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

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Unsteady, Compressible, Reactive Navier-Stokes Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0,$$

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u} + p\mathbf{I} - \boldsymbol{\tau}) = \mathbf{0},$$

$$\frac{\partial}{\partial t}\left(\rho\left(e + \frac{\mathbf{u}\cdot\mathbf{u}}{2}\right)\right) + \nabla \cdot \left(\rho\mathbf{u}\left(e + \frac{\mathbf{u}\cdot\mathbf{u}}{2}\right) + (p\mathbf{I} - \boldsymbol{\tau})\cdot\mathbf{u} + \mathbf{q}\right) = 0,$$

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \mathbf{u} Y_i + \mathbf{j}_i) = \overline{M_i}\,\dot{\omega}_i\,,$$

$$p = \mathcal{R}T\sum_{i=1}^{N}\frac{Y_i}{\overline{M_i}}, \qquad e = e\left(T, Y_i\right), \qquad \dot{\omega}_i = \dot{\omega}_i\left(T, Y_i\right),$$

$$\mathbf{j}_i = \rho \sum_{\substack{k=1 \\ k\neq i}}^{N} \frac{\overline{M_i} D_{ik} Y_k}{\overline{M}}\left(\frac{\nabla y_k}{y_k} + \left(1 - \frac{\overline{M_k}}{\overline{M}}\right)\frac{\nabla p}{p}\right) - \frac{D_i^T \nabla T}{T},$$

$$\boldsymbol{\tau} = \mu\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T - \frac{2}{3}(\nabla\cdot\mathbf{u})\,\mathbf{I}\right),$$

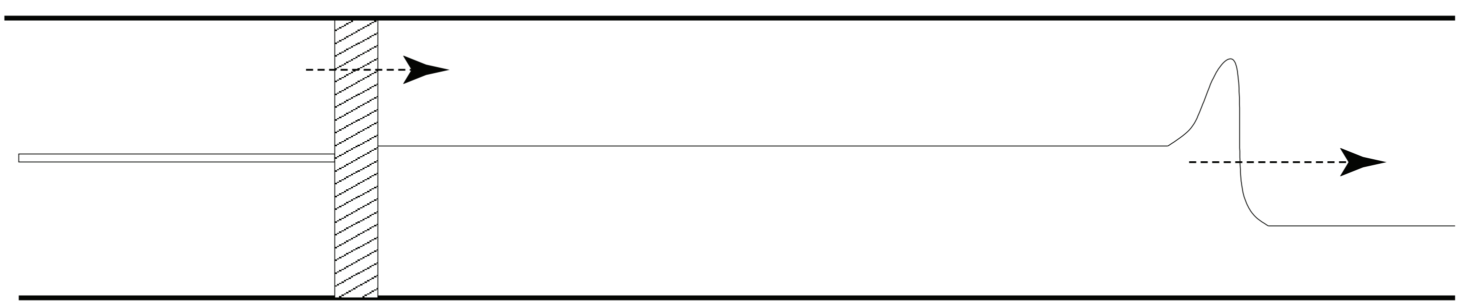
$$\mathbf{q} = -k\nabla T + \sum_{i=1}^{N}\mathbf{j}_i h_i - \mathcal{R}T\sum_{i=1}^{N}\frac{D_i^T}{\overline{M_i}}\left(\frac{\nabla\overline{y}_i}{\overline{y}_i} + \left(1 - \frac{\overline{M_i}}{\overline{M}}\right)\frac{\nabla p}{p}\right).$$

