On the Development of Hydrogen-Air Detonations

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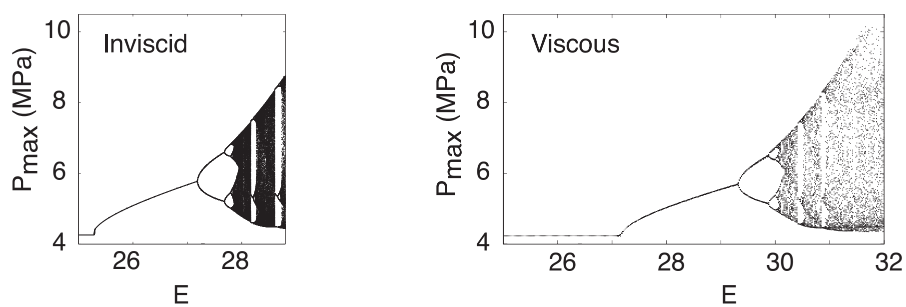
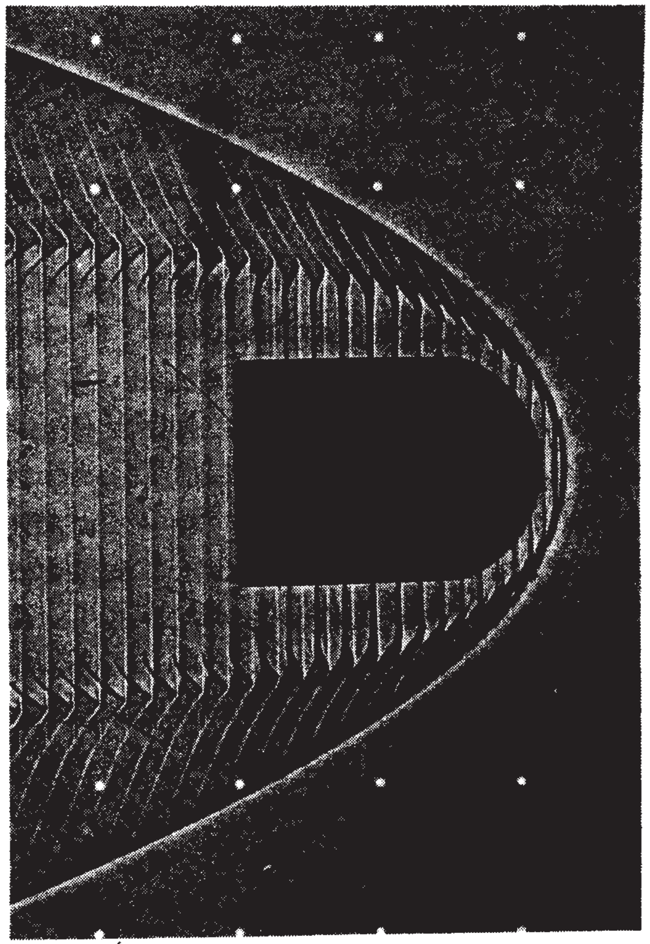
Motivation

- It is often argued that viscous forces and diffusive effects are small, do not affect detonation dynamics, and thus can be neglected.
- Using a one-step kinetics model, we (*JFM*, 2012) showed that when the viscous length scale is similar to that of the finest reaction scale, viscous effects play a critical role in determining the long time behavior of the detonation.



- Does this viscous effect on pulsating detonations extend to a model that utilizes a detailed kinetics mechanism that has multiple reaction length scales and an induction zone length that is several orders of magnitude larger than the viscous scale?

Validation: 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 $f \approx 1.1$
- For $f = 1.1$, the predicted frequency of $0.97\ MHz$ agrees with observed frequency and the prediction by Yungster and Radhakrishan of $1.06\ MHz$

Model: Reactive Navier-Stokes (NS) Equations

- Unsteady, compressible, one-dimensional
- Detailed mass action kinetics with Arrhenius temperature-dependency
- Ideal mixture of calorically imperfect ideal gases
- Physical viscosity and thermal conductivity
- Multicomponent mass diffusion with Soret and DuFour effects

Case Examined

- Initially quiescent stoichiometric mixture of $2H_2 + O_2 + 3.76N_2$ at $1\ atm$ and $293.15\ K$ accelerated using a piston
- Form of piston velocity was chosen to force a detonation to form $\sim 1\ \mu s$

$$u_p = u_{p_i}\left(1 + \tanh\left[a\left(t - t_a\right)\right]\right) - \left(u_{p_i} - u_{p_f}\right)\left(1 + \tanh\left[b\left(t - t_b\right)\right]\right),$$

$$u_{p_i} = 1650\, m/s,\ a = 10^8\ 1/s,\ b = 10^7\ 1/s,\ t_a = 10^{-7}\ s,\ t_b = 10^{-6}\ s.$$

