Nonlinear dynamics of hydrogen-air detonations with detailed kinetics and diffusion

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Unsteady, Compressible, Reactive Navier-Stokes Equations

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \]
\[ \frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{uu} + p \mathbf{I} - \mathbf{\tau}) = 0, \]
\[ \frac{\partial}{\partial t} \left( \rho \left( e + \frac{\mathbf{u} \cdot \mathbf{u}}{2} \right) \right) + \nabla \cdot \left( \rho \mathbf{u} \left( e + \frac{\mathbf{u} \cdot \mathbf{u}}{2} \right) + (p \mathbf{I} - \mathbf{\tau}) \cdot \mathbf{u} + \mathbf{q} \right) = 0, \]
\[ \frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \mathbf{u} Y_i + j_i) = \overline{M_i} \dot{\omega}_i, \]
\[ p = \mathcal{R} T \sum_{i=1}^{N} \frac{Y_i}{M_i}, \quad e = e (T, Y_i), \quad \dot{\omega}_i = \dot{\omega}_i (T, Y_i), \]
\[ j_i = \rho \sum_{\substack{k=1 \atop k \neq i}}^{N} \frac{M_i D_{ik} Y_k}{M} \left( \frac{\nabla y_k}{y_k} + \left( 1 - \frac{M_k}{M} \right) \frac{\nabla p}{p} \right) - \frac{D_i T}{T} \nabla T, \]
\[ \mathbf{\tau} = \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right), \]
\[ \mathbf{q} = -k \nabla T + \sum_{i=1}^{N} j_i h_i - \mathcal{R} T \sum_{i=1}^{N} \frac{D_i T}{M_i} \left( \frac{\nabla y_i}{y_i} + \left( 1 - \frac{M_i}{M} \right) \frac{\nabla p}{p} \right). \]
Computational Methods

- Inviscid
  - Shock-fitting: Fifth order algorithm adapted from Henrick et al. (J. Comp. Phys., 2006)
  - Shock-capturing: Second order min-mod algorithm

- Viscous
  - Wavelet method (WAMR), developed by Vasilyev and Paolucci (J. Comp. Phys., 1996 & 1997)
  - User-defined threshold parameter controls error

- All methods used a fifth order Runge-Kutta scheme for time integration

- See Romick, Aslam, Powers, JFM, 2012
Case Examined

- Overdriven detonations with ambient conditions of 0.421 atm or 1 atm and 293.15 K
- Initial stoichiometric mixture of $2H_2 + O_2 + 3.76N_2$
- $D_{CJ} \sim 1972$ m/s
- Overdrive is defined as $f = \frac{D_o^2}{D_{CJ}^2}$
- Overdrives of $1.018 < f < 1.150$ were examined
- (Some cases were easier defined by piston velocity)
Typical Stable Steady Wave Profile

\[ f = 1.15 \]
For high enough overdrives, the detonation relaxes to a steady propagating wave in the inviscid case as well as in the diffusive case.
A single fundamental frequency oscillation occurs at a frequency of 0.97 $MHz$.
This frequency agrees with the experimental observations of Lehr (Astro. Acta, 1972).

**Organ pipe oscillation between shock and end of reaction zone:** $\nu \simeq \frac{a}{\ell} = \frac{(1000 \text{ m/s})}{(0.0001 \text{ m})} \simeq 10 MHz$. 
Lehr’s High Frequency Instability

- Stoichiometric mixture of $2\text{H}_2 + \text{O}_2 + 3.76\text{N}_2$ at 0.421 atm
- Observed 1.04 MHz frequency for projectile velocity corresponding to $f \approx 1.10$
- For $f = 1.10$, the predicted frequency of 0.97 MHz agrees with observed frequency and the prediction by Yungster and Radhakrishnan of 1.06 MHz

(Astro. Acta, 1972)
The addition of viscosity has a stabilizing effect, decreasing the amplitude of the oscillations. The pulsation frequency relaxes to 0.97 MHz.
As the overdrive is lowered, multiple frequencies appear, and the amplitude of the oscillations continues to grow. These multiple frequencies persist at long time.
Harmonic Analysis - PSD

- Harmonic analysis can be used to extract the multiple frequencies of a signal.
- The discrete one-sided mean-squared amplitude Power Spectral Density (PSD) for the pressure was used:

\[
\Phi_d(0) = \frac{1}{N^2} |P_o|^2,
\]

\[
\Phi_d(\bar{f}_k) = \frac{2}{N^2} |P_k|^2, \quad k = 1, 2, \ldots, (N/2 - 1),
\]

\[
\Phi_d(N/2) = \frac{1}{N^2} |P_{N/2}|^2,
\]

where \(P_k\) is the standard discrete Fourier Transform of \(p\),

\[
P_k = \sum_{n=0}^{N-1} p_n \exp \left( -\frac{2\pi i nk}{N} \right), \quad k = 0, 1, 2, \ldots, N/2.
\]
Viscous H₂-Air Harmonics: Effect of Overdrive

(a) 

(b) 

(c) 

(d) 

\( \Phi_d(\nu) \) (dB)
Viscous H₂-Air Harmonics: Effect of Overdrive

(a) $\Phi_d(\nu)$ (dB)

(b) $\tilde{\Phi}_d(\nu)$ (dB)

(c) $\hat{\Phi}_d(\nu)$ (dB)

(d) $\Phi_d(\nu)$ (dB)

$\nu$ (MHz)

$\nu_l$, $2\nu_l$, $\nu_h - 2\nu_l$, $\nu - \nu_l$, $\nu_h$, $\nu_h + \nu_l$

$\nu_v$, $2\nu_v$, $3\nu_v$, $4\nu_v$

$\frac{1}{2}\nu_v$, $\frac{3}{2}\nu_v$, $2\nu_v$, $3\nu_v$, $4\nu_v$, $5\nu_v$

$\frac{3}{2}\nu_v$, $2\nu_v$, $3\nu_v$
Bifurcation Diagram for Hydrogen-Air Detonation

(a) $P_{\text{peak}}/P_{\text{avg}}$

(b) $\nu$ (MHz)

Low Frequency | Dual Mode | High Frequency | Stable

$\overline{u}_p$ (cm/s)
2D extension to DDT in thin channel (with extra nitrogen dilution)
Conclusions

- Long time behavior of a one-dimensional hydrogen-air detonation becomes more complex as the overdrive is decreased.

- Harmonic analysis has revealed the first harmonic frequency moderately lowers as the overdrive is lowered.

- At the second bifurcation there is a drastic shift in the fundamental frequency from 0.71 MHz to 0.11 MHz.

- The fundamental instability is dictated by reaction/advection; diffusion provides a small amplitude reduction and phase shift.

- Diffusion plays a larger role modulating high frequency modes.

- Fully resolved two-dimensional dynamics are difficult, and we are beginning to find results.