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

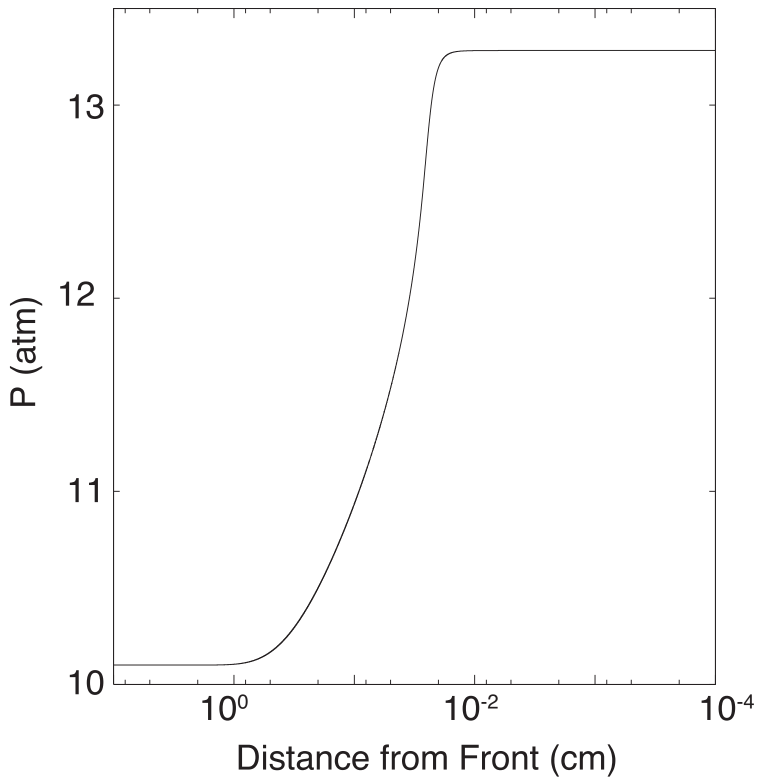
Case Examined

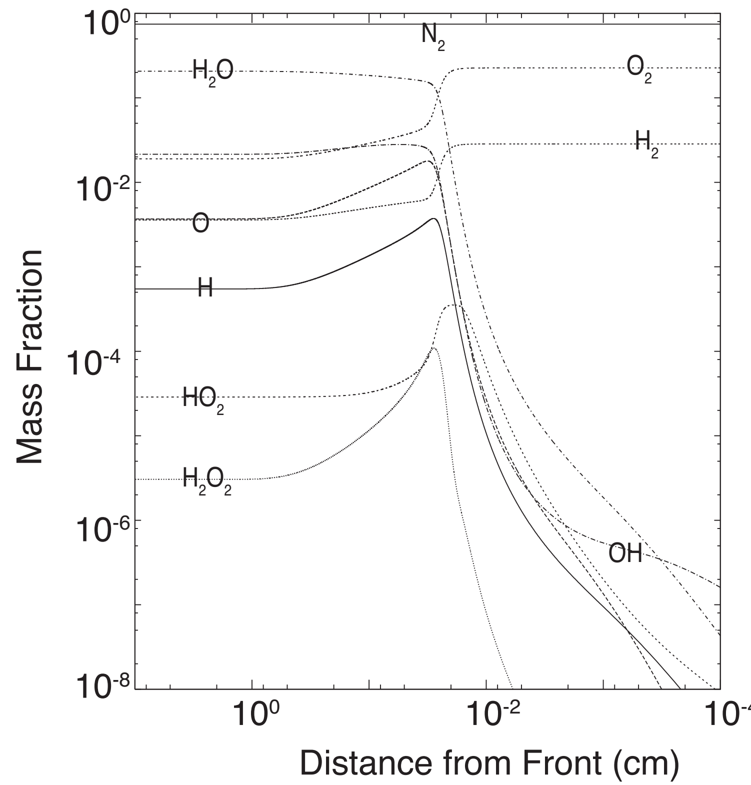
- Overdriven detonations with ambient conditions of 0.421 atm or 1 atm and 293.15 K
- Initial stoichiometric mixture of $2H_2 + O_2 + 3.76N_2$
- $D_{CJ} \sim 1972$ m/s
- Overdrive is defined as $f = D_o^2/D_{CJ}^2$
- Overdrives of $1.018 < f < 1.150$ were examined
- (Some cases were easier defined by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