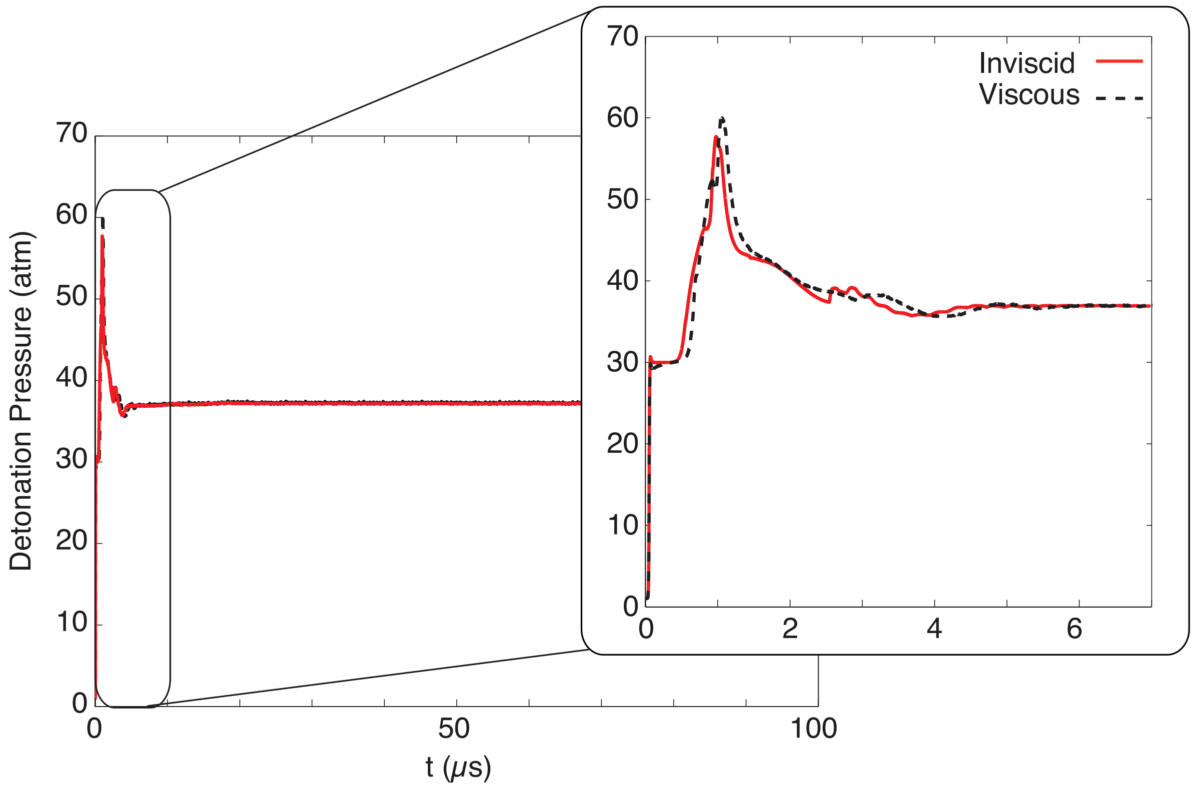
- Final piston velocities $1200\ m/s < u_{p_f} < 1500\ m/s$ were examined

Computational Methods

- Viscous, Shock-Capturing
  - Wavelet Adaptive Multiresolution Representation (WAMR) method was used, developed by Vasilyev and Paolucci (*J. Comp. Phys.*, 1996 & 1997)
  - User-defined threshold parameter controls error
  - Fifth order Runge-Kutta scheme for temporal integration
  - Direct Numerical Simulation
- Inviscid, Shock-Capturing - viscosity, mass diffusion, and thermal conductivity are all set to zero
  - Uniform spatial grid
  - Second order min-mod coupled with Lax-Friedrichs scheme
  - Second order Runge-Kutta scheme for temporal integration

