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Title:	Dynamics of Unsteady Inviscid and Viscous Detonations in Hydrogen-Air
Author(s):	Christopher M. Romick, Z# 259510 Tariq D. Aslam, Z# 115318 Joseph M. Powers
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Dynamics of Unsteady Inviscid and Viscous Detonations in Hydrogen-Air

Christopher M. Romick*
University of Notre Dame, Notre Dame, Indiana, 46556-5637, USA

Tariq D. Aslam†
Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

Joseph M. Powers‡
University of Notre Dame, Notre Dame, Indiana, 46556-5637, USA

ABSTRACT

The dynamics of one-dimensional, overdriven, hydrogen-air detonations predicted in the inviscid limit as well as with the inclusion of mass, momentum, and energy diffusion were investigated. A series of shock-fitted calculations was performed in which the overdrive was varied in the inviscid limit. The 0.97 MHz frequency of oscillation predicted for a $f = 1.1$ overdriven detonation agrees well with the value of1.04 MHz observed by Lehr in the equivalent shock-induced combustion experiment around a spherical projectile. As the initial overdrive is lowered, the long time behavior of the system becomes more complex, causing the amplitude of pulsations to increase and oscillations at multiple frequencies to appear. When the viscous analog of these detonations was simulated, it was found that viscous effects slightly alter the structure of a stable detonation and can significantly decrease the amplitude of pulsations in an unstable detonation.

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Christopher M. Romick,
University of Notre Dame, Notre Dame, IN
Tariq D. Aslam,
Los Alamos National Laboratory, Los Alamos, NM
and
Joseph M. Powers
University of Notre Dame, Notre Dame, IN

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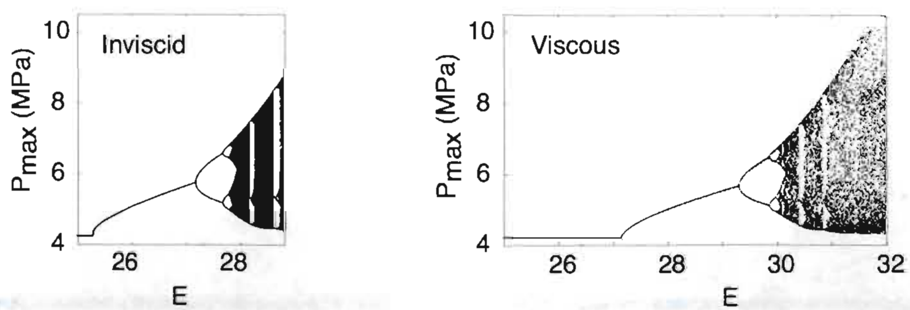
Motivation

- Standard result from non-linear dynamics: small scale phenomena can influence large scale phenomena and vice versa.
- What are the risks of using reactive Euler instead of reactive Navier-Stokes?
- Might there be risks in using numerical viscosity, LES, and turbulence modeling, all of which filter small scale physical dynamics?

Motivation

- It is often argued that viscous forces and diffusive effects are small, do not affect detonation dynamics, and thus can be neglected.
- Tsuboi *et al.*, (*Comb. & Flame*, 2005) report, even when using micron grid sizes, that some structures cannot be resolved.
- Powers, (*JPP*, 2006) showed that two-dimensional detonation patterns are grid-dependent for the reactive Euler equations, but relax to a grid-independent structure for comparable Navier-Stokes calculations.
- Using an one-step kinetics model, we (*49th AIAA ASM*, 2011) 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
- This suggests grid-dependent numerical viscosity may be problematic and one may want to consider the introduction of physical diffusion.



Review of hydrogen detonation

- Powers & Paolucci (*AIAA J.*, 2005) studied the reaction length scales of a steady, inviscid hydrogen detonation and found the finest length scales on the order of sub-microns to microns and the largest on the order of centimeters with ambient conditions of $1\ atm$ and $298\ K$.
- These small scales are continuum manifestations of molecular collisions.
- This range of scales must be resolved to capture the dynamics.

Review of hydrogen detonation

- Sussman (Ph.D. Thesis, 1995) performed one-dimensional simulations using only 20 points in the induction zone.
- Using a massively parallel computing environment, Oran *et al.* (*Comb. & Flame*, 1998) studied the development of detonation cells in a low-pressure hydrogen mixture in two dimensions.
- Eckett (Ph.D. Thesis, 2001) found that 150 points in the induction zone were necessary capture the dynamics of an overdriven, inviscid detonation at an ambient pressure of $1\ atm$.
- Singh *et al.* (*Comb. Theory & Mod.*, 2001) simulated a one-dimensional, unsteady, viscous, detonation in a hydrogen-oxygen-argon mixture using an adaptive mesh.

Review of hydrogen detonation

- Yungster and Radhakrishan (*Comb. Theory & Mod.*, 2004) found that a minimum resolution of near micron was necessary to capture the dynamics in the inviscid limit at ambient pressure of $0.197\ atm$.
- Daimon and Matsuo (*Phys. Fluids*, 2007) found that as the overdrive is lowered, the long time behavior of the detonation became more complex.
- Using an adaptive mesh in a parallel computing environment, Ziegler *et al.* (*J. Comp. Phys.*, 2011) examined a viscous double-Mach reflection detonation and found that even with a resolution near a micron only qualitative convergence was achieved.

Model: Reactive Navier-Stokes Equations

- unsteady,
- 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

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 Dynamics
  - High-order shock-fitting algorithm adapted from Henrick *et al.* (*J. Comp. Phys.*, 2006).
  - Equations transformed to a shock-attached frame, jump conditions enforced at shock boundary, and fifth order Runge-Kutta used for time integration.
- Viscous Dynamics
  - Wavelet Adaptive Multiresolution Representation (WAMR) method first developed by Vasilyev and Paolucci (*J. Comp. Phys.*, 1996,1997) employed.
  - An adaptive mesh refinement technique using wavelet functions which have compact support in both space and time enables the use of many less points to accurately represent a flow field.

Case Examined

- Overdriven detonations with ambient conditions of $0.421\ atm$ and $293.15\ K$
- Initial stoichiometric mixture of $2H_2 + O_2 + 3.76N_2$
- $D_{CJ} \sim 1961\, m/s$
- Overdrive is defined as $f = D_o^2/D_{CJ}^2$
- Overdrives of $1.025 < f < 1.150$ were examined

Continuum Scales

- The mean-free path scale is the cut-off minimum length scale associated with continuum theories.
- A simple estimate for this scale is given by Vincenti and Kruger (1967):

$$\lambda = \frac{\overline{M}}{\sqrt{2}\pi \mathcal{N}_A \rho d^2} \sim \mathcal{O}\left(10^{-6}\ cm\right). \quad (1)$$