Typical Stable Steady Wave Profile

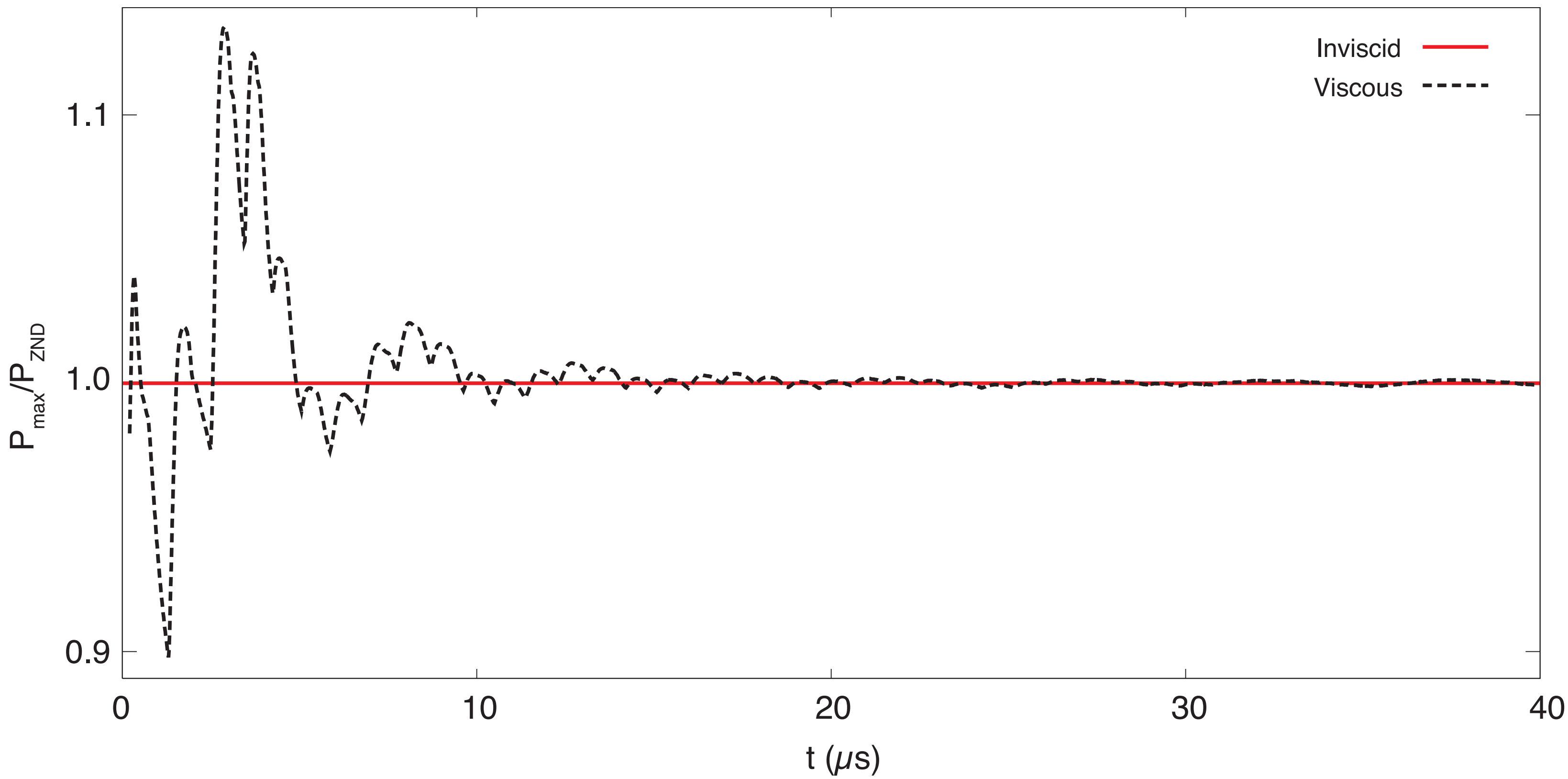
$f = 1.15$





Stable Detonation at High Overdrive

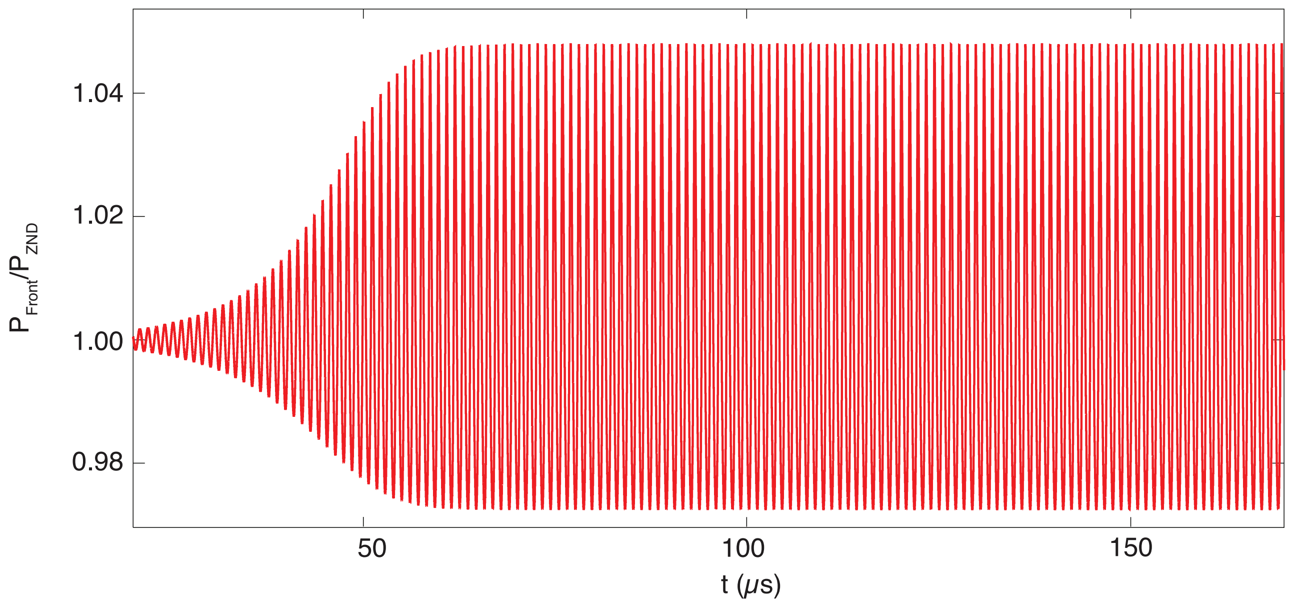
$f = 1.15$



For high enough overdrives, the detonation relaxes to a steady propagating wave in the inviscid case as well as in the diffusive case.