Stable Detonation

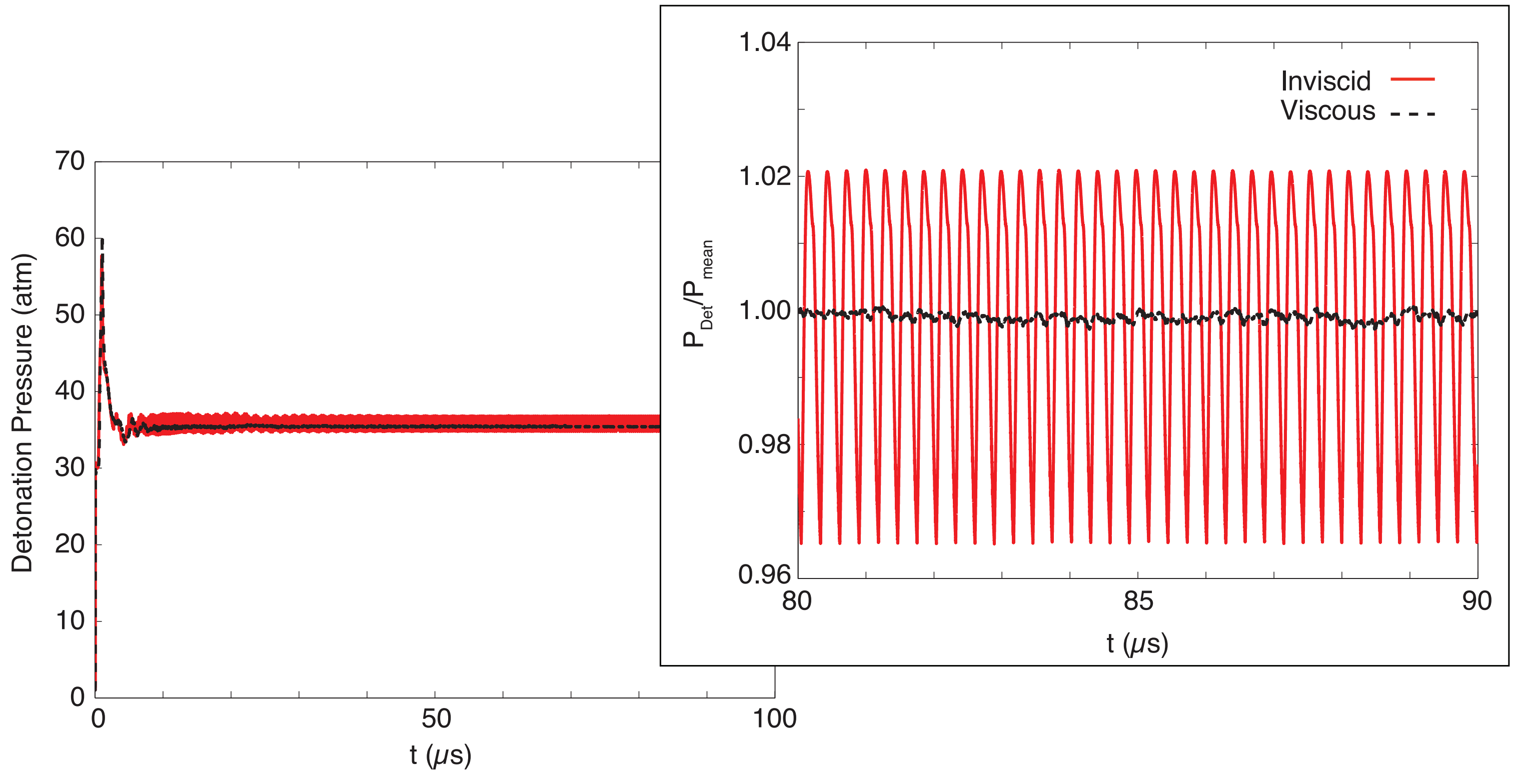
$u_{p_f} = 1500\, m/s$



The viscous case smooths the initialization; due to this slightly weaker shock, it takes longer to ignite the detonation. This delay increases the von Neumann spike. Additionally, the viscosity causes the detonation to take longer to relax to steady state.

