LES OF A STRATIFIED TURBULENT BURNER WITH A THICKENED FLAME MODEL COUPLED TO ADAPTIVE MESH REFINEMENT AND DETAILED CHEMISTRY

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Regulation on pollutants emissions become stricter
=> Need for highly accurate numerical tools to design systems

Large-Eddy Simulation (LES) routinely used in the industry

New technologies with low emissions based on lean premixed and stratified combustion regimes
Large-Eddy Simulation (LES): **Large resolved scales** + **small modelled scales**

**ISSUE 1:** The flame structure is not resolved on the LES grid as the LES grid size is typically larger than the flame.

**ISSUE 2:** Interactions between unresolved turbulent structures and the flame front have to be modeled.

\[ \delta_l^0 \ll \Delta x \quad \Delta x \]

*(Typically 0.5 to a few mm)*
THICKENED FLAME MODEL (TFM)

- The flame front is artificially thickened to ensure sufficient resolution

\[ F = \max \left( \frac{n_{res} \Delta x}{\delta_l^0}, 1 \right) \]

- Subgrid scale (SGS) interactions described by a wrinkling factor:

\[ \Xi_\Delta = \frac{A}{A_0} \]

- Turbulent flame speed propagation:

\[ S_T = \Xi_\Delta S_l^0 \]
Performance of the TFM model decreases when the mesh size increases (less flame/turbulence interactions resolved; more is modelled)

- LES is expensive => mesh resolution is limited

Opportunity: Adaptive Mesh Refinement (AMR)
  - Idea: Refine the mesh only where necessary and hence reduce computational costs

**OBJECTIVE:** couple TFM and AMR to propose a model for highly accurate simulation of gas turbines at low computational cost
I. TFM-AMR model: coupling Thickened Flame Model with Adaptive Mesh Refinement

II. Validation of TFM-AMR on planar laminar flames

III. Simulation of the Cambridge stratified burner

IV. Conclusion
**ADAPTIVE MESH REFINE MENT: PRINCIPLE**

- **AMR inputs**
  - AMR sensor
  - AMR level

**AMR algorithm**

Generation of new grid using user-defined criterion

**LES SOLVER**

- Equations solved on current AMR mesh
- Solving TFM model equations:

\[
\frac{\partial \bar{Y}_k}{\partial t} + \frac{\partial \bar{u} \bar{Y}_k}{\partial x} = \frac{1}{\rho} \left( \frac{\mu}{S_c} + (1 - \hat{S}) \frac{\mu}{S_t} \frac{\partial \bar{Y}_k}{\partial x} \right) + \bar{\omega} \frac{\phi}{F} \rho \bar{\omega}_k
\]

- Resolved fields and modeling variables
  - \( \bar{Y}_k, \bar{T}, \bar{u}, F, \ldots \)

**Updated refined mesh**
Dynamic TFM modeling framework: We only thicken in the flame

=> Definition of a flame sensor $S$

Redefinition of the thickening factor:

$$F = F_{max} + (S - 1)F_{max}$$

AMR is activated when $S > 0$ (equivalently: $F > 1$)
TFM-AMR MODEL: AMR LEVEL DEFINITION

- AMR mesh size: \( \Delta x = \Delta_x^{\text{Base}} / 2^{n_{AMR}} \)

  \( \Rightarrow \) Thickening factor in flame region: \( F_{max} = \max \left( \frac{n_{res}\Delta_x^{\text{Base}}}{2^n_{AMR}\delta_0^0(\phi)}, 1 \right) \)

- **Default strategy:** set a constant AMR refinement level when the AMR sensor is active

**Solution retained:** adapt the AMR level to local flame conditions to optimize the number of added nodes.
**Set-up:** planar laminar flame propagation

Laminar flame propagation speed:

\[
S_c(t) = \frac{1}{\rho_u(y^u_{fuel} - y^b_{fuel})} \int_{x=-\infty}^{+\infty} \rho \dot{\omega}_{fuel}(x, t) \, dx
\]

**Numerical set-up:**
- Solver: CONVERGE
- Equivalence ratio: \( \phi = 0.75 \)
- 30 species skeletal mechanism for \( CH_4 \)
PLANAR LAMINAR FLAME SIMULATIONS

