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<table>
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<th>04 Jan 2016</th>
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<tbody>
<tr>
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<td>Briefing Charts</td>
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**4. TITLE AND SUBTITLE**

Application of Detailed Chemical Kinetics to Combustion Instability Modeling

**6. AUTHOR(S)**

Harvazinski, Matt; Talley, Doug; Sankaran, Venke

**7. Performing Organization NAME(S) and ADDRESS(ES)**

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For presentation at AIAA SciTech 2016 (January 2016) PA Case Number: #15705; Clearance Date: #12/15/2015
This document contains in-house research only which is relevant to work done on this contract

**14. ABSTRACT**

Briefing Charts

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<table>
<thead>
<tr>
<th>a. REPORT</th>
<th>b. ABSTRACT</th>
<th>c. THIS PAGE</th>
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<tbody>
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**17. LIMITATION OF ABSTRACT**

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**19a. NAME OF RESPONSIBLE PERSON**

E. Weber

**19b. TELEPHONE NO**

N/A
Application of Detailed Chemical Kinetics to Combustion Instability Modeling

Matt Harvazinski, Doug Talley, Venke Sankaran

Air Force Research Laboratory
*Edwards AFB, CA*
Challenges of Combustion Instability

Combustion instability is an organized, oscillatory motion in a combustion chamber sustained by combustion.

Irreparable damage can occur in less than 1 second.

Damaged engine injector faceplate caused by combustion instability

“Combustion instabilities have been observed in almost every engine development effort, including even the most recent development programs”


Distribution A: approved for public release; distribution unlimited.
Prior Work – Kinetics Used

• Simulations:
  1) 3D real geometry
  2) Unsteady
  3) Long run-times
  4) Coupled physics
• 1-4 have forced the use of simplified kinetics
  – Global reactions

\[
\begin{align*}
\text{CH}_4 + 2\text{O}_2 & \rightarrow 2\text{H}_2\text{O} + \text{CO}_2 \\
2\text{CH}_4 + 3\text{O}_2 & \rightarrow 2\text{CO} + 4\text{H}_2\text{O} \\
2\text{CO} + \text{O}_2 & \leftrightarrow 2\text{CO}_2 \\
2\text{CH}_4 + \text{O}_2 & \rightarrow 2\text{CO} + 4\text{H}_2 \\
\text{CH}_4 + \text{H}_2\text{O} & \rightarrow \text{CO} + 3\text{H}_2 \\
2\text{H}_2 + \text{O}_2 & \leftrightarrow \text{H}_2\text{O} \\
\text{CO} + \text{H}_2\text{O} & \leftrightarrow \text{CO}_2 + \text{H}_2
\end{align*}
\]
Global mechanisms can be tuned but have limited parameters to adjust.

The flowfields contain widely varying parameters, making tuning to operating conditions difficult at best.

Mixture fraction for the same operating condition at different times.

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Single Step Results

Simulation

Experiment

Amplitudes under predicted by 10%,
Frequencies over predicted by 15% (or more)

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Two-dimensional Study

2D study showed substantial improvement in amplitudes with detailed kinetics, BUT, 2D predictions were always worse compared with 3D.

Sardeshmukh et al. 2015
### Current Work: Detailed kinetics in 3D

<table>
<thead>
<tr>
<th></th>
<th>Global</th>
<th>Detailed GRI-1.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of reactions</td>
<td>1</td>
<td>177</td>
</tr>
<tr>
<td>Number of species</td>
<td>4</td>
<td>31</td>
</tr>
<tr>
<td>Number of cores</td>
<td>960</td>
<td>21,600</td>
</tr>
<tr>
<td>Core hours per ms</td>
<td>11,520</td>
<td>259,200</td>
</tr>
</tbody>
</table>

Extremely Expensive!  
22.5× more than Global

---

**CVRC Experiment**

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Experimental Results

Unsteady pressure for a translating test

PSD power for the first mode

Harvazinski et al. 2013

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Instability Mechanism

- **Flow Disruption**
- **Heat Release Moves Downstream**
- **Unburnt Accumulated Fuel**

**Unstable: Cyclic Fuel Disruption and Heat Release**

**Marginally Stable: Continuous Heat Release**

**Combustion Reinitiated from Returning Post Wave**

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A similar delay is observed for the marginally stable operating point.
Fluctuating Pressure

Marginally Stable

Unstable

More cycle to cycle variability

Steep-fronted waves

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PSD Analysis – Marginally Stable

Global simulation – 40 ms (35 ms of data used for analysis)
Detailed Simulation – 20 ms (15 ms of data used for analysis)

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### Detailed Comparison

**Marginally Stable**

<table>
<thead>
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<th>Mode</th>
<th>Experiment</th>
<th>Global</th>
<th>Detailed</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>$f$, Hz</td>
<td>$p'_{ptp}$, kPa</td>
<td>$f$, Hz</td>
</tr>
<tr>
<td>1</td>
<td>1379</td>
<td>121.70</td>
<td>1.00</td>
</tr>
<tr>
<td>2</td>
<td>2734</td>
<td>5.86</td>
<td>1.98</td>
</tr>
<tr>
<td>3</td>
<td>3882</td>
<td>16.03</td>
<td>2.82</td>
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- Error in the frequency is reduced from 20% to 11%
- Error in 1st mode amplitude goes from 6% too high to 18% too high
- Amplitudes of the harmonic also show an increase

