LES of industrial turbulent reacting flows: modeling effects and challenges

L.Y.M. Gicquel

B. Cuenot, E. Riber, G. Staffelbach, A. Dauptain, N. Odier
F. Duchaine, O. Vermorel, J. Dombard, A. Misdiaris
T. Poinsot

1 CERFACS - CFD combustion team, Toulouse
2 CNRS - IMFT, Toulouse
† http://www.cerfacs.fr/~lgicquel
Combustion: An engineering science at the cross-road between chemistry & fluid mechanics with strong technological / industrial and societal implications.
Turbulent reacting flows have been from the beginning studied and theoretically addressed as true/pure multi-scale multi-physics problems:

### DNS
- Chemical reactions
- Turbulence

### LES
- Flame Flow/Obstacle interactions

### Large scale industrial problems
- Geometrical complexities

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- ~100 μm
- ~1 mm
- ~10 mm
- ~100 mm
- ~1 m
- ~10 m
- ~100 m
- ~1 km

- ~1 ms
- ~10 ms
- ~1 s
- ~10 s
- ~1 min
- ~10 min
- ~1 h
- ~1 jour
Recent industrial achievement by SAFRAN SHE


- Industrial burner with 1.1B elements for the geometry
- Turbulent compressible, gaseous reacting LES

Selective refinement (chamber only) based on the Pampa Library using MMG3D (collaboration with C. Lachat & C. Dobrzynski, A. Froelhy from INRIA)

<table>
<thead>
<tr>
<th>Case</th>
<th># of cells</th>
<th>360 equiv # of cells</th>
<th>Δ_{cell}</th>
<th>F_{max}</th>
</tr>
</thead>
<tbody>
<tr>
<td>mesh 1</td>
<td>11M</td>
<td>220M</td>
<td>Δ₀</td>
<td>100</td>
</tr>
<tr>
<td>mesh 2</td>
<td>33M</td>
<td>660M</td>
<td>Δ₀/2</td>
<td>50</td>
</tr>
<tr>
<td>mesh 3</td>
<td>220M</td>
<td>4400M</td>
<td>Δ₀/4</td>
<td>25</td>
</tr>
<tr>
<td>mesh 4</td>
<td>1030M</td>
<td>20600M</td>
<td>Δ₀/7</td>
<td>14</td>
</tr>
</tbody>
</table>

CCRT supercomputing center: COBALT grand challenges
Twelve years to do:

- ~1,500 times on the number of cells and ~250 times on the number of procs
- improved reduced chemistry model PLUS NOx and CO (crude models)
- homogeneous vs heterogeneous multi perforated plate model
- full transfer to the industry
I ] HPC & turbulent reacting flow CFD

II ] Ignition / transient turbulent reacting flows

2.1 GT context: engine ignition prediction
2.2 Explosion: deflagrating fronts

III ] Difficulty of the initial phase

IV ] GT applications: emission predictions & multi-phase flows

Conclusions and perspectives
II. Ignition / transient turbulent reacting flows

Ignition = fully transient laminar/turbulent reacting flow

Aeronautical GT's:
- Ignition = first design phase
  => light around time: fctt of the burner size…
- Safety issues

Fuel plants:
- Security issue / risk management

Deepwater horizon, 2010
Buncefield, 2005

L = inter-injector?
Common features & differences

Single sector configuration

Multi sector configuration

EARLY STAGES OF IGNITION

PROPAGATION PHASE

L = inter-injector?


II.1 Light around phase - turbulent combustion dominated problem

- Low injector spacing (SP9)
- High injector spacing (SP26)
Evolution of the luminous signal (CH emissions vs. Heat release images):

- Large spacing:
  - Experimental variability
  - Large overall ignition time

- Low spacing:
  - High repeatability
  - Rapid ignition process
• Ignition times for each injector

- SP9

- SP16

• Ignition time between two consecutive injectors

- Good estimation of the ignition times for each injectors
- 2 distinct propagation modes (inj/inj propagation times)
II.2 ] Deflagration problem - fully transient and transitioning problem

Experiments Conducted by

Medium scale problem: i.e L ~1.5 m

LES

Time: 1.0
SGS modeling impact on the predictions

- **Reaction rate:**
  - Fixed resolved contribution regardless of the modeling
  - Modeling effectively scales the SGS contribution and thereof the net consumption rate (⇒ shift in time)
  - Different modeling = different turbulent combustion flame speeds
  - Faster combustion = higher peak pressure

⇒ High sensitivity to SGS model !!