SIMULATION 1: TFM on a regular mesh

SIMULATION 2: TFM-AMR with $F_{\text{target}} = 5$ on coarse mesh

SIMULATION 3: TFM-AMR with $F_{\text{target}} = 2.5$ on coarse mesh

$\delta_l^0 \approx 0.5\text{mm}$

$\Delta_x = 0.5\text{mm}$

$\Delta_x^{\text{AMR}} = 0.5\text{mm}$

$\Delta_x = 1\text{mm}$

$\Delta_x^{\text{AMR}} = 0.25\text{mm}$

$\Delta_x = 1\text{mm}$
RESULTS: LAMINAR FLAME PROPAGATION

: TFM on standard mesh
(\(\Delta_x = 0.5\)mm)

: TFM-AMR (\(F_{\text{target}} = 5 \Rightarrow \Delta_x = 0.5\)mm in flame)

: TFM-AMR (\(F_{\text{target}} = 2.5 \Rightarrow \Delta_x = 0.25\)mm in flame)
RESULTS: LAMINAR FLAME STRUCTURE

- Reference laminar flame
- TFM on standard mesh ($\Delta x = 0.5\text{mm}$)
- TFM-AMR ($F_{target} = 5 \Rightarrow \Delta x = 0.5\text{mm in flame}$)
- TFM-AMR ($F_{target} = 2.5 \Rightarrow \Delta x = 0.25\text{mm in flame}$)
III. VALIDATION ON A 3-D BURNER: EXPERIMENTAL SET-UP

Cambridge SwB burner (Sweeney et al., 2012):

OPERATING CONDITIONS
Flow:
- Inner/Outer tube speeds: \( U_i = 8.31, U_o = 18.7 \)
- Reynolds numbers: \( Re_i = 5960, Re_o = 11500 \)

Flame:

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Inlet mixtures</th>
</tr>
</thead>
<tbody>
<tr>
<td>SwB1 (premixed)</td>
<td>( \phi_i = 0.75; \phi_o = 0.75 )</td>
</tr>
<tr>
<td>SwB5 (stratified)</td>
<td>( \phi_i = 1.0; \phi_o = 0.5 )</td>
</tr>
</tbody>
</table>

NUMERICAL SET-UP
Solver: CONVERGE CFD SOFTWARE
Chemistry:
- 30 species skeletal mechanism
- SAGE chemistry solver with adaptive zoning to speed up calculations

Physical models:
- Turbulence model: SIGMA
- SGS wrinkling model: algebraic Charlette
VALIDATION STRATEGY

Non-reacting flow simulation on coarse LES grid

Default option (used in other CFD codes): embedding in a large area

New methodology: AMR on coarse LES grid

Comparison to validate the TFM-AMR strategy

Flame simulation with TFM and embedded refined grid

Flame simulation with TFM and AMR

\[ F_{\text{target}} = 5 \Rightarrow \Delta x = 0.5 \text{mm for } \phi = 0.75 \]
TFM-AMR MODEL BEHAVIOR
Dilution by air co-flow
$\Rightarrow \phi$ is decreased
$\Rightarrow n_{AMR}^* \approx 1$

Region of premixed burning
($\phi = 0.75$)
$\Rightarrow n_{AMR}^* = 2$
COMPARISON WITH EXPERIMENT: TEMPERATURE

- SwB1 (premixed)
- SwB5 (stratified)

- Embedded TFM
- TFM-AMR ($F_{\text{target}} = 5$)
COMPARISON WITH EXPERIMENT: CARBON MONOXIDE

- **SwB1 (premixed)**
  - $z = 10$ mm
  - $z = 50$ mm

- **SwB5 (stratified)**
  - $z = 10$ mm
  - $z = 50$ mm

**Legend:**
- **Blue Line:** Embedded TFM
- **Green Line:** TFM-AMR ($F_{target} = 5$)
AMR refinement study:

TFM-AMR with $F_{target} = 5$

TFM-AMR with $F_{target} = 2.5$

AMR $n_{AMR} = 2$
($\Delta x = 0.5 \text{mm}$)

AMR $n_{AMR} = 3$
($\Delta x = 0.25 \text{mm}$)
TEMPERATURE STATISTICS

SwB1 (premixed)  SwB5 (stratified)  SwB1 (premixed)  SwB5 (stratified)

$z = 10\text{mm}$  $z = 10\text{mm}$  $z = 10\text{mm}$  $z = 10\text{mm}$

$z = 50\text{mm}$  $z = 50\text{mm}$  $z = 50\text{mm}$  $z = 50\text{mm}$

$\text{mean } \bar{T} [K]$  $\text{mean } \bar{T} [K]$  $\text{RMS } T [K]$  $\text{RMS } T [K]$

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: TFM-AMR ($F_{target} = 5$)