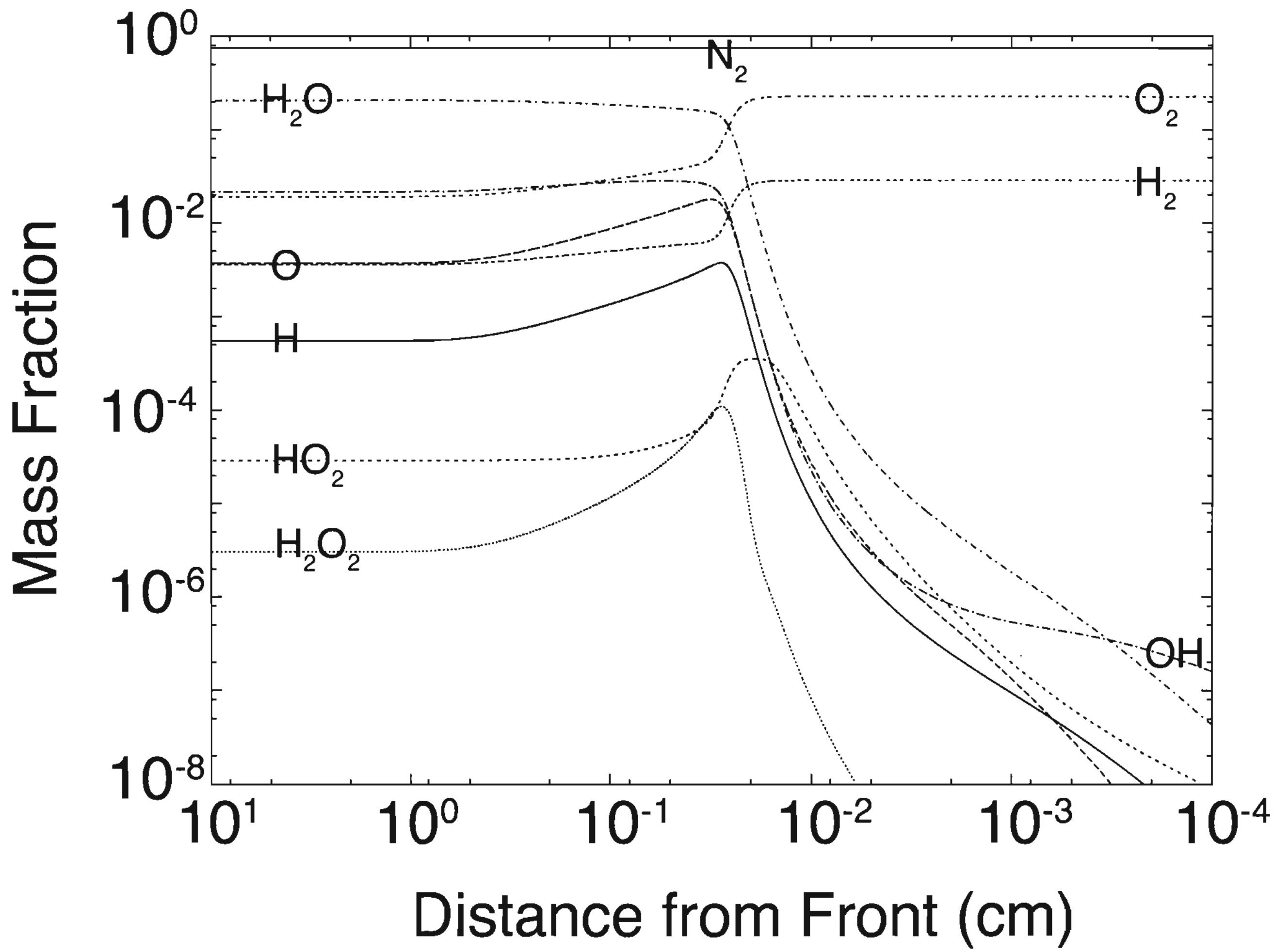
- The finest reaction length scale is $L_r \sim \mathcal{O}\left(10^{-4}\ cm\right)$.
- A simple estimate of a viscous length scale is:

$$L_\mu = \frac{\nu}{c} = \frac{6 \times 10^{-1}\ cm^2/s}{9 \times 10^4\ cm/s} \sim \mathcal{O}\left(10^{-5}\ cm\right). \quad (2)$$