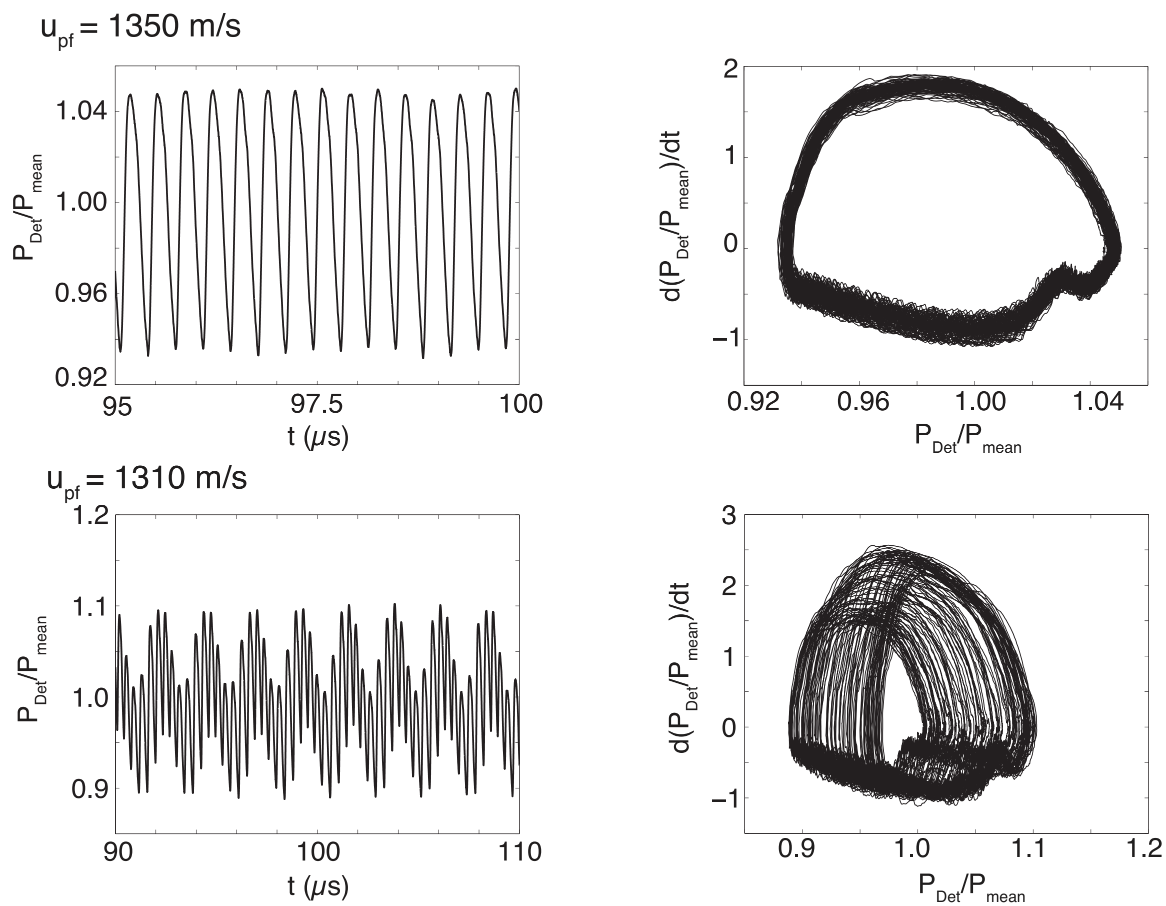
Unstable Detonation

$u_{p_f} = 1420\, m/s$



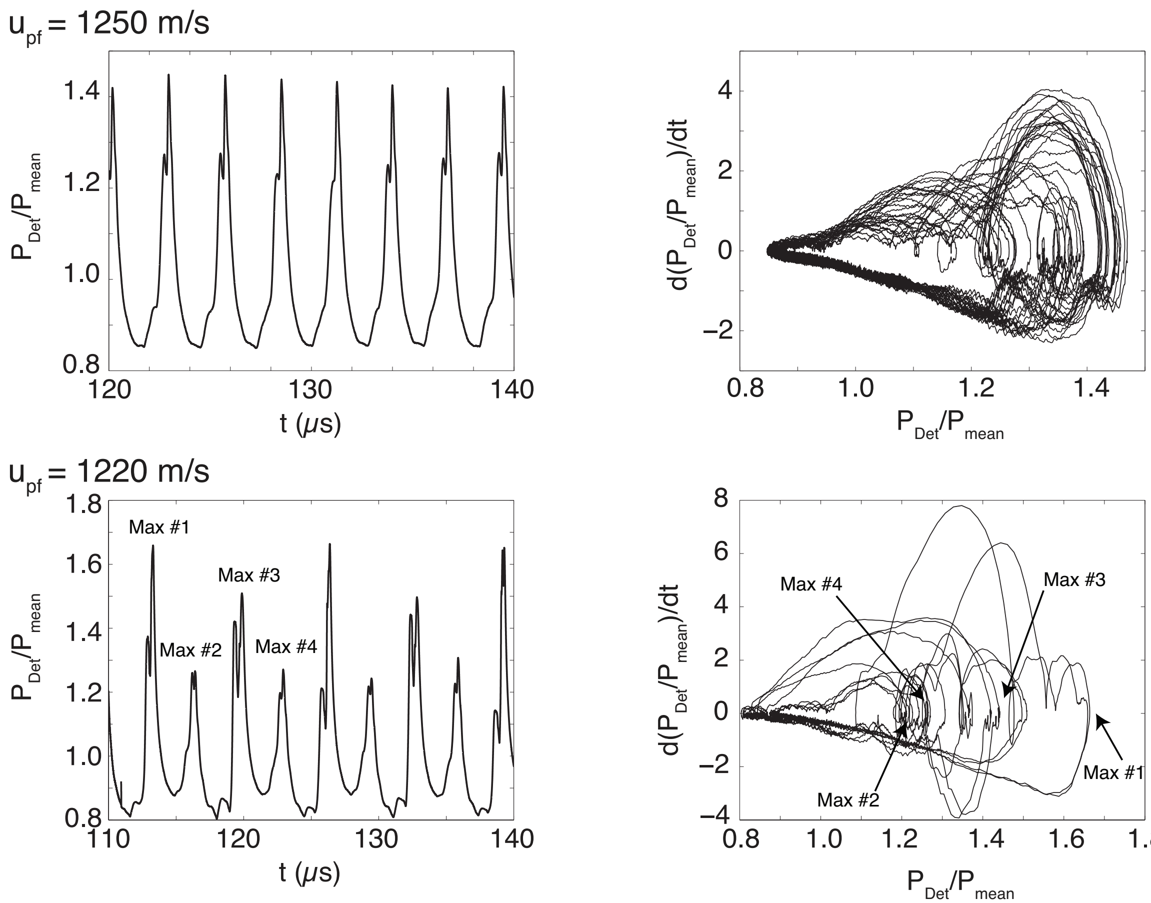
The addition of physical viscosity delays the onset of the initial appearance of instability. The small variations present in the viscous case are due to the detonation traversing a non-uniform grid and will be reduced as the tolerance of the WAMR is reduced.