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: TFM-AMR ($F_{target} = 2.5$)
CARBON MONOXIDE STATISTICS

\[ \text{mean } \tilde{Y}_{CO} [-] \]

\[ \text{RMS } \tilde{Y}_{CO} [-] \]

- SwB1 (premixed)
  - \( z = 10 \text{mm} \)
  - \( z = 50 \text{mm} \)

- SwB5 (stratified)
  - \( z = 10 \text{mm} \)
  - \( z = 50 \text{mm} \)

\[ \text{TMM-AMR (} F_{\text{target}} = 5) \]

\[ \text{TMM-AMR (} F_{\text{target}} = 2.5) \]
COMPUTATIONAL COSTS

CPU cost / CPU cost on reference mesh

\[ \Delta_{x}^{\text{flame}} = 1mm \quad \Delta_{x}^{\text{flame}} = 0.5mm \quad \Delta_{x}^{\text{flame}} = 0.25mm \]

- Static embedding
- TFM-AMR
CONCLUSION AND PERSPECTIVES

A new model based on the coupling between Thickened Flame Model (TFM) and Adaptive Mesh Refinement (AMR) has been developed for premixed and stratified combustion.

TFM-AMR model has been validated on the Cambridge swirled burner in premixed and stratified operating conditions.

Conclusions:
- TFM-AMR leads to an optimization of the flame simulation providing iso-resolution at lower computational cost compared to conventional simulations.
- For similar costs, TFM-AMR enables to perform simulations with a better mesh resolution and hence improving predictions.

Perspectives:
- In depth study of unresolved turbulence / flame interactions when using TFM-AMR
- Extension of TFM-AMR to spray combustion
REFERENCES

RESULTS: NON-REACTING FLOW

- Simulation on coarse grid
- Simulation on refined grid
FLAME THICKENING

- **Thickening factor**: the flame is broadened by a factor 

\[ \mathcal{F} = \max \left( \frac{n_{res} \Delta x}{\delta_l^0(\phi)}, 1 \right) \]

Where \( n_{res} \) is the number of grid points in the flame thickness.

- **Scaling laws**: 

\[ \delta_l^0 \propto \sqrt{\frac{D_{th}}{\dot{\Omega}}} \quad \text{and} \quad S_l^0 \propto \sqrt{D_{th} \dot{\Omega}} \]

- **Modeling requirements**: 

\[ \delta_l^0 \rightarrow \mathcal{F} \delta_l^0 \quad \text{and} \quad S_l^0 \rightarrow S_l^0 \]

  - Diffusion multiplied by \( \mathcal{F} \) and reaction rates by \( 1/\mathcal{F} \)

- **Transport equation for species mass fractions**:

\[
\frac{\partial \rho \tilde{Y}_k}{\partial t} + \frac{\partial \rho \tilde{u} \tilde{Y}_k}{\partial x} = \frac{\partial}{\partial x} \left( \mathcal{F} \frac{\mu}{Sc} \frac{\partial \tilde{Y}_k}{\partial x} \right) + \frac{1}{\mathcal{F}} \rho \tilde{\omega}_k
\]

\[D_{th}: \text{Heat diffusivity}\]

\[\dot{\Omega}: \text{Mean reaction rate}\]
Final transport equation for species mass fractions (TFM model):

\[
\frac{\partial \rho \tilde{Y}_k}{\partial t} + \frac{\partial \rho \tilde{u} \tilde{Y}_k}{\partial x} = \frac{\partial}{\partial x} \left( \mathcal{F} \Xi \Delta \frac{\mu}{S_c} + (1 - \hat{S}) \frac{\mu_t}{S_{ct}} \frac{\partial \tilde{Y}_k}{\partial x} \right) + \frac{\Xi \Delta}{\mathcal{F}} \overline{\rho \omega_k}
\]

- Resolution of the flame front thickness
- Accurate turbulent propagation speed
- Only flame front is thickened
TFM-AMR MODELING STRATEGY: AMR LEVEL COMPUTATION

Principle:
- Setting a target flame thickening value $F_{target}$
- Computing the theoretical AMR level $n^*_{AMR}$ to reach the $F_{target}$ value

Relationship between $n^*_{AMR}$ and $F_{target}$:

$$\frac{\delta_l^0(\phi)F_{target}}{n_{res}} = \frac{\Delta_{Base}}{2^n_{AMR}}$$

Theoretical AMR level:

$$n^*_{AMR} = \frac{1}{\log(2)} \log \left( \frac{n_{res} \Delta_{Base}}{\delta_l^0(\phi)F_{target}} \right)$$