- $\lambda < L_\mu < L_r$

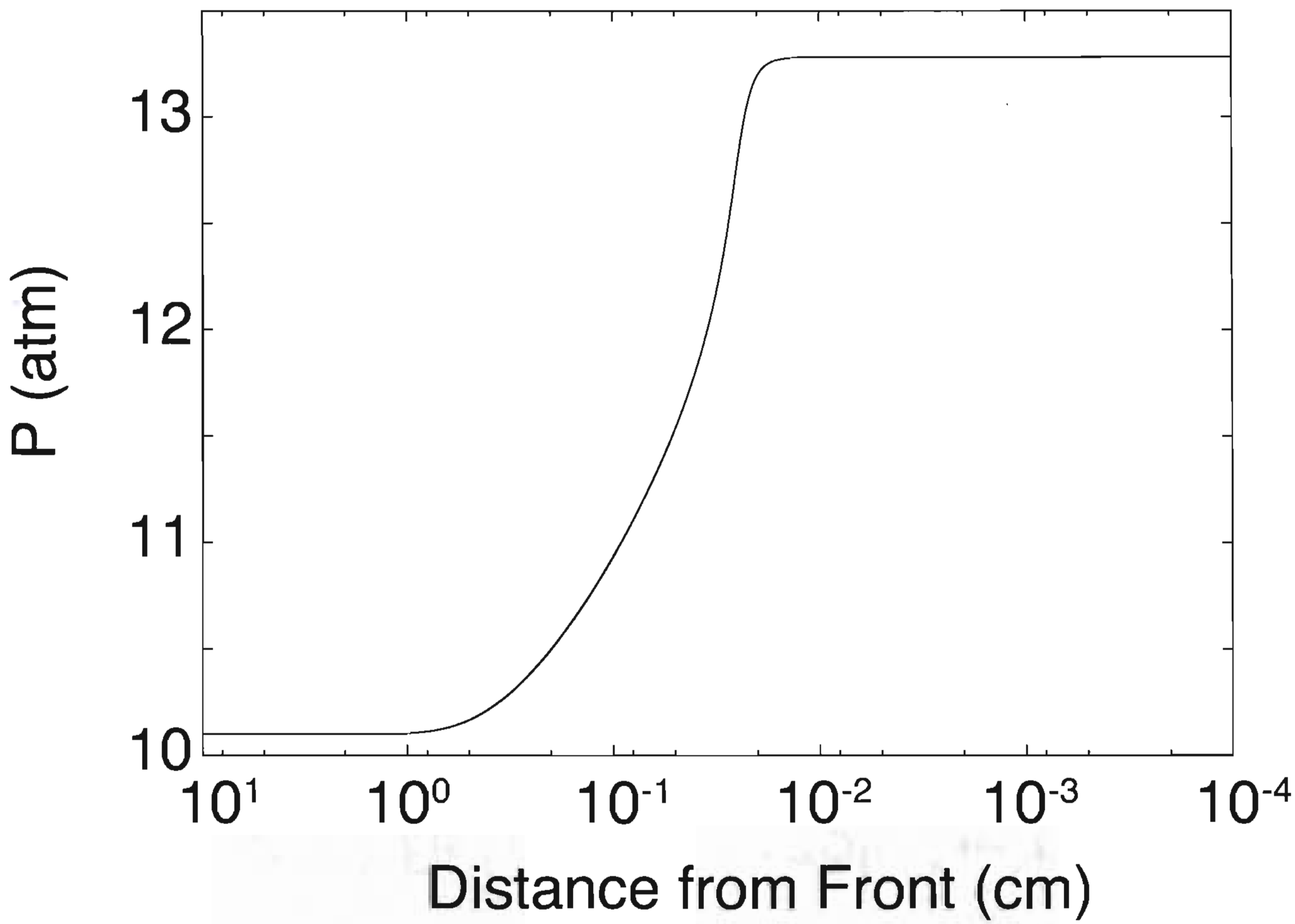
Inviscid Steady-State: Mass Fractions

$f = 1.15$



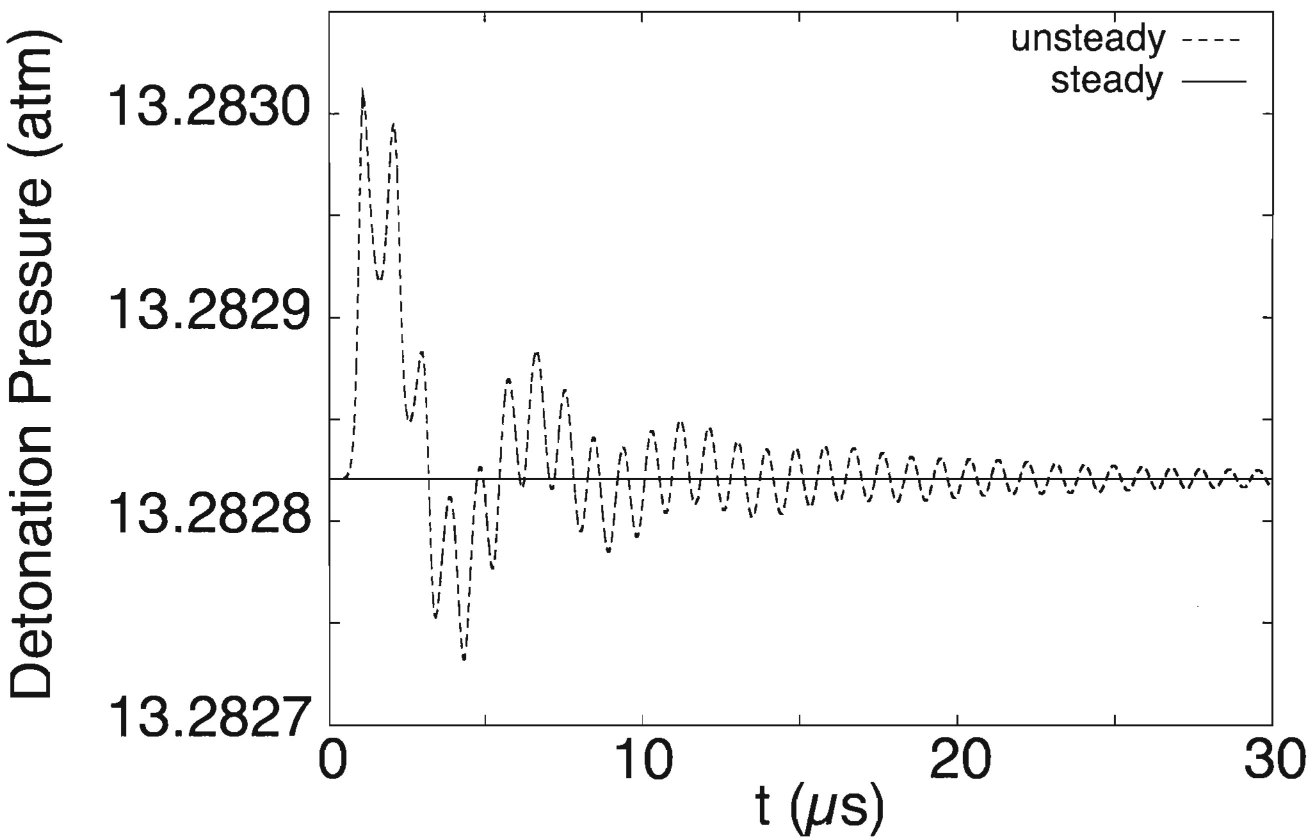
Inviscid Steady-State: Pressure

$f = 1.15$

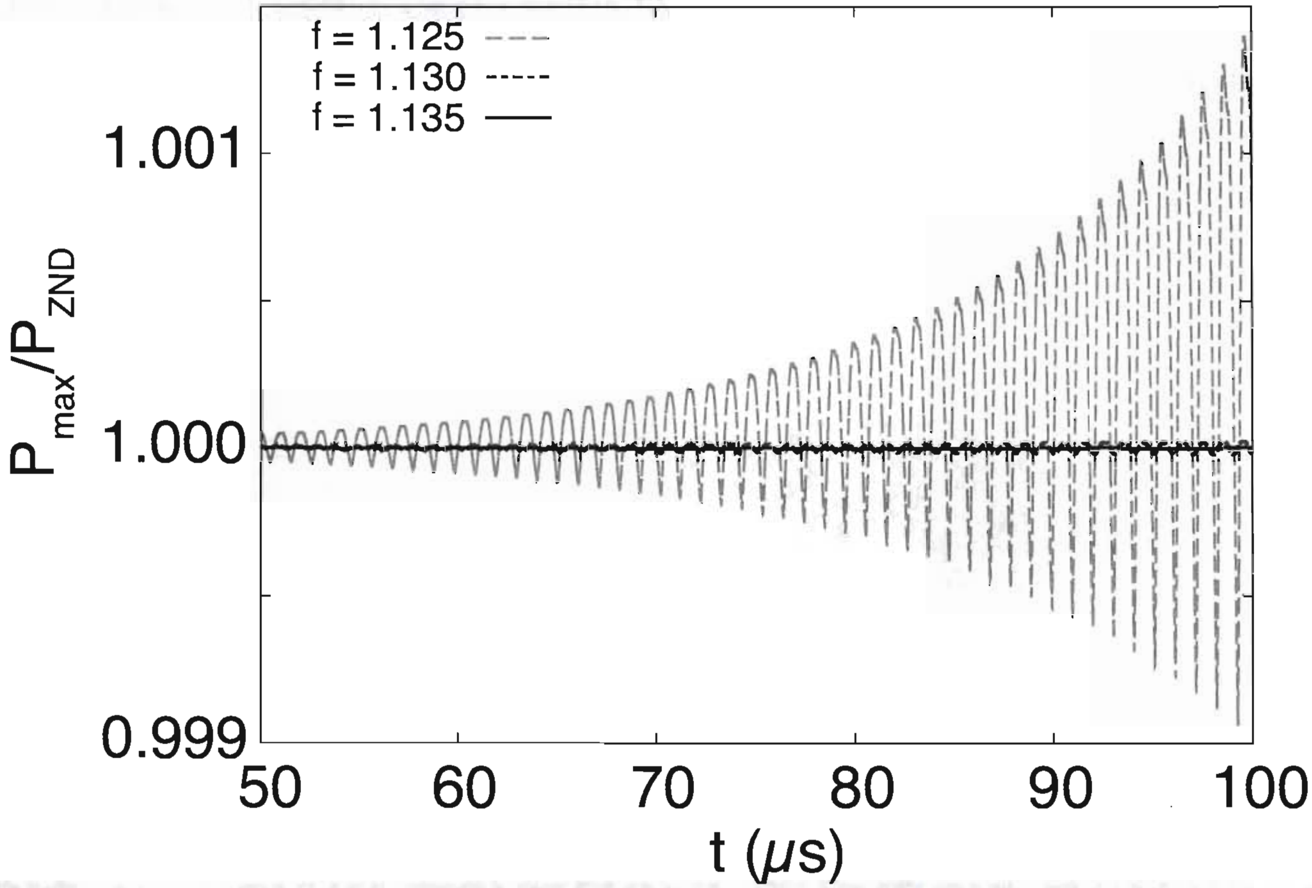


Inviscid Transient Behavior: Stable Detonation

$f = 1.15$

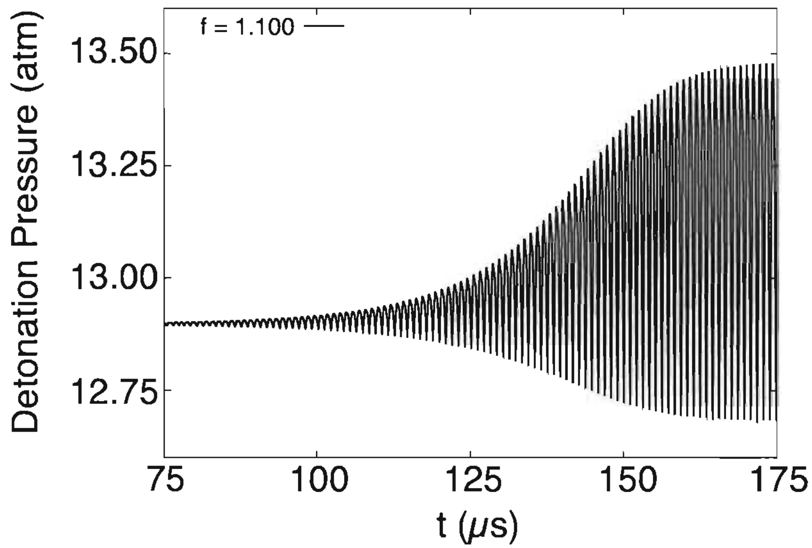


Near Neutral Stability



Inviscid Transient Behavior : Unstable Detonation

