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Verified Calculation of Nonlinear Dynamics of Viscous Detonation *

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The dynamics of one-dimensional detonations predicted by a one-step irreversible Arrhenius kinetic model with the inclusion of mass, momentum, and energy diffusion were investigated. A series of calculations in which activation energy is varied, holding the length scales of diffusion and reaction constant, was performed. As in the inviscid case, as the activation energy increases, the system goes through a period-doubling process and eventually undergoes a transition to chaos. Within the chaotic regime, there exist regions of low frequency limit cycles. The addition of diffusion significantly delays the onset of instability and strongly influences the dynamics in the unstable regime. Because the selected reaction and viscous length scales are representative of real physical systems, the common use of reactive Euler equations to predict detonation dynamics in the unstable and marginally stable regimes is called into question; reactive Navier-Stokes may be a more appropriate model in such regimes.

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Introduction

- 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?

Introduction-Continued

- It is often argued that viscous forces and diffusion are small effects which 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.
- This suggests grid-dependent numerical viscosity may be problematic.

Introduction-Continued

- Powers & Paolucci (*AIAA J*, 2005) studied the reaction length scales of inviscid H_2-O_2 detonations and found the finest length scales on the order of sub-microns to microns and the largest on the order of centimeters for atmospheric ambient pressure.
- This range of scales must be resolved to capture the dynamics.
- In a one-step kinetic model only a single chemical length scale is induced compared to the multiple length scales of detailed kinetics.
- By choosing a one-step model, the effect of the interplay between chemistry and transport phenomena can more easily be studied.

Review

- In the one-dimensional inviscid limit, one step models have been studied extensively.
- Erpenbeck (*Phys. Fluids*, 1962) began the investigation into the linear stability almost fifty years ago.
- Lee & Stewart (*JFM*, 1990) developed a normal mode approach, using a shooting method to find unstable modes.
- Bourlioux *et al.* (*SIAM JAM*, 1991) studied the nonlinear development of instabilities.

Review-Continued

- Kasimov & Stewart (*Phys. Fluids*, 2004) used a first order shock-fitting technique to perform a numerical analysis.
- Ng *et al.* (*Comb. Theory and Mod.*, 2005) developed a coarse bifurcation diagram showing how the oscillatory behavior became progressively more complex as activation energy increased.
- Henrick *et al.* (*J. Comp. Phys.*, 2006) developed a more detailed bifurcation diagram using a fifth order mapped WENO shock-fitting technique.

One-Dimensional Unsteady Compressible Reactive Navier-Stokes Equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0,$$

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}\left(\rho u^2 + P - \tau\right) = 0,$$

$$\frac{\partial}{\partial t}\left(\rho\left(e + \frac{u^2}{2}\right)\right) + \frac{\partial}{\partial x}\left(\rho u\left(e + \frac{u^2}{2}\right) + j^q + (P - \tau)\, u\right) = 0,$$

$$\frac{\partial}{\partial t}(\rho Y_B) + \frac{\partial}{\partial x}\left(\rho u Y_B + j_B^m\right) = \rho r.$$

Equations were transformed to a steady moving reference frame.

Constitutive Relations

$$P = \rho R T,$$

$$e = \frac{p}{\rho\,(\gamma - 1)} - q Y_B,$$

$$r = H(P - P_s) a\,(1 - Y_B)\, e^{-\frac{\tilde{E}}{p/\rho}},$$

$$j_B^m = -\rho \mathcal{D} \frac{\partial Y_B}{\partial x},$$

$$\tau = \frac{4}{3} \mu \frac{\partial u}{\partial x},$$

$$j^q = -k \frac{\partial T}{\partial x} + \rho \mathcal{D} q \frac{\partial Y_B}{\partial x}.$$

with $D = 10^{-4} \frac{m^2}{s}$, $k = 10^{-1} \frac{W}{mK}$, and $\mu = 10^{-4} \frac{Ns}{m^2}$, so for $\rho_o = 1 \frac{kg}{m^3}$, $Le = Sc = Pr = 1$.