Lower Overdrive: High Frequency Instability

$f = 1.10$

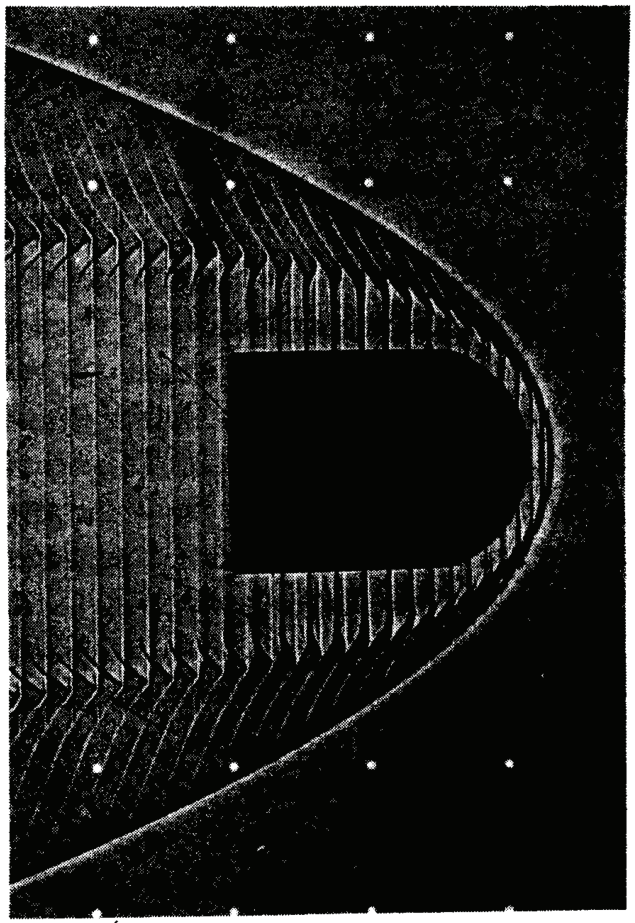


A single fundamental frequency oscillation occurs at a frequency of $0.97\ MHz$.

This frequency agrees with the experimental observations of Lehr (*Astro. Acta*, 1972).

Organ pipe oscillation between shock and end of reaction zone: $\nu \simeq a/\ell$ = (1000 m/s)/(0.0001 m)$\simeq$ 10 MHz.

Lehr's High Frequency Instability

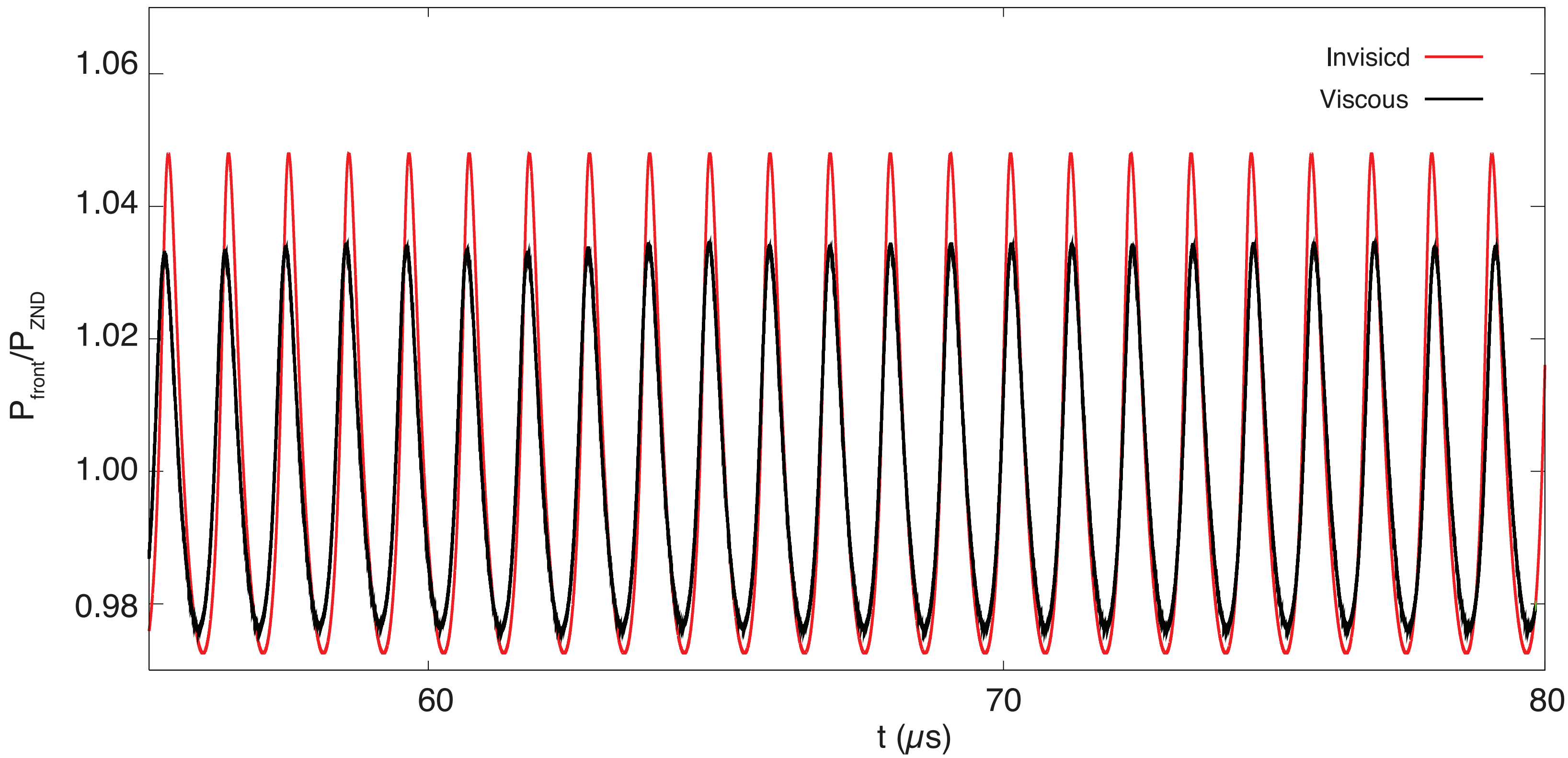


(*Astro. Acta*, 1972)