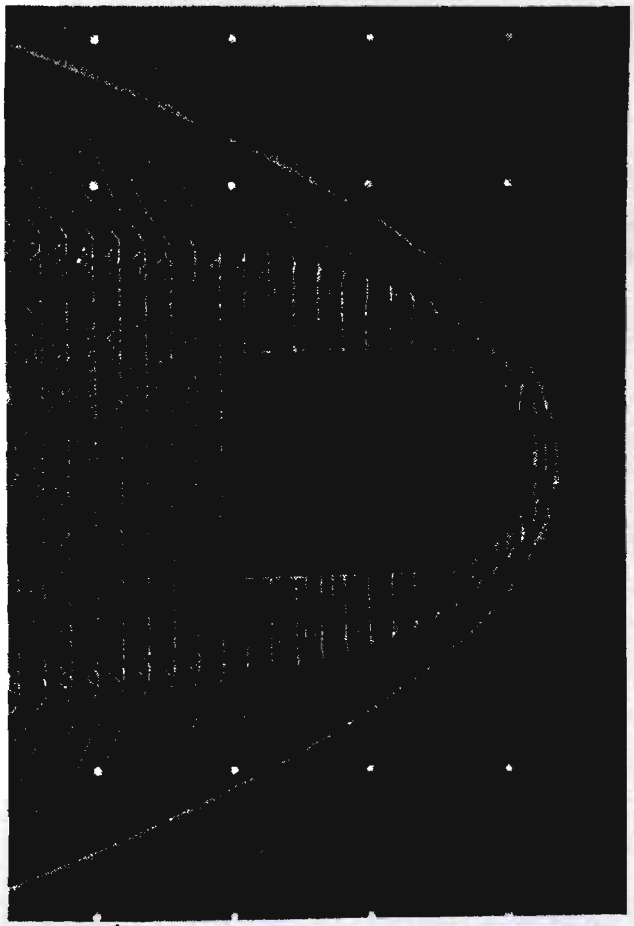
$f = 1.10$



- Frequency of $0.97\ MHz$ agrees well with both the frequency, $1.04\ MHz$, observed by Lehr (*Astro. Acta, 1972) in experiments and the frequency,* $1.06\ MHz$, *predicted by Yungster and Radhakrishan.*

- The maximum detonation front pressure predicted, $13.5\ atm$, is similar to the value of $14.0\ atm$ found by Daimon and Matsuo.