Does not fully explain the reason why a constant delay exists between the various ignition times
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Conclusions and perspectives
III Initial phase issues

Major issues:
- it is not clear what is the initial state of these flow problems
- we do not know what and how much energy is deposited…
  => pseudo deterministic / stochastic description
  => difficult to know what really counts…

Very few data is available on the experimental side and most of the time it is time or spatially integrated….}

IGNITION SYSTEM STUDIES
Small scale / lab-scale configuration
<1ms
- Plasma physics
- Ignition chemistry
- Heat transfer

IGNITION TRANSIENT STUDIES (NUMERICS / LES)

Effect of stretch on the fuel consumption speed

\[ S_c = S_L^0 - \mathcal{L}_a^c \kappa \]

with
\[ \kappa = \frac{1}{S} \frac{\partial S}{\partial t} \] (stretch)

\[ \mathcal{L}_a^c = \frac{1}{2} \beta (L_{\text{fuel}} - 1) \delta_L^0 \]

\[ \left( \frac{T_{FG}}{T_{BG} - T_{FG}} \right) \int_0^{\frac{T_{BG} - T_{FG}}{T_{FG}}} \frac{\ln(1 + x)}{x} dx \]
1/ Potential importance in deflagration simulations:

- Stretch definitely can play a role in the early instants (always spheric and laminar)
- Thermo diffusive instabilities can appear here !
  ⇒ Impact on the local transition to turbulence (?)
- Stretch is also present when the flame front reaches obstacles…

2/ Potential importance in GT simulations:

- Stretch is rapidly present and strongly impact the initial kernel behavior (quenching…)
- As the flame propagates in the turbulent flow, it faces very different turbulent flow states…
Potential chemistry modeling issues

Thermo-chemical model and its impact

Flame propagation: C3H8, 0 array

<table>
<thead>
<tr>
<th>φ =1</th>
<th>$S_L^0$</th>
<th>$T_{ad}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>GRI-MECH</td>
<td>38.4 cm/s</td>
<td>2275 K</td>
</tr>
<tr>
<td>2-steps</td>
<td>38.4 cm/s</td>
<td>2289 K</td>
</tr>
<tr>
<td>1-step</td>
<td>38.4 cm/s</td>
<td>2400 K</td>
</tr>
</tbody>
</table>

- $\phi = 1$: same laminar flame speed
- 1-step adiab. Temp. overestimated by 5%

$$S_d = \frac{\rho_{GF}}{\rho_{GB}} \cdot S_L^0$$
overshot

Characteristic diag.: C3H8, 3-arrays
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Conclusions and perspectives
IV] Application to a GT: pollutant emissions & multi-phase flows

Today reduced chemistry schemes are accessible in terms of tools and CPU

Analytically Reduced Chemistry (ARC) for C3H8 / air combustion

**Pepiot-Desjardins / Jerzembeck** skeletal scheme

Derived from the LLNL comprehensive mechanisms
- 99 transported species
- 669 reactions

Reference mechanism => skeletal mechanism:
- DRGEP

Skeletal mechanism => reduced scheme:
- QSSA using the LOI criterion

**ARC C3H8-22-12qss:**
- 22 transported species
- 173 reactions
- 12 QSS species

LES
OH Concentration

OH PLIF [1]

Heat release rate

3 Bars

6 Bars

HRR/\rho \ [W/kg]
Exhaust pollutant concentrations

- **NO**
  - Satisfactory prediction
  - Slight under-prediction
  - Trend correctly recovered
- **CO**
  - Significant over-prediction

Deterioration of **NO prediction**

- Improvement of temperature prediction
- Significant improvement of **CO prediction** at the exit: driven by equilibrium
Single burner setup: SICCA-Spray

EM2C laboratory (Paris)

Multi-phase reacting flows

Steady operating conditions
- cold non-reacting
- reacting spray flame

Thermo acoustically unstable configuration

Wall interaction model: SLIP
Wall interaction model: FILM

CERFACS
Conclusions & perspectives

Current progresses in LES @ CERFACS include more and more complexity

=> In terms of chemistry: ARC schemes needed to predict pollutants will improve the quality of the laminar flame speed predictions for simple flames provided that these schemes are properly constructed from adequate reference schemes.

=> ARC will however not alleviate the dependency of the turbulent combustion closure to the laminar flame speed (and thickness) for non-planar flames… i.e. how to properly incorporate stretch and strain effects

=> Multi-phase flames clearly add complexity: depending on the droplets, different regimes of combustion appear and their effect on the flame thickness and speed are not fully understood…