- Shock-induced combustion experiment (*Astro. Acta*, 1972)
- Stoichiometric mixture of $2H_2 + O_2 + 3.76N_2$ 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 Radhakrishan of 1.06 MHz

High Frequency Mode - Viscous vs. Inviscid

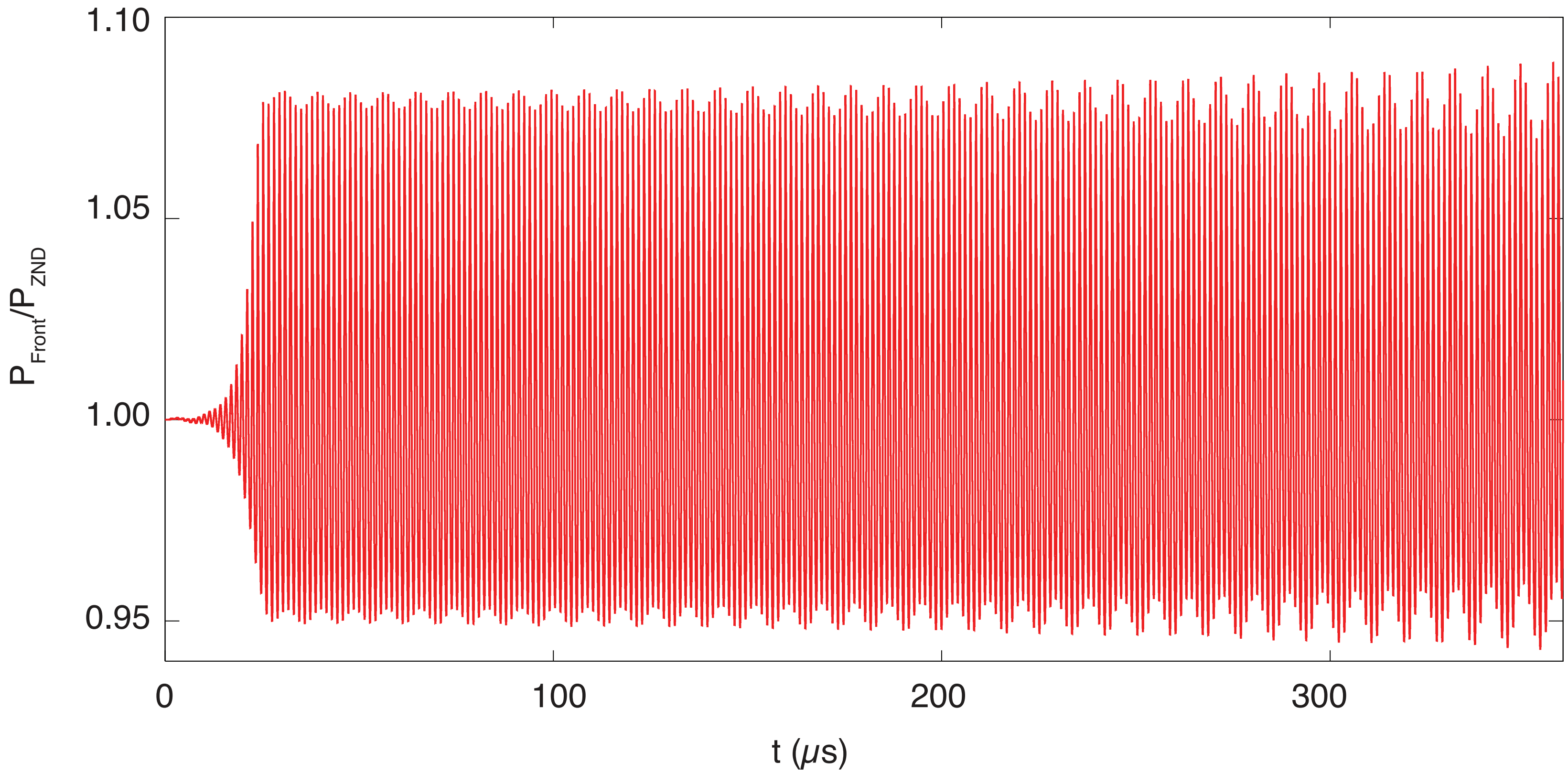
$f = 1.10$



The addition of viscosity has a stabilizing effect, decreasing the amplitude of the oscillations. The pulsation frequency relaxes to 0.97 MHz.