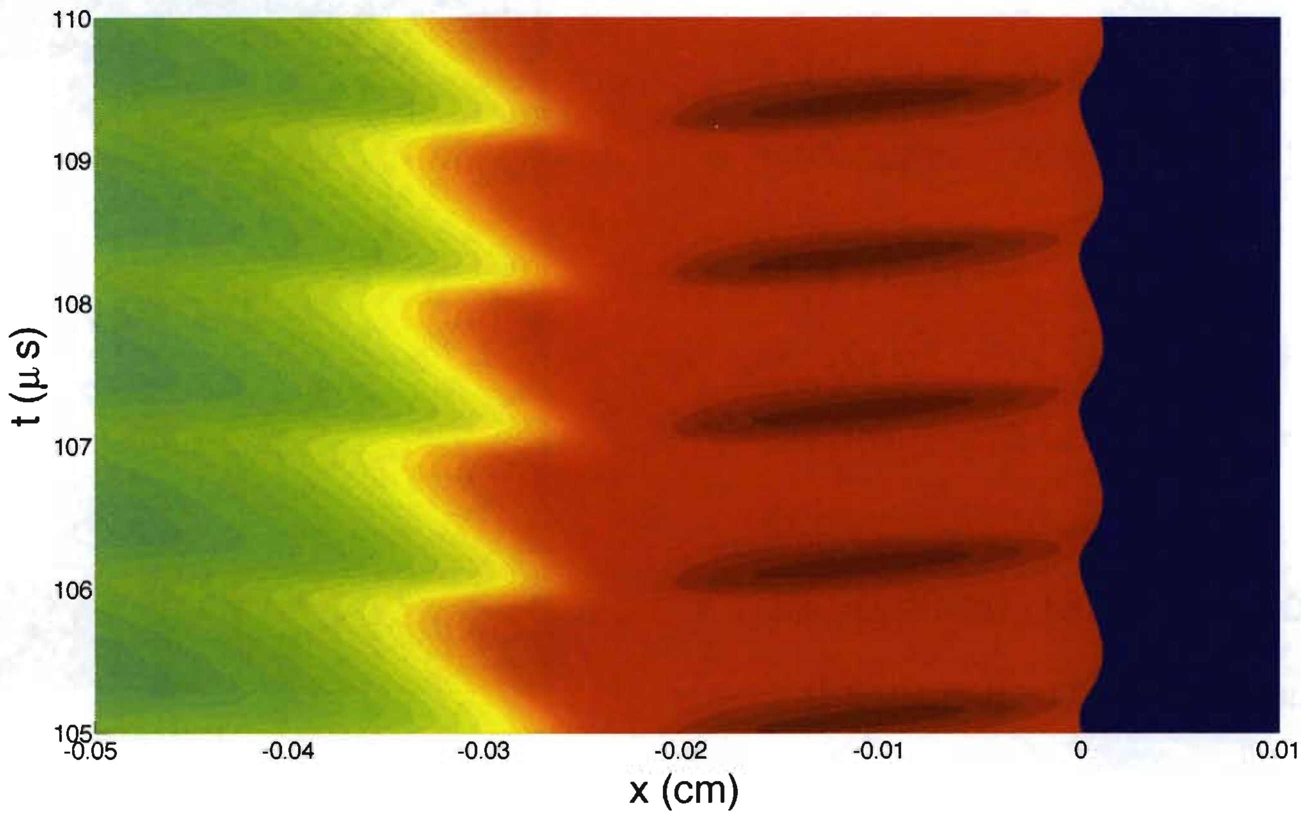
Lehr's High Frequency Instability



- Experiment of shock-induced combustion in flow around a sphere-cylinder projectile in an ambient stoichiometric mixture of $2H_2 + O_2 + 3.76N_2$ at $0.421\,atm$.
- Projectile velocity yields an equivalent overdrive of $f \approx 1.1$
- The observed frequency was approximately $1.04\,MHz$

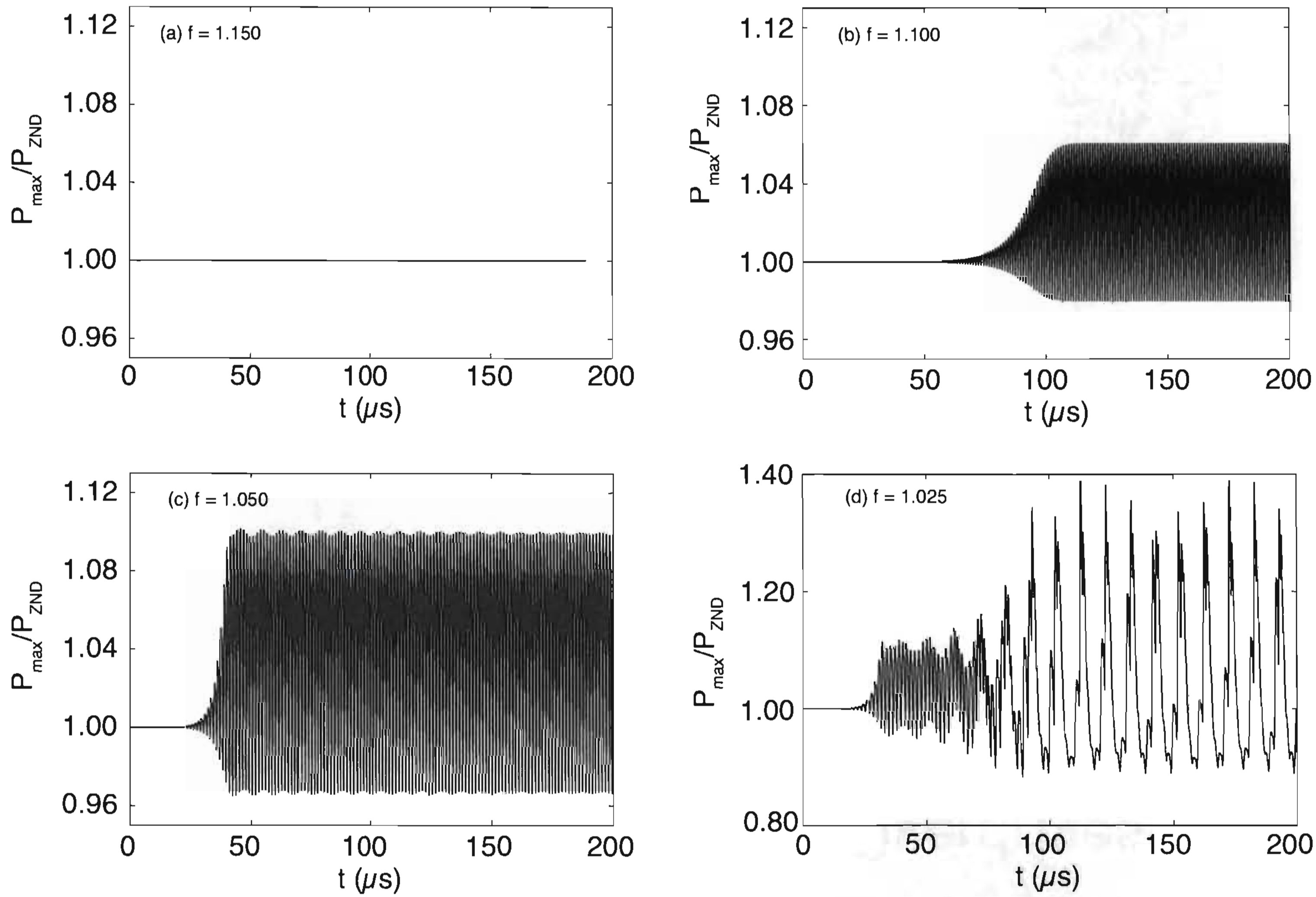
Unstable, Inviscid Detonation: x-t Diagram