Effect of Reducing Piston Velocity - Viscous



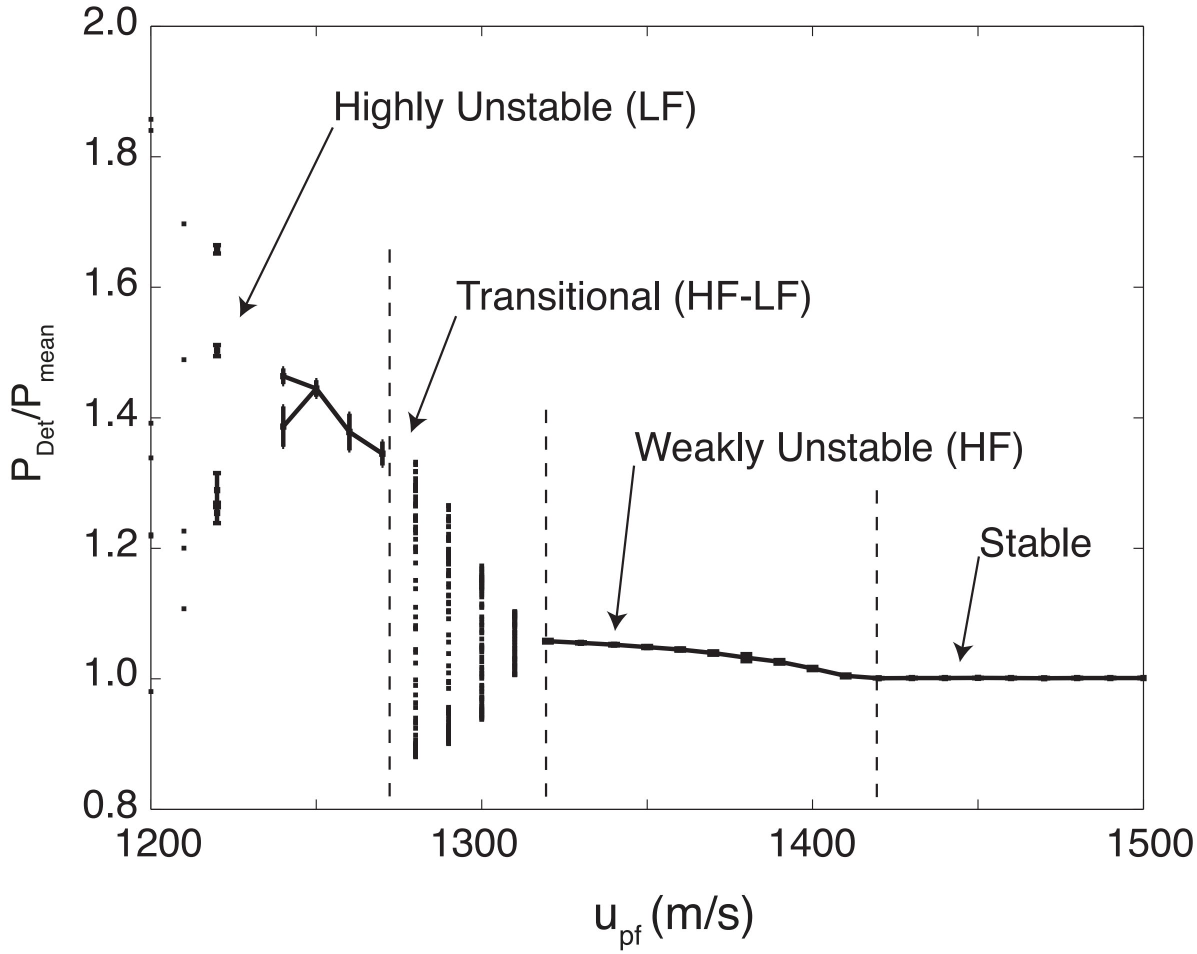
Even with the addition of physical viscosity the detonation still becomes unstable ($f_{1350\ m/s} = 2.94\ MHz$). Eventually there is a transition to multiple dominant frequencies of oscillation.