Low Frequency Mode Appearance

$f = 1.035$



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

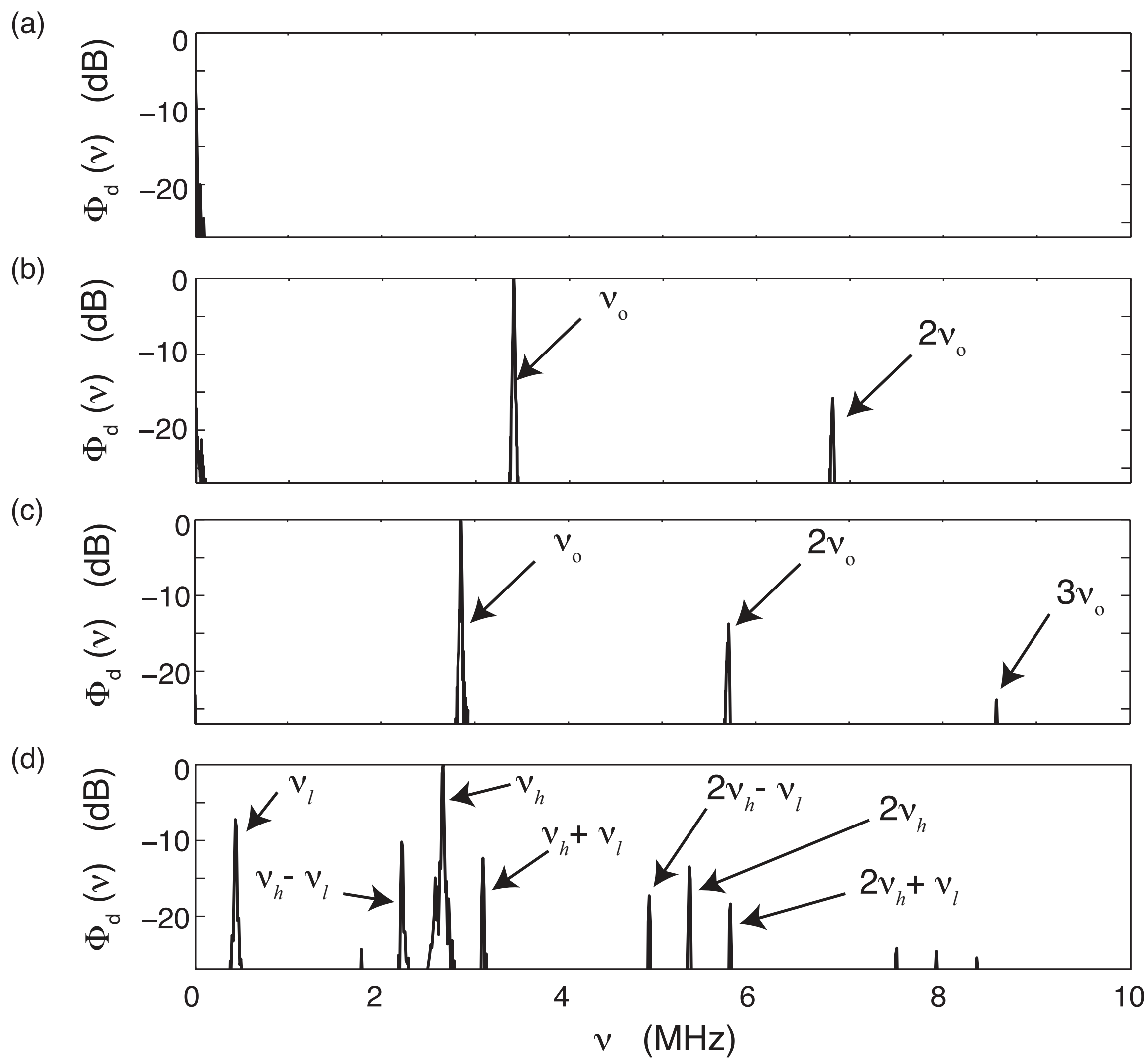
- Harmonic analysis can be used to extract the multiple frequencies of a signal
- The discrete one-sided mean-squared amplitude Power Spectral Density (PSD) for the pressure was used

$$\Phi_d(0) = \frac{1}{N^2}|P_o|^2,$$
$$\Phi_d(\bar{f}_k) = \frac{2}{N^2}|P_k|^2, \qquad k = 1, 2, \ldots, (N/2-1),$$
$$\Phi_d(N/2) = \frac{1}{N^2}|P_{N/2}|^2,$$