$f = 1.10$

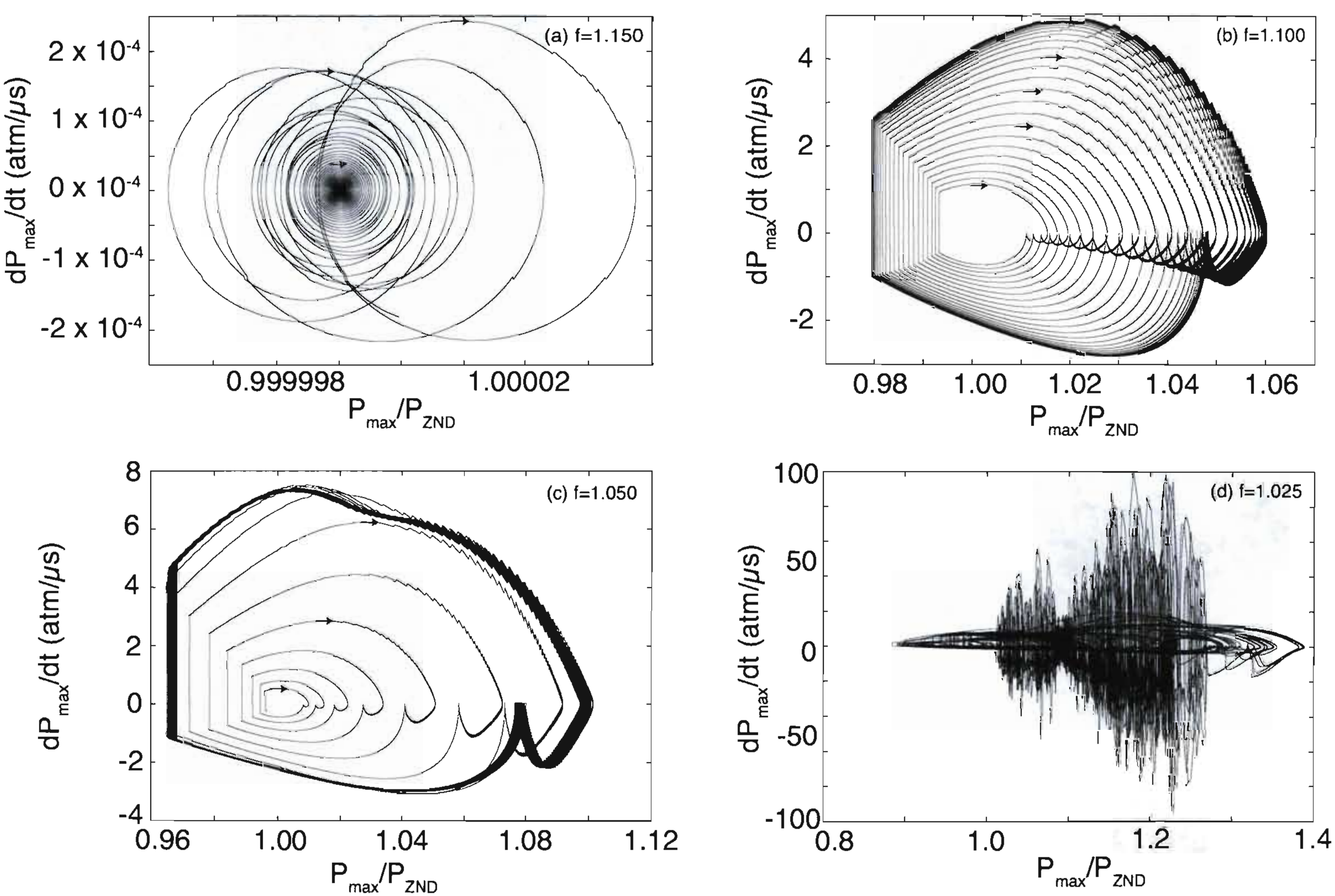


A x-t diagram of density in a Galilean reference frame traveling at $2057\ m/s$.

Inviscid Transient Behavior: Various Overdrives

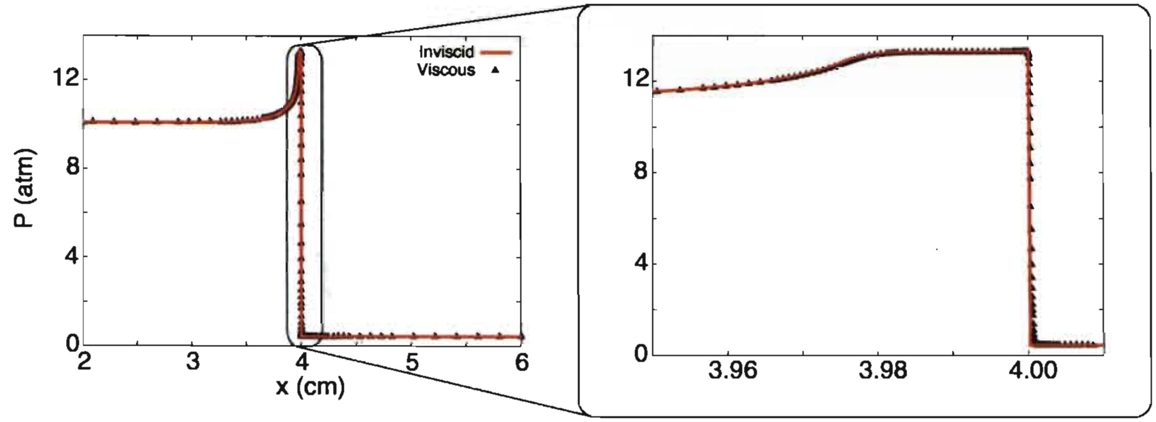


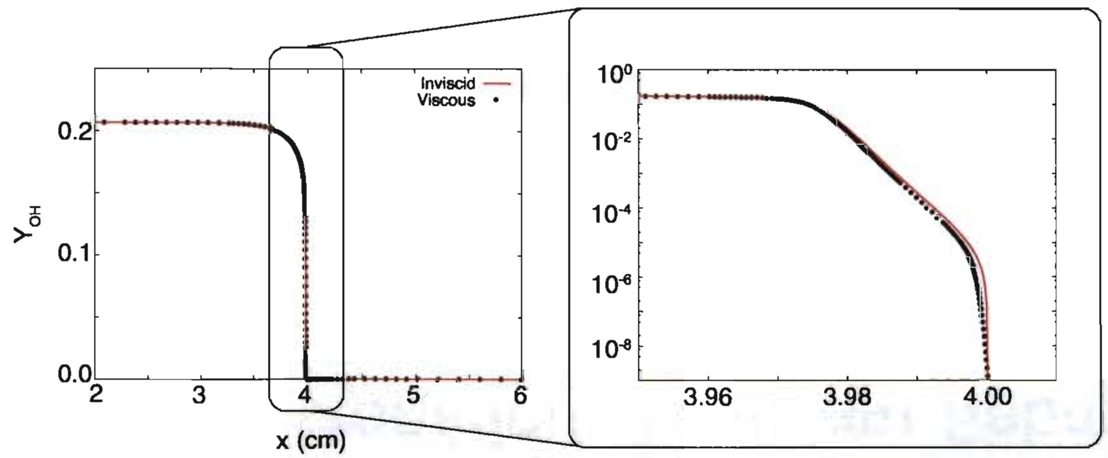
Inviscid Phase Portraits: Various Overdrives