Effect of Reducing Piston Velocity - Viscous



The lower frequency ($f_{1250\ m/s} = 0.362\ MHz$) becomes the dominant mode at lower velocities; at this lower frequency a period doubling behavior is predicted.

Bifurcation Plot - Viscous



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

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

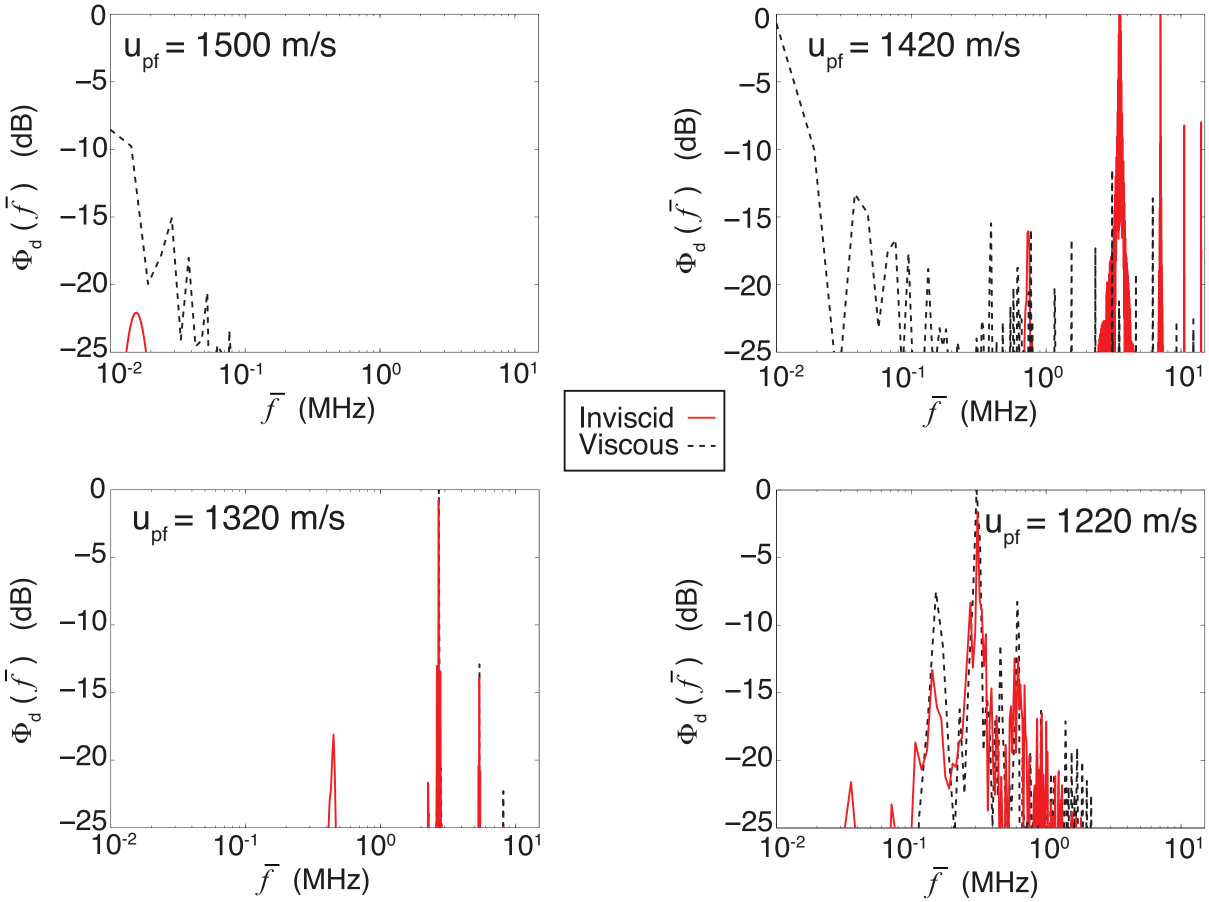
$$\Phi_d(\bar{f}_k) = \frac{2}{N^2}|P_k|^2, \qquad k = 1, 2, \ldots, (N/2-1),$$