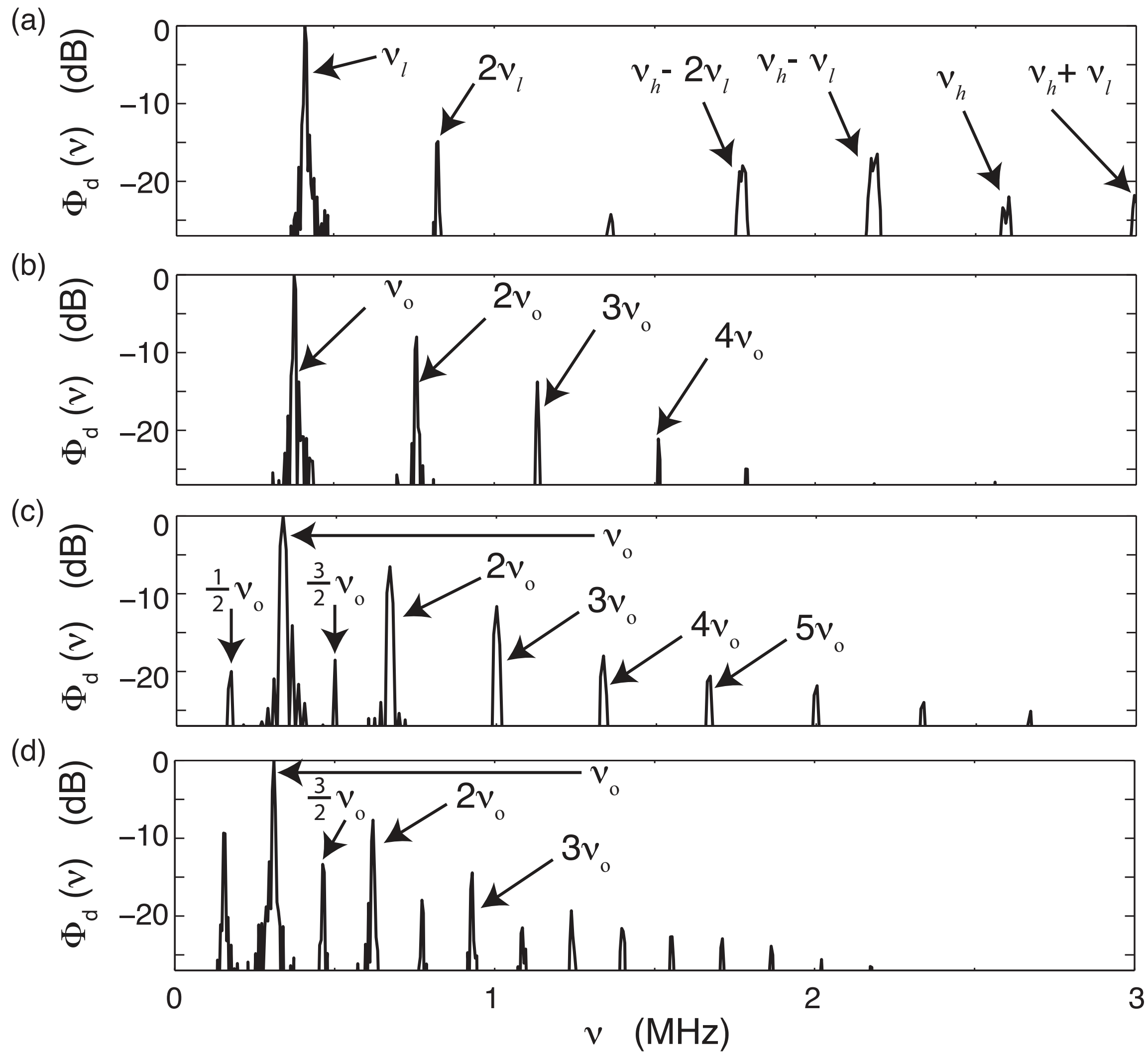
where P_k is the standard discrete Fourier Transform of p,

$$P_k = \sum_{n=0}^{N-1} p_n \exp\left(-\frac{2\pi \imath n k}{N}\right), \qquad k = 0, 1, 2, \ldots, N/2.$$

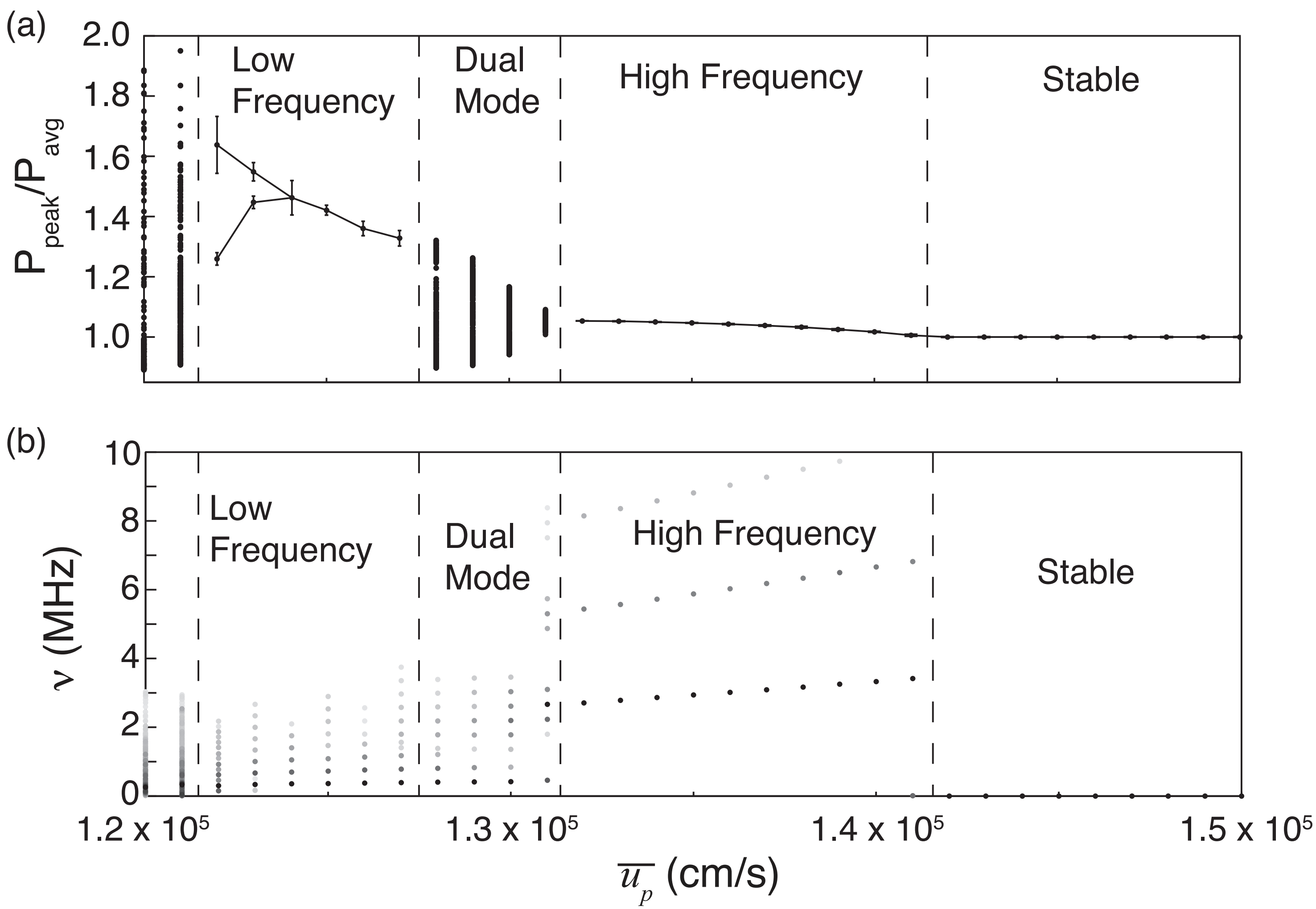
Viscous H_2-Air Harmonics: Effect of Overdrive