Stable, Viscous Detonation: Long Time Structure

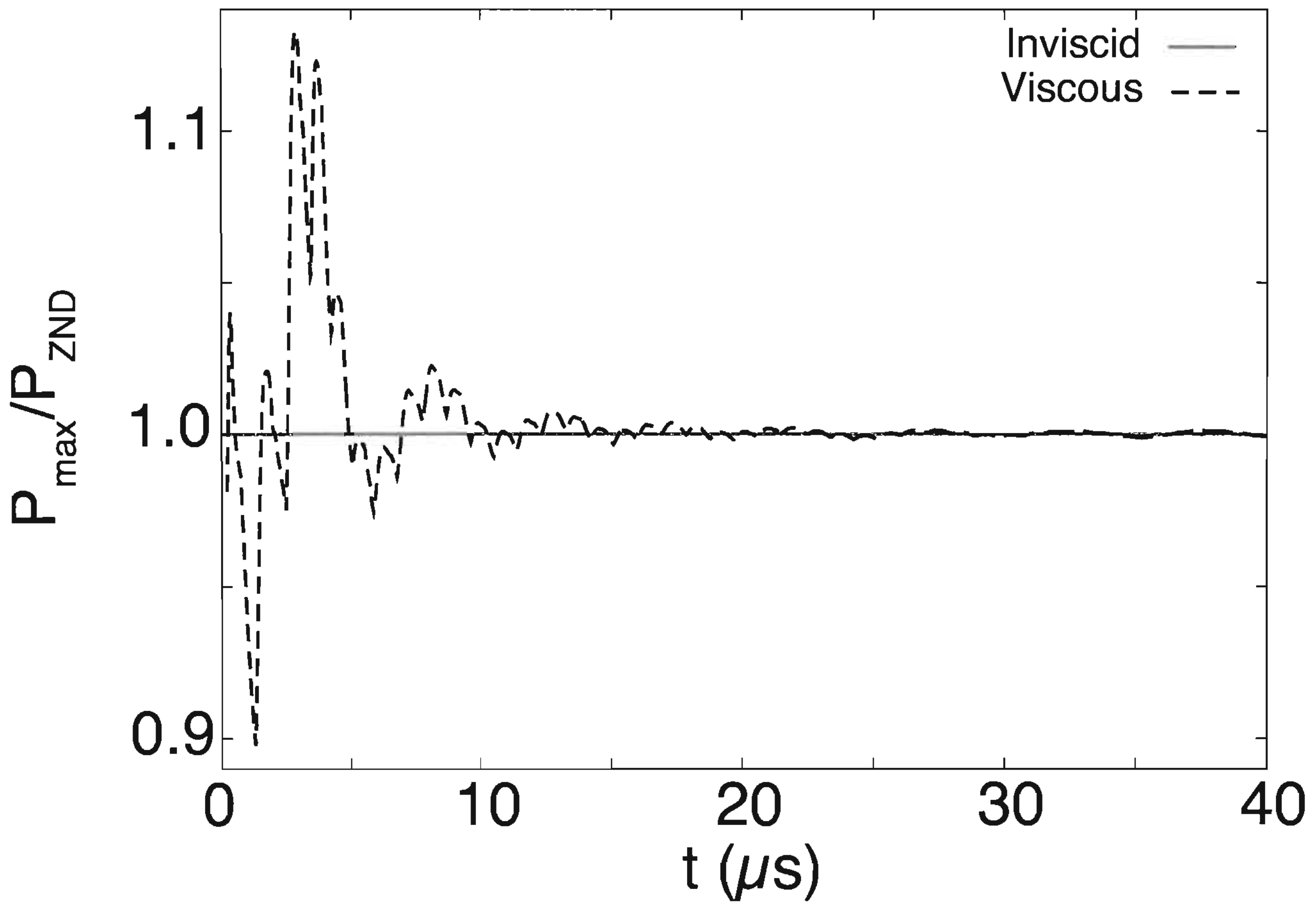
$f = 1.15$





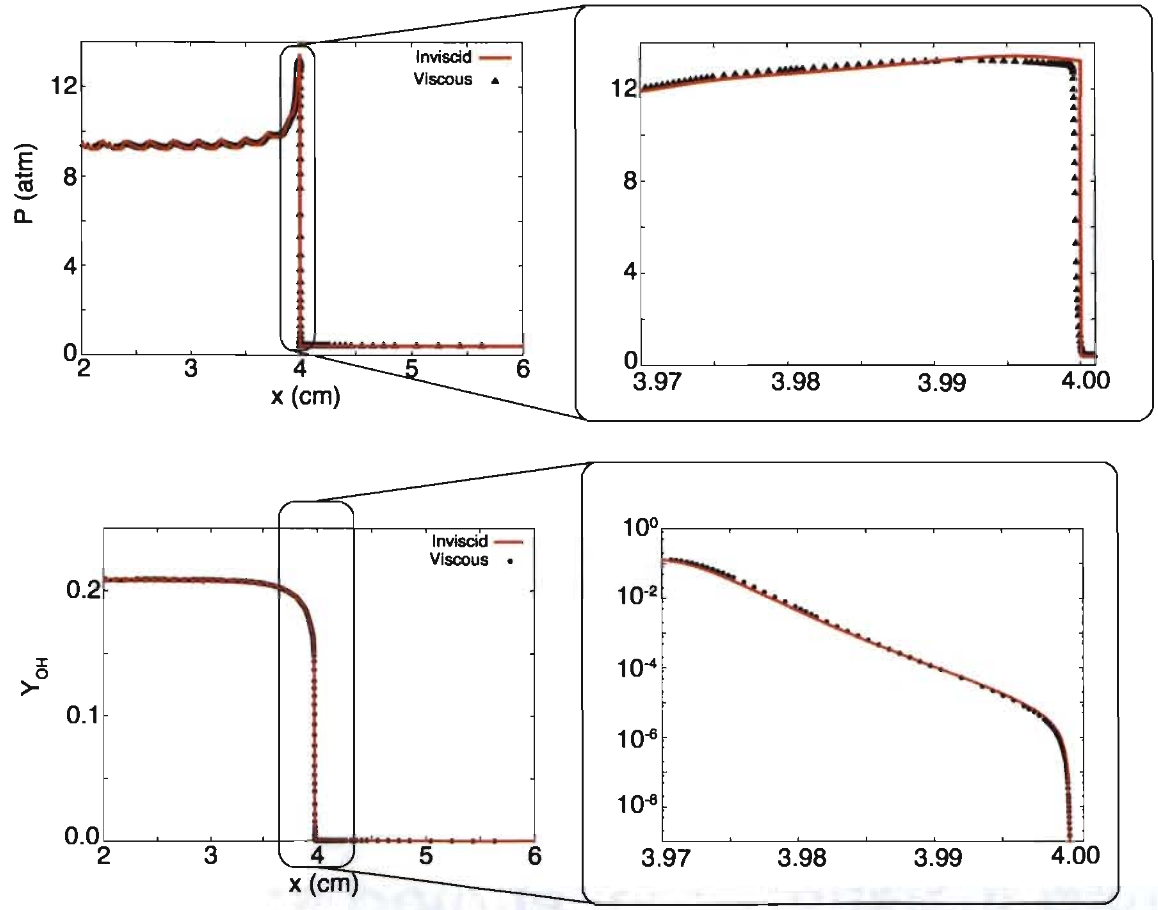
Stable, Viscous Detonation: Transient Behavior