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

where P_k is the standard discrete Fourier Transform of p,

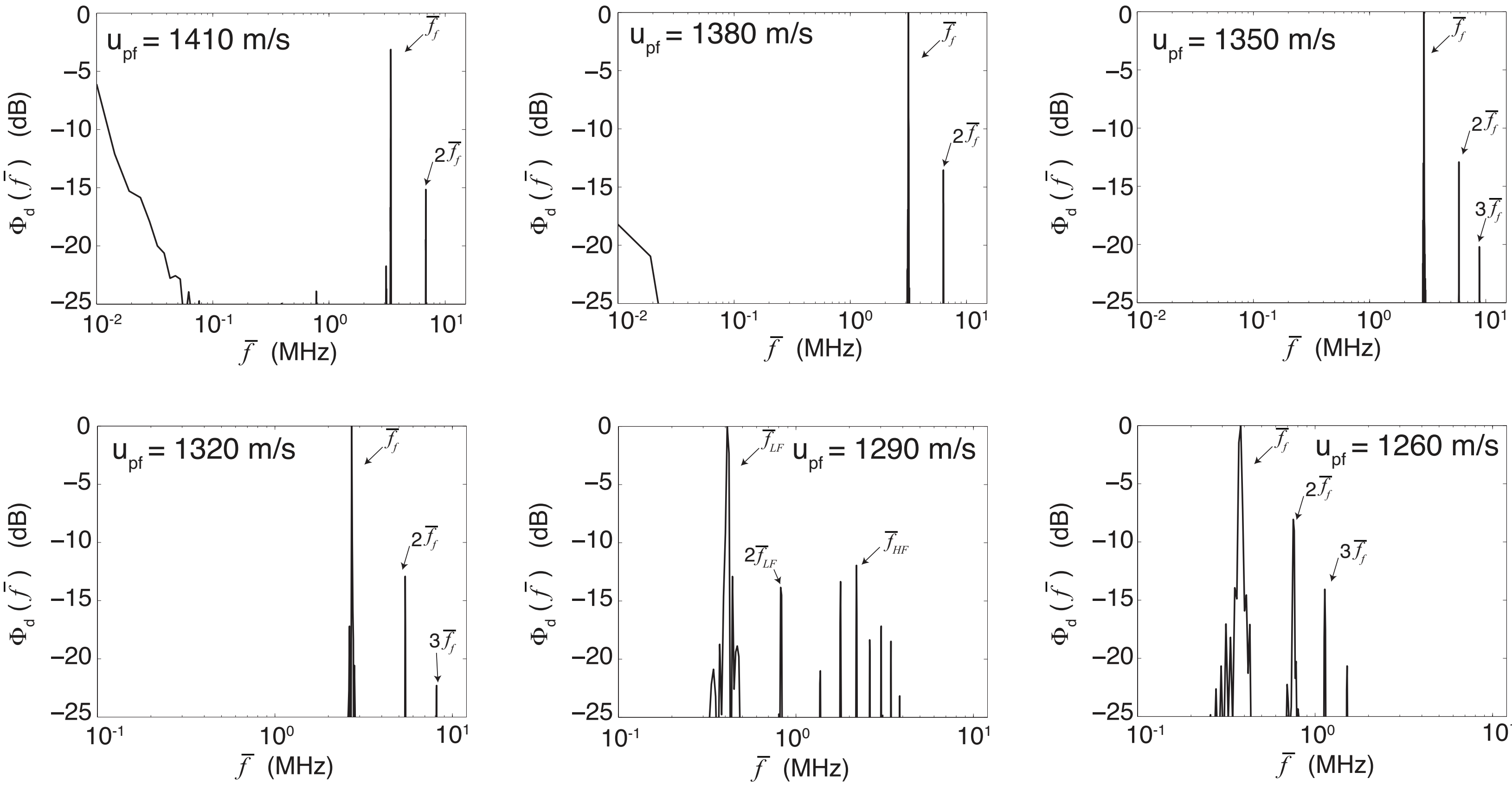
$$P_k = \sum_{n=0}^{N-1} p_n \exp\left(-\frac{2\pi\imath nk}{N}\right), \qquad k = 0, 1, 2, \ldots, N/2.$$

