray cases]
Diffusion flamelet, but only for the “diffusion-part”:

\[
\chi Z \frac{dY_F^d}{dZ^2} = -\dot{\omega}_F^d(Z, \chi Z)
\]

\[
\mathcal{I}_d^{DNS} = \int_{L_y} (1 - \xi_p) \dot{\omega}_F dy
\]

\[
\mathcal{I}_d^{Eq.38} = \int_{L_y} (1 - \xi_p) \dot{\omega}_F^d(Z, \chi Z) dy
\]

Gaseous

Spray
Flame decomposition:

\[
\bar{\omega}_F = \xi_p \bar{\omega}_F^p + (1 - \xi_p) \bar{\omega}_F^d
\]

Modeled decomposition:

\[
\bar{\omega}_F = \bar{\alpha}_p \bar{\omega}_F^p + \bar{\alpha}_d \bar{\omega}_F^d
\]

Modeled coefficients:

\[
\bar{\alpha}_p = \frac{\xi_p \bar{\omega}_F^p}{\bar{\omega}_F^p} \quad \bar{\alpha}_d = \frac{(1 - \xi_p) \bar{\omega}_F^d}{\bar{\omega}_F^d}
\]
Modeled decomposition:


\[
\overline{\dot{\omega}}_F = \overline{\alpha}_p \overline{\dot{\omega}}^p_F + \overline{\alpha}_d \overline{\dot{\omega}}^d_F
\]