Low-Dimensional Manifolds in Direct Numerical Simulations of Autoigniting Mixing Layers

Jeroen van Oijen, Ugur Göktolga, Philip de Goey

4th IWMRRF
San Francisco, June 2013
MILD combustion

- Promising combustion concept
  - High efficiency
  - Low emissions
  - Homogeneous temperature
  - Low noise

- Preheated and diluted reactants
  - Exhaust gas recirculation
  - High initial T: autoignition
  - Low flame T: low NO_x emissions

Courtesy IFRF
Objective

Develop a numerical model for MILD combustion
• Flamelet based chemical reduction (FGM)
• Large eddy simulation (LES)

Multi-scale approach
• Detailed simulations of micro-scale reaction structures ($10^{-4}$ m)
  • Reveal fundamental processes
  • Develop reduced chemistry model (FGM)
• Simulation of lab-scale flames ($10^{-2}$ m)
  • Develop turbulent combustion model (LES/FGM)
• Application in industrial-scale burner systems ($10^{0}$ m)
Jet-in-Hot-Coflow (JHC) burners

- Berkeley, Cabra et al.
- Adelaide, Dally et al.
- Delft, Oldenhof et al.
- …
DNS of turbulent mixing layers

- Investigate reaction structures
- Compressible equations
- Detailed chemistry: DRM19
- Constant non-unity Lewis numbers
- Compact finite difference
  - 6th order diffusion terms
  - 5th order convective terms
- Low-storage 3rd order RK
  - Time step equals 10 ns
Numerical implementation

- 2D domain 20x20 mm
- 521x521 grid points, $h=38\mu m$
  - Validated with 1041x1041
- Conditions similar to experiments of Dally et al. 2002
- $U_{fu} - U_{ox} = 67$ m/s
  - Re = 3850
- Three cases (HM1/2/3)

<table>
<thead>
<tr>
<th>Oxidizer</th>
<th>$Y_{O_2}$</th>
<th>$Y_{N_2}$</th>
<th>$Y_{H_2O}$</th>
<th>$Y_{CO_2}$</th>
<th>$Z_{st}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$ (K)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1300</td>
<td>0.03</td>
<td>0.85</td>
<td>0.065</td>
<td>0.055</td>
<td>$0.67 \times 10^{-2}$</td>
</tr>
<tr>
<td>1300</td>
<td>0.06</td>
<td>0.82</td>
<td>0.065</td>
<td>0.055</td>
<td>$1.34 \times 10^{-2}$</td>
</tr>
<tr>
<td>1300</td>
<td>0.09</td>
<td>0.79</td>
<td>0.065</td>
<td>0.055</td>
<td>$1.99 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

**DNS results 2D mixing layer**

<table>
<thead>
<tr>
<th>$H_2$</th>
<th>$H$</th>
<th>$\Delta T = T - T_{\text{mix}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$t = 0.00 \text{ ms}$

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
</table>

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
</table>

HM1: $Y_{O_2} = 0.03$

$K_a = \tau_{ig} / \tau = O(10)$

Green lines: $Z_{st} = 0.0067$
Ignition time

- Maximum $Y_H$ and temperature rise $\Delta T$ as a function of time
- Comparison with laminar mixing layer and 0D homogeneous ignition
Scalar dissipation rate

Grey dots: Scatter
Symbols: Cond. average log $\chi$
Bold line: Laminar

$t = 0.2$ ms
Scatter plots in mixture fraction space

$t = 0.2\, \text{ms}$

$t = 0.4\, \text{ms}$
Scatter plot conditioned at $Z = Z_{st}$

Progress variable $Y$ is a normalized linear combination of reaction products.
Igniting laminar mixing layer with FGM

- Assume a 2D manifold $Y = f(Z, \mathcal{V})$
- Create 2D manifold from 1D igniting mixing layers $Y(x, t) \mapsto Y(Z, \mathcal{V})$
- Solve transport equations for controlling variables $Z, \mathcal{V}$
FGM validation: scalar dissipation rate

- Temperature rise in 1D igniting counterflow flames (Cabra exp.)
- FGM created with strain rate $a = 100 \text{ s}^{-1}$
- Comparison FGM (dashed) vs detailed chemistry (solid)
LES of JHC: $H_2$ addition

$CH_4$

$25\% H_2$

Artega Mendez & Roekaerts
TU Delft, The Netherlands

E. Abtahizadeh
Conclusions

- MILD combustion occurs in thin reaction diffusion layers
- Due to the very low values of $Z_{st}$, the reaction layers lie at the edge of the turbulent mixing layer
- Ignition chemistry appears to proceed along a lower-dimensional manifold
- A 2D FGM can accurately predict the ignition delay time
  - Counterflow flames: various strain rates
  - JHC flames: capture effect of $H_2$ addition
Outlook

- More realistic DNS
  - Include variations in coflow composition and temperature
  - Include turbulence in the coflow
  - 3D turbulence
- Validating FGM in DNS
- Quantitative comparison of LES/FGM results with experiments
- Investigate fuel effects
- $\text{NO}_x$ predictions
Thank you!

- My coworkers
- Dutch Technology Foundation