Inviscid vs. Viscous - Frequency Domain



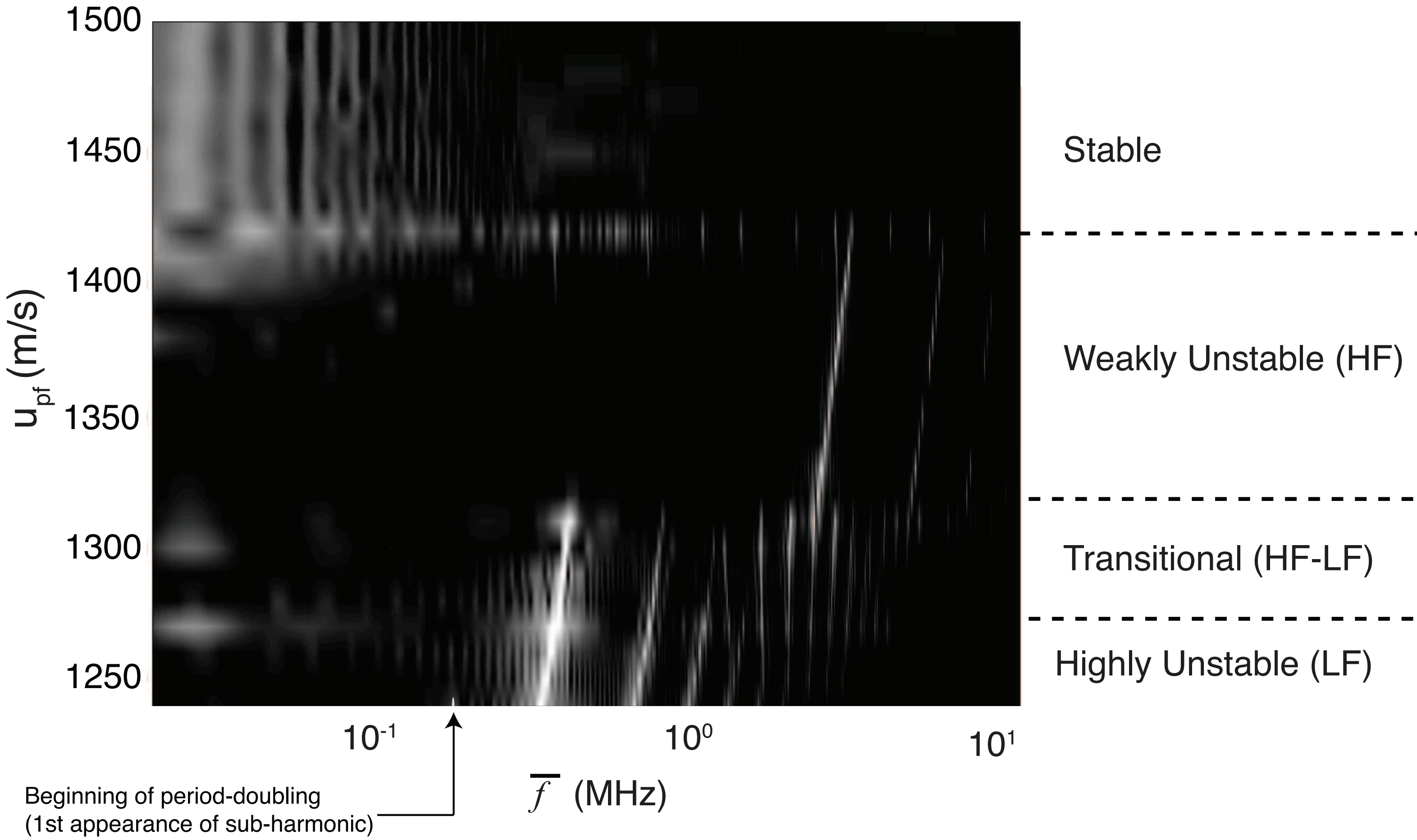
The inviscid case under goes a transition to instability before the viscous case; it also enters the dual mode oscillations before the viscous case. At the lower piston velocities the inviscid case appears to be chaotic sooner.

Evolution of Frequencies - Viscous



Below the stability point the main frequency blue-shifts; eventually there is an appearance of dual mode behavior. After the transition region, the low frequency begins to dominate.

Overview of the Frequency Domain - Viscous



Conclusions

- Long time behavior of a hydrogen-air detonation becomes more complex as the final piston velocity is decreased; four phenomena are predicted:
  - a stable detonation,
  - a single dominant high frequency mode oscillatory detonation,
  - a dual mode oscillatory detonation,
  - a mode dominated by a low frequency.
- A phenomena similar to period-doubling occurs in the low frequency dominated mode
- Harmonic analysis has revealed the first harmonic frequency blue-shifts as the piston velocity is lowered in the high frequency mode.
- Physical diffusion causes a delay of the bifurcation limits.