The Dynamics of Unsteady Detonation in Ozone

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Motivation

- Computational tools are critical in design of aerospace vehicles which employ high speed reactive flow.
- Small structures are continuum manifestations of molecular collisions.
- We explore the transient behavior of detonations with fully resolved detailed kinetics.
Verification and Validation

- **verification**: solving the equations right (math).

- **validation**: solving the right equations (physics).

- Main focus here on verification

- Some limited validation possible, but detailed validation awaits more robust measurement techniques.

- Verification and validation always necessary but never sufficient: finite uncertainty must be tolerated.
Model: Reactive Euler Equations

- one-dimensional,
- unsteady,
- inviscid,
- detailed mass action kinetics with Arrhenius temperature dependency,
- ideal mixture of calorically imperfect ideal gases
Model: Reactive Euler PDEs

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) = 0, \\
\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u^2 + p) = 0, \\
\frac{\partial}{\partial t} \left( \rho \left( e + \frac{u^2}{2} \right) \right) + \frac{\partial}{\partial x} \left( \rho u \left( e + \frac{u^2}{2} + \frac{p}{\rho} \right) \right) = 0, \\
\frac{\partial}{\partial t} (\rho Y_i) + \frac{\partial}{\partial x} (\rho u Y_i) = M_i \omega_i, \\
p = \rho \mathcal{R} T \sum_{i=1}^{N} \frac{Y_i}{M_i}, \\
e = e(T, Y_i), \\
\dot{\omega}_i = \dot{\omega}_i(T, Y_i).
\]
Computational Methods

• Steady wave structure
  – LSODE solver with IMSL DNEQNF for root finding
  – Ten second run time on single processor machine.

• Unsteady wave structure
  – Shock fitting coupled with a high order method for continuous regions
  – see Henrick, Aslam, Powers, *J. Comp. Phys.*, 2006, for full details on shock fitting
Outline of Shock Fitting Method

• Transform from lab frame to shock-attached frame
  – example mass equation becomes
  \[
  \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} \left( \rho (u - D) \right) = 0
  \]

• In interior, approximate spatial derivatives with fifth order Lax-Friedrichs discretization

• At shock boundary, one-sided high order differences are utilized
Outline of Shock Fitting Method

- Note that some form of an approximate Riemann solver must be used to determine the shock speed, \( D \), and thus set a valid shock state.
- At downstream boundary, a zero gradient (constant extrapolation) approximation is utilized.
- Fifth order Runge-Kutta time integration is employed.
## Ozone Reaction Kinetics

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$a_f^{R}, a_r^f$</th>
<th>$\beta_f^{f}, \beta_r^f$</th>
<th>$E_f^{f}, E_r^f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_3 + M \leftrightarrow O_2 + O + M$</td>
<td>$6.76 \times 10^6$</td>
<td>2.50</td>
<td>$1.01 \times 10^{12}$</td>
</tr>
<tr>
<td></td>
<td>$1.18 \times 10^2$</td>
<td>3.50</td>
<td>0.00</td>
</tr>
<tr>
<td>$O + O_3 \leftrightarrow 2O_2$</td>
<td>$4.58 \times 10^6$</td>
<td>2.50</td>
<td>$2.51 \times 10^{11}$</td>
</tr>
<tr>
<td></td>
<td>$1.18 \times 10^6$</td>
<td>2.50</td>
<td>$4.15 \times 10^{12}$</td>
</tr>
<tr>
<td>$O_2 + M \leftrightarrow 2O + M$</td>
<td>$5.71 \times 10^6$</td>
<td>2.50</td>
<td>$4.91 \times 10^{12}$</td>
</tr>
<tr>
<td></td>
<td>$2.47 \times 10^2$</td>
<td>3.50</td>
<td>0.00</td>
</tr>
</tbody>
</table>

Validation: Comparison with Observation


- \( p_o = 1.01325 \times 10^6 \text{ dyne/cm}^2, T_o = 298.15 \text{ K}, \)
  \( Y_{O_3} = 1, Y_{O_2} = 0, Y_O = 0. \)

<table>
<thead>
<tr>
<th>Value</th>
<th>Streng, <em>et al.</em></th>
<th>this study</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_{CJ} )</td>
<td>1.863 \times 10^5 \text{ cm/s}</td>
<td>1.936555 \times 10^5 \text{ cm/s}</td>
</tr>
<tr>
<td>( T_{CJ} )</td>
<td>3340 \text{ K}</td>
<td>3571.4 \text{ K}</td>
</tr>
<tr>
<td>( p_{CJ} )</td>
<td>3.1188 \times 10^7 \text{ dyne/cm}^{2}</td>
<td>3.4111 \times 10^7 \text{ dyne/cm}^{2}</td>
</tr>
</tbody>
</table>

Slight overdrive to preclude interior sonic points.
Stable Strongly Overdriven Case: Length Scales

\[ D_0 = 2.5 \times 10^5 \text{ cm/s}. \]
Mean-Free-Path Estimate

• The mixture mean-free-path scale is the cutoff *minimum* length scale associated with continuum theories.

• A simple estimate for this scale is given by *Vincenti and Kruger, ’65*:

\[ \ell_{mfp} = \frac{M}{\sqrt{2N} \pi d^2 \rho} \sim 10^{-7} \text{ cm}. \]
Stable Strongly Overdriven Case: Mass Fractions

\[ D_o = 2.5 \times 10^5 \text{ cm/s}. \]
Stable Strongly Overdriven Case: Temperature

\[ D_o = 2.5 \times 10^5 \text{ cm/s}. \]
Stable Strongly Overdriven Case: Pressure

\[ D_o = 2.5 \times 10^5 \, cm/s. \]
Stable Strongly Overdriven Case: Transient Behavior for Various Resolutions

Initialize with steady structure of $D_o = 2.5 \times 10^5 \text{ cm/s}$. 

![Graph showing transient behavior for various resolutions](image-url)
3 Cases Near Neutral Stability: Transient Behavior

![Graph showing transient behavior with different values of D0.](image)
Slightly Unstable Case: Transient Behavior

Initialized with steady structure, $D_o = 2.4 \times 10^5 \text{ cm/s}$.
Case After Bifurcation: Transient Behavior

Initialized with steady structure of $D_o = 2.1 \times 10^5 \text{ cm/s.}$
Long Time $D_{\text{max}} / D_0$ versus $D_{\text{min}} / D_0$
# Effect of Resolution on Unstable Moderately Overdriven Case

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>Numerical Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1 \times 10^{-7} \text{ cm}$</td>
<td>Unstable Pulsation</td>
</tr>
<tr>
<td>$2 \times 10^{-7} \text{ cm}$</td>
<td>Unstable Pulsation</td>
</tr>
<tr>
<td>$4 \times 10^{-7} \text{ cm}$</td>
<td>Unstable Pulsation</td>
</tr>
<tr>
<td>$8 \times 10^{-7} \text{ cm}$</td>
<td>$O_2$ mass fraction $&gt; 1$</td>
</tr>
<tr>
<td>$1.6 \times 10^{-6} \text{ cm}$</td>
<td>$O_2$ mass fraction $&gt; 1$</td>
</tr>
</tbody>
</table>

- Algorithm failure for insufficient resolution
- At low resolution, one misses critical dynamics
Conclusions

- Unsteady detonation dynamics can be accurately simulated when sub-micron scale structures admitted by detailed kinetics are captured with ultra-fine grids.
- Shock fitting coupled with high order spatial discretization assures numerical corruption is minimal.
- Predicted detonation dynamics consistent with results from one-step kinetic models.
- At these length scales, diffusion will play a role and should be included in future work.