Case Examined

Let us examine this one-step kinetic model with:

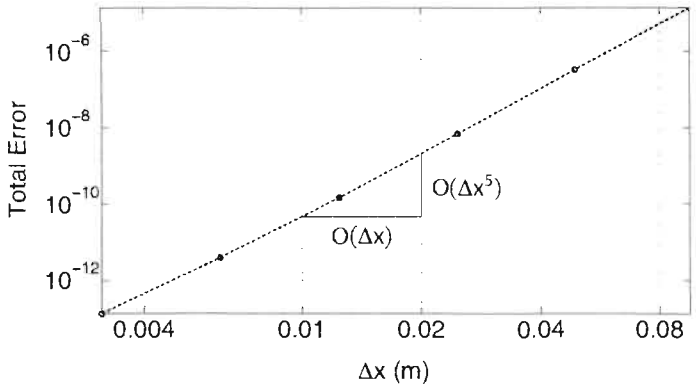
- a fixed reaction length, $L_{1/2} = 10^{-6}\ m$, which is similar to the finest length scale of H_2-O_2.
- a fixed the diffusion length, $L_\mu = 10^{-7}\ m$; mass, momentum, and energy diffusing at the same rate.
- an ambient pressure, $P_o = 101325\ Pa$, ambient density, $\rho_o = 1\ kg/m^3$, heat release $q = 5066250\ m^2/s^2$, and $\gamma = 6/5$.
- a range of activation energies were examined $(25 \leq E \leq 32)$ and thus a range for the collision frequency factor $(1.145 \times 10^{10}\ 1/s \leq a \leq 3.54 \times 10^{10}\ 1/s)$.

Numerical Method

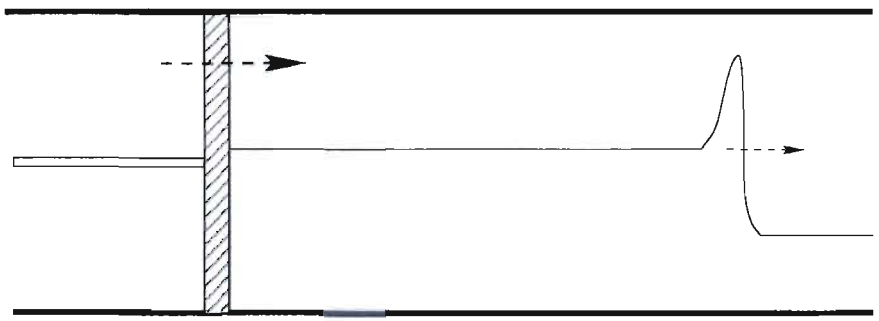
- Finite difference, uniform grid
  $\left(\Delta x = 2.50 \times 10^{-8} m, N = 8001, L = 0.2\, mm\right)$.
- Computation time = 192 hours for $10\ \mu s$ on an AMD $2.4\ GHz$ with $512\ kB$ cache.
- A point-wise method of lines aproach was used.
- Advective terms were calculated using a combination of fifth order WENO and Lax-Friedrichs.
- Sixth order central differences were used for the diffusive terms.
- Temporal integration was accomplished using a third order Runge-Kutta scheme.

Method of Manufactured Solutions (MMS)

- A solution form is assumed, and special sources terms are added to the governing equations.
- With these sources terms, the assumed solution satisfies the modified equations.
- Fifth order and third order convergence is acheived for space and time, respectively.