$f = 1.15$



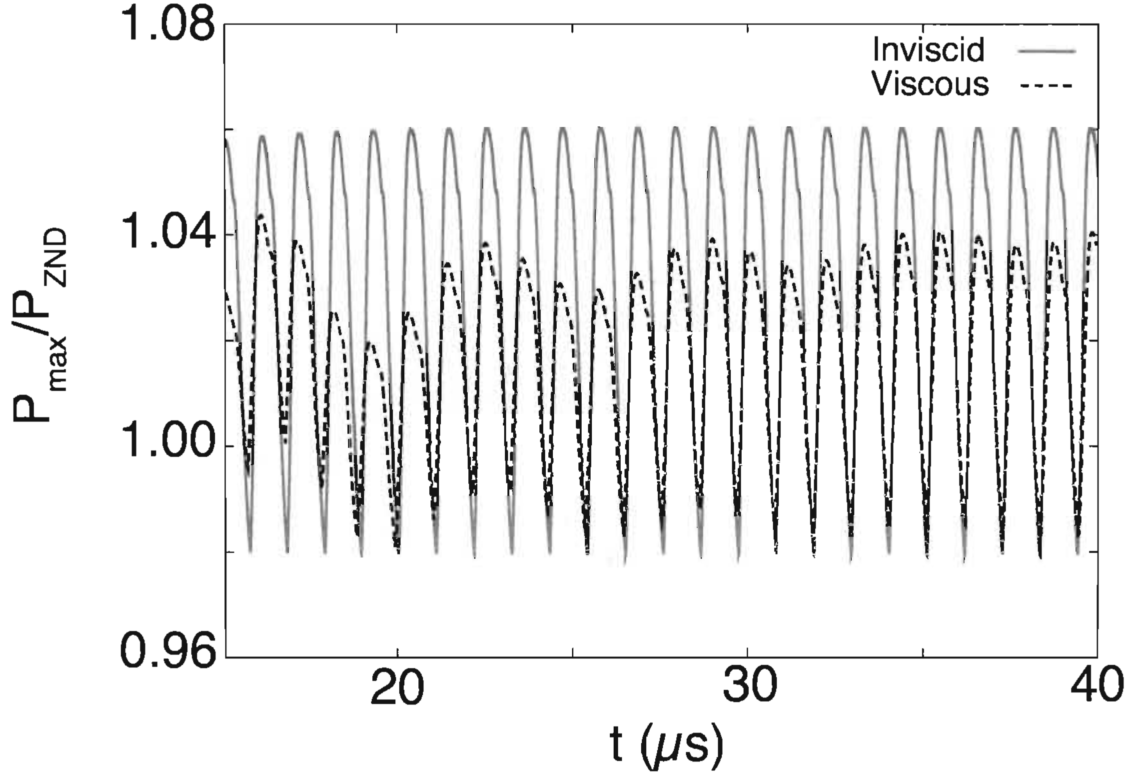
Unstable, Viscous Detonation: Long Time Structure

$f = 1.10$



Unstable, Viscous Detonation: Transient Behavior

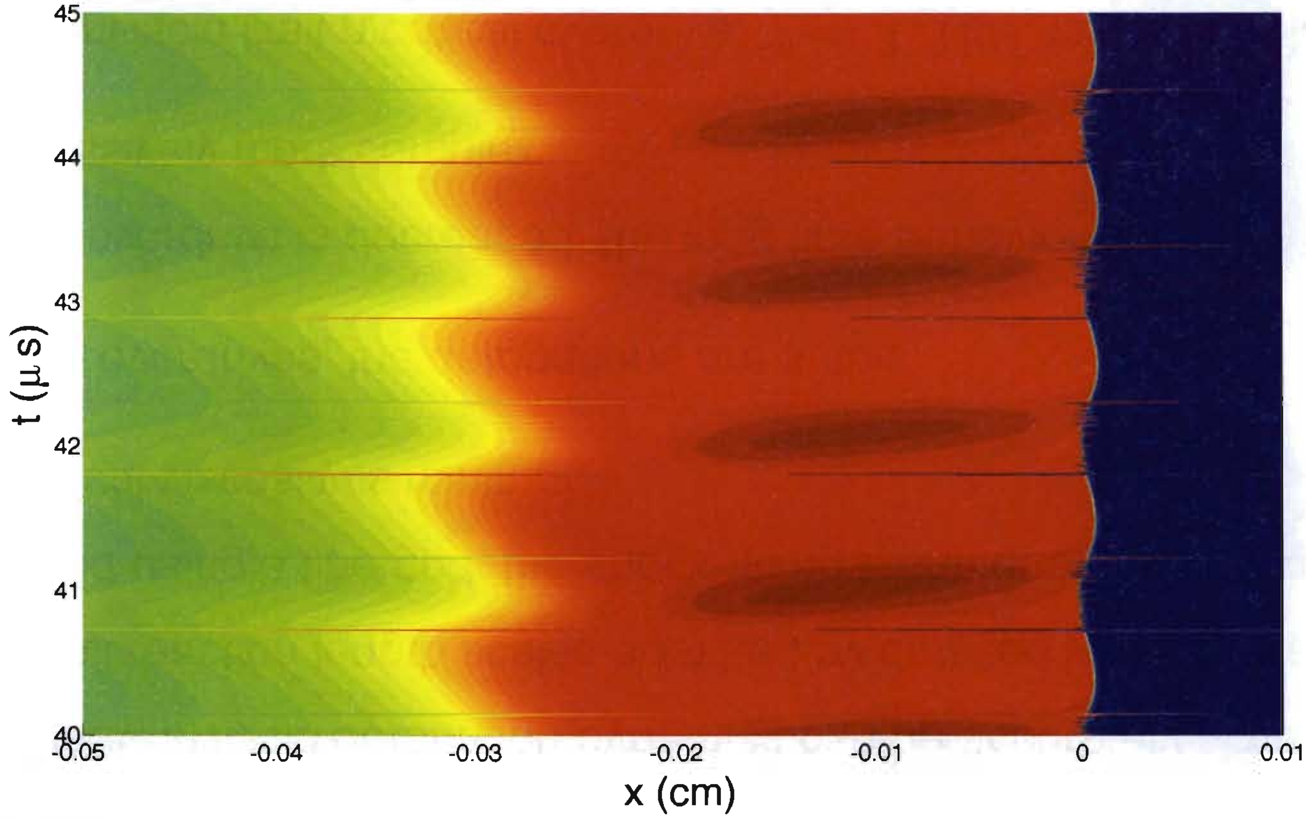
$f = 1.10$



The addition of viscous effects have a stabilizing effect, decreasing the amplitude of the oscillations by $\sim 25\%$.

Unstable, Viscous Detonation: x-t Diagram

$f = 1.10$



A x-t diagram of density in a Galilean reference frame traveling at $2057\ m/s$.

Conclusions

- Unsteady, inviscid detonation dynamics can be accurately simulated when all reaction length scales admitted by detailed kinetics are fully resolved using a fine grid; the shock-fitting technique used assures numerical viscosity is minimal.
- At high overdrives, the detonations are stable.
- As the overdrive is decreased, the long time behavior becomes progressively more complex.
- In the inviscid limit a critical overdrive, $f = 1.130$, is found below which oscillations at a single frequency appear.
- As the overdrive is lowered, the amplitude of these oscillations increases.

Conclusions

- Lowering the overdrive yet further gives rise to oscillations at multiple frequencies.
- The predicted $0.97\ MHz$ frequency for a $f = 1.10$ overdriven detonation agrees well with the frequency of $1.04\ MHz$ observed by Lehr in his experiments of shock-induced combustion flow around spherical projectiles.
- The structure of the overdriven detonation relative to the inviscid limit is modulated by the addition of mass, momentum, and energy diffusion.
- The addition of viscous effects has a stabilizing effect on the long time behavior of a detonation; the amplitude of the oscillations is significantly reduced.