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Global simulation – 40 ms (35 ms of data used for analysis)
Detailed Simulation – 20 ms (15 ms of data used for analysis)
## Detailed Comparison

### Unstable Stable

<table>
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<tr>
<td></td>
<td>$f$, Hz</td>
<td>$f$, Hz</td>
<td>$f$, Hz</td>
</tr>
<tr>
<td></td>
<td>$p'_{ptp}$, kPa</td>
<td>$p'_{ptp}$, kPa</td>
<td>$p'_{ptp}$, kPa</td>
</tr>
<tr>
<td></td>
<td>$f_i/f_1$</td>
<td>$f_i/f_1$</td>
<td>$f_i/f_1$</td>
</tr>
<tr>
<td>1</td>
<td>1324</td>
<td>1543</td>
<td>1467</td>
</tr>
<tr>
<td></td>
<td>387.15</td>
<td>349.10</td>
<td>416.79</td>
</tr>
<tr>
<td></td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>2</td>
<td>2655</td>
<td>3114</td>
<td>2933</td>
</tr>
<tr>
<td></td>
<td>89.29</td>
<td>87.55</td>
<td>130.41</td>
</tr>
<tr>
<td></td>
<td>2.01</td>
<td>2.01</td>
<td>2.00</td>
</tr>
<tr>
<td>3</td>
<td>3979</td>
<td>4629</td>
<td>4400</td>
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<tr>
<td></td>
<td>46.37</td>
<td>36.25</td>
<td>64.88</td>
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<tr>
<td></td>
<td>3.01</td>
<td>3.00</td>
<td>3.00</td>
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Error in the frequency is reduced from 15% to 10%

Error in 1st mode amplitude goes from 10% too low to 7% too high

Amplitudes of the harmonic also show an increase

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Detailed Results - Unstable

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Detailed Cycle Evaluation

Global

Detailed

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Time 1

Global

(b) Time 1.

Heat Release, MW/m³

0 10000 20000 30000 40000 50000

Detailed

(b) Time 1.

Heat Release, MW/m³

0 10000 20000 30000 40000 50000

Static Pressure, Pa

1.2E+06 1.4E+06 1.6E+06 1.8E+06

CH₄ Mass Fraction

0.0 0.2 0.4 0.6 0.8 1.0

(a) Time 1.

Static Pressure, Pa

1.2E+06 1.4E+06 1.6E+06 1.8E+06

CH₄ Mass Fraction

0.0 0.2 0.4 0.6 0.8 1.0

(a) Time 1.

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Time 4

Global

Detailed

(h) Time 4.

(h) Time 4.

(g) Time 4.

(g) Time 4.

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Time 5

Global

Detailed

(i) Time 5.

(ii) Time 5.

Distribution A: approved for public release; distribution unlimited.
Time 6

Global

Detailed

(l) Time 6.

(l) Time 6.

(k) Time 6.

(k) Time 6.

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Detailed Results – Marginally Stable

Distribution A: approved for public release; distribution unlimited.
Detailed Cycle Evaluation

Global

Detailed

Distribution A: approved for public release; distribution unlimited.
Time 1

Global

Heat Release, MW/m³

0 10000 20000 30000 40000 50000

(b) Time 1.

Detailed

Heat Release, MW/m³

0 10000 20000 30000 40000 50000

(b) Time 1.

Static Pressure, Pa

1.2E+06 1.4E+06 1.6E+06 1.8E+06

(a) Time 1.

CH₄ Mass Fraction

0.0 0.2 0.4 0.6 0.8 1.0

Static Pressure, Pa

1.2E+06 1.4E+06 1.6E+06 1.8E+06

(a) Time 1.

CH₄ Mass Fraction

0.0 0.2 0.4 0.6 0.8 1.0

Distribution A: approved for public release; distribution unlimited.
Time 2

Global

(d) Time 2.

Detailed

(d) Time 2.

(c) Time 2.

(c) Time 2.

Distribution A: approved for public release; distribution unlimited.
Time 3

Global

(f) Time 3.

Detailed

(f) Time 3.

(e) Time 3.

(e) Time 3.

Distribution A: approved for public release; distribution unlimited.
Time 5

Global

Detailed

(j) Time 5.

(j) Time 5.

(i) Time 5.

(i) Time 5.

Distribution A: approved for public release; distribution unlimited.
Time 6

Global

Detailed

(l) Time 6.

(l) Time 6.

(k) Time 6.

(k) Time 6.

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Summary and Conclusions

• A comparison of global and detailed kinetics mechanisms was completed for two operating conditions of a rocket injector

• Detailed kinetics showed higher amplitudes and lower frequencies
  — Frequencies still do not match experimental values, heat transfer is the remaining unknown

• The cyclic heat release of the unstable case was predicted by both mechanisms
Summary and Conclusions

• Similar results between both mechanisms suggest that in this configuration:
  – The flow is mixing dominated
  – The coupling between pressure and heat release is captured sufficiently by the global mechanism
  – Differences in the heat release locations is a secondary effect and does not drive the instability

• The prior improvement observed in the 2D simulations suggests that the poor ability to predict mixing in 2D is the key problem, not the simplicity of the kinetics.
Questions

Acknowledgments

All computing resources were provided by the DoD high performance computing modernization program. Substantial resources for the detailed chemistry simulations were obtained through the TI-14 and TI-15 Capability Applications Project, Phase II.

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