Method

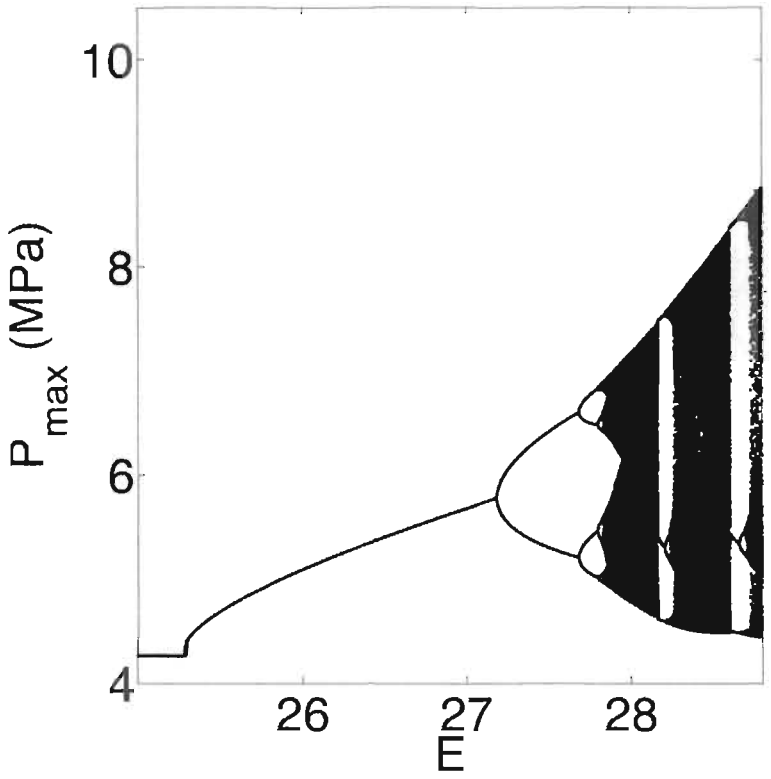


- Initialized with inviscid ZND solution.
- Moving frame travels at the CJ velocity.
- Integrated in time for long time behavior.

Inviscid Limit

- Lee and Stewart revealed for $E < 25.26$ the steady ZND wave is linearly stable. Henrick *et al.* found the stability limit at $E_0 = 25.265 \pm 0.005$.
- The system goes through a bifurcation process, transitioning to a period-1 limit cycle.
- A period-doubling begins at $E_1 \approx 27.2$. The point where this period-doubling behavior accumulates is $E_\infty \approx 27.8324$.
- After this period-doubling region, there is a likely a chaotic regime with pockets of order, having periods of 5, 6, and 3.
- The period-doubling behavior and transition to chaos predicted has striking similarilities to that of the logistic map.

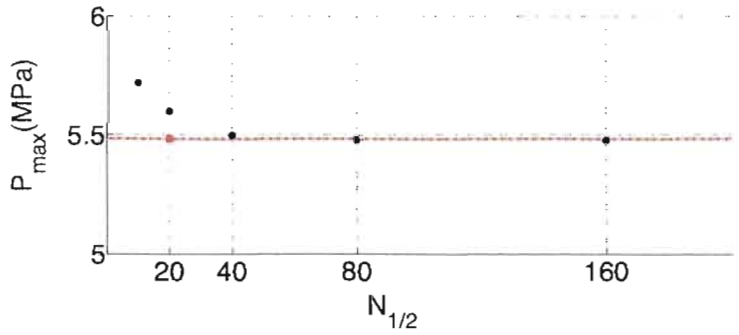
Bifurcation Diagram (Inviscid)



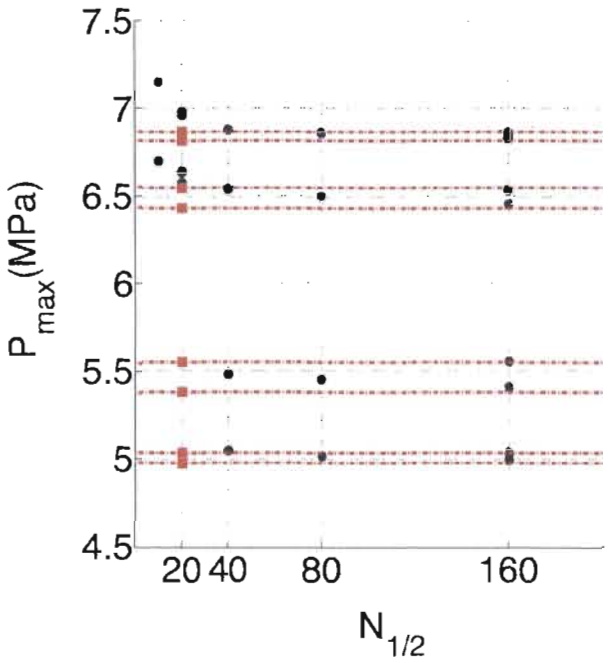
Note: The bifurcation plot was constructed using $N_{1/2} = 20$ in combination with a shock-fitting technique of Henrick *et al.*

Inviscid Limit - Shock-capturing vs. Shock-fitting

- At lower activation energies where the behavior is simpler, shock-capturing compares well with shock-fitting with similar resolutions.
- At $E = 26.64$, shock-fitting predicts a period-1 oscillating detonation $(P_{max} = 5.48\ MPa)$.
- Shock-capturing using $N_{1/2} = 20$, yields an relative difference of 2.1% and using $N_{1/2} = 40$ this relative difference is reduced to 0.34%

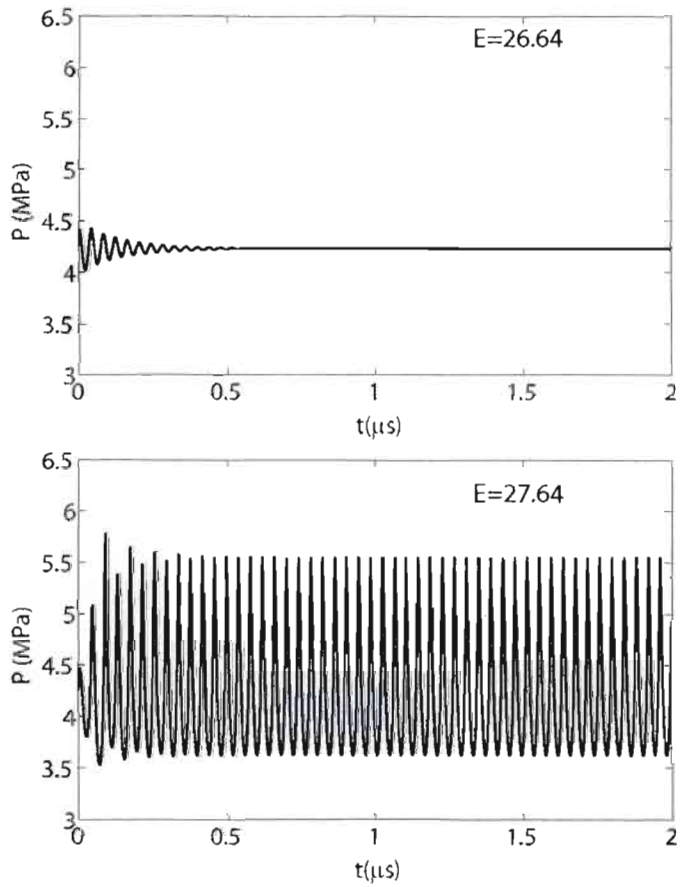


Inviscid Limit - Shock-capturing vs. Shock-fitting



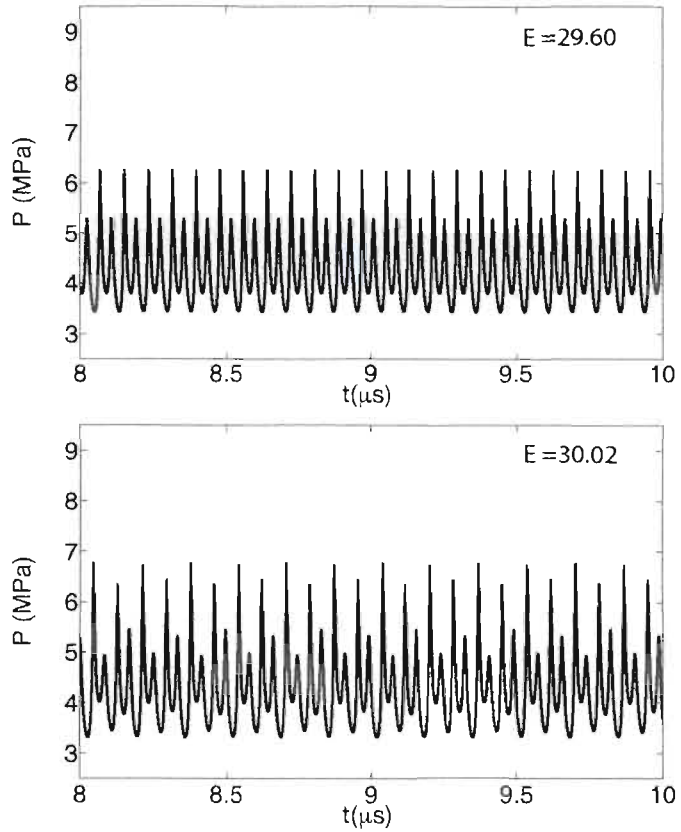
- At a higher activation energy, $(E = 27.82)$, shock-fitting predicts a period-8 detonation, where as shock-capturing using $N_{1/2} = 40$ predicts a period-4 detonation. To reconcile this difference, the resolution of the shock-capturing technique must be increased to $N_{1/2} \approx 160$.
- Numerical diffusion is playing an important role in determining the behavior of the system. Let's add physical diffusion and see how that affects the behavior of the system.

Effect of Diffusion on Limit Cycle Behavior



- Recall the stability limit for the ZND wave was found to be $E_0 = 25.265 \pm 0.005$ in the inviscid case
- In the viscous case $E = 26.66$ is still stable; however, above $E_0 \approx 27.14$ a period-1 limit cycle can be realized.

Period-Doubling Phenomena



- As in the inviscid limit the viscous case goes through a period-doubling phase.
- However the addition of diffusion delays this transition from $E_1 \approx 27.2$ to $E_1 \approx 29.32$.

Effect of Diffusion on Transition to Chaos

- With the ratio of $L_\mu / L_{1/2} = 1/10$, the accumulation point of bifurcation is delayed until $E_\infty \approx 30.0327$.
- For $E > 30.0327$, a region exists with many relative maxima in the detonation pressure; it is likely the system is in the chaotic regime.

Approximations to Feigenbaum's Constant

$$\delta_\infty = \lim_{n\to\infty} \delta_n = \lim_{n\to\infty} \frac{E_n - E_{n-1}}{E_{n+1} - E_n}$$

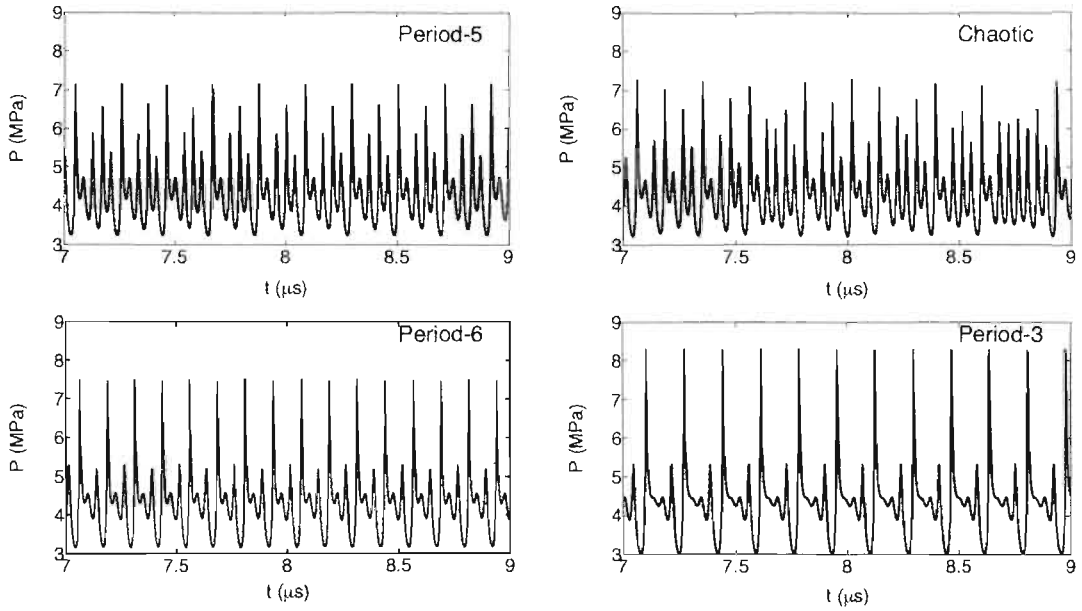
Feigenbaum predicted $\delta_\infty \approx 4.669201.$

	Inviscid	Inviscid	Viscous	Viscous
n	E_n	δ_n	E_n	δ_n
0	25.2650	-	27.14	-
1	27.1875	3.86	29.32	3.89
2	27.6850	4.26	29.88	4.67
3	27.8017	4.66	30.00	-
4	27.82675	-	-	-

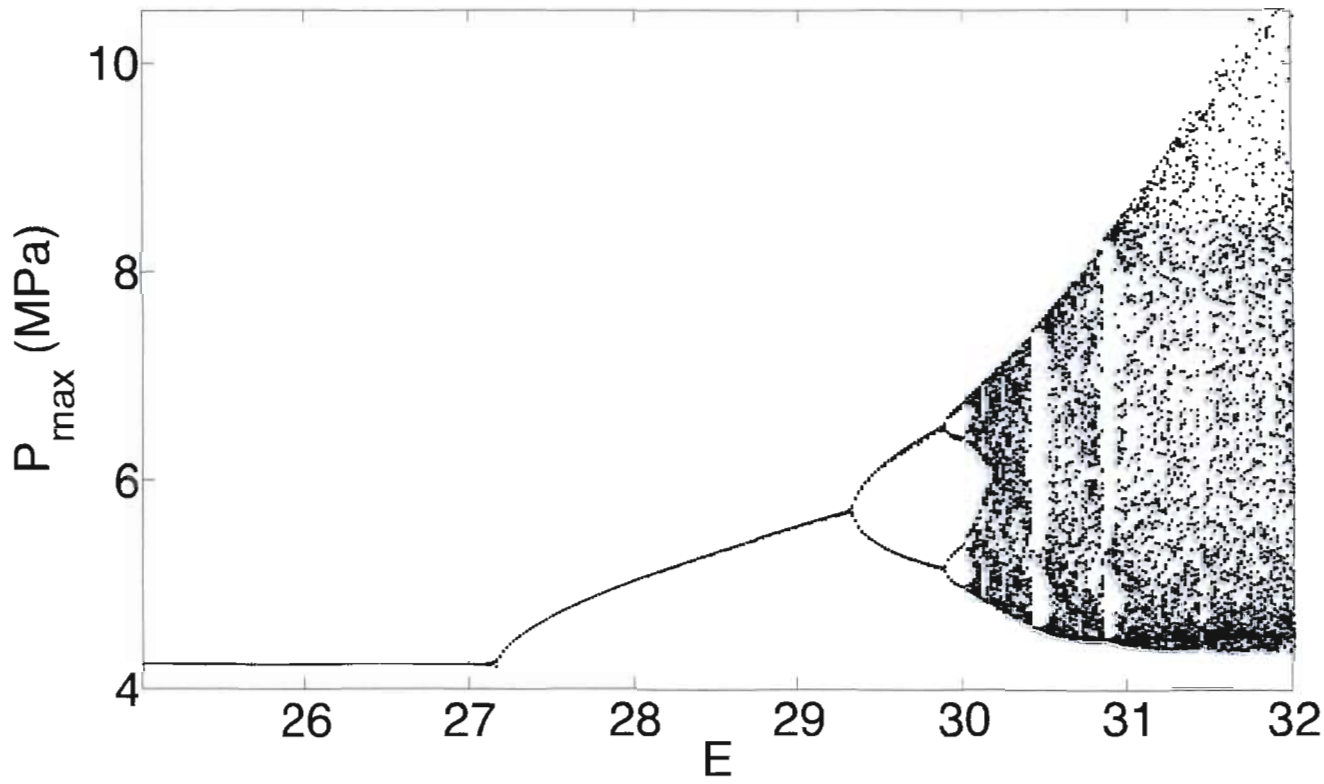
Chaos and Order

- The period-doubling behavior and transition to chaos predicted in the inviscid limit is also observed in the diffusive case.
- Within this chaotic region, there exist pockets of order with periods of 5, 6, and 3 present.