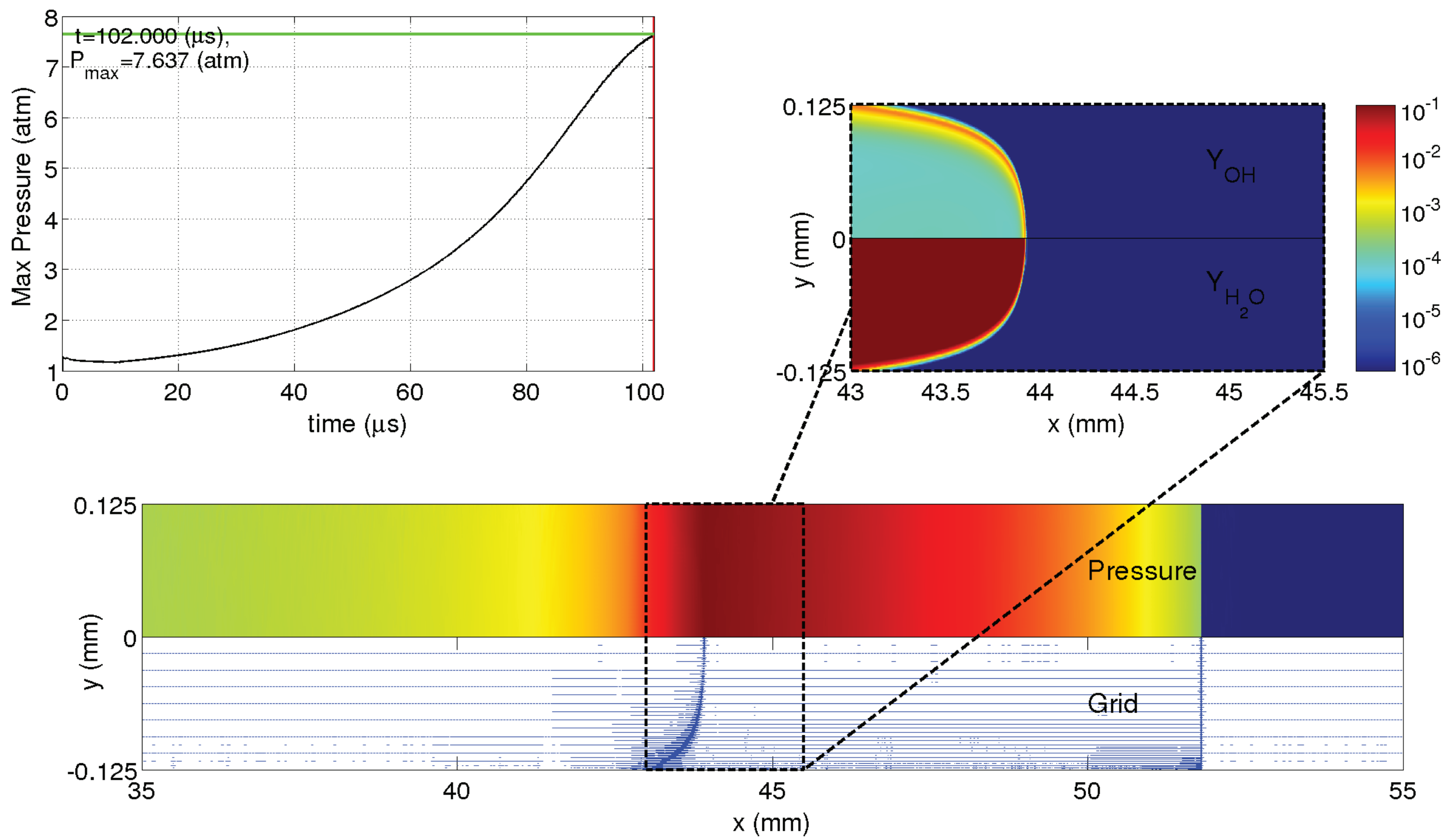
Viscous H_2-Air Harmonics: Effect of Overdrive



Bifurcation Diagram for Hydrogen-Air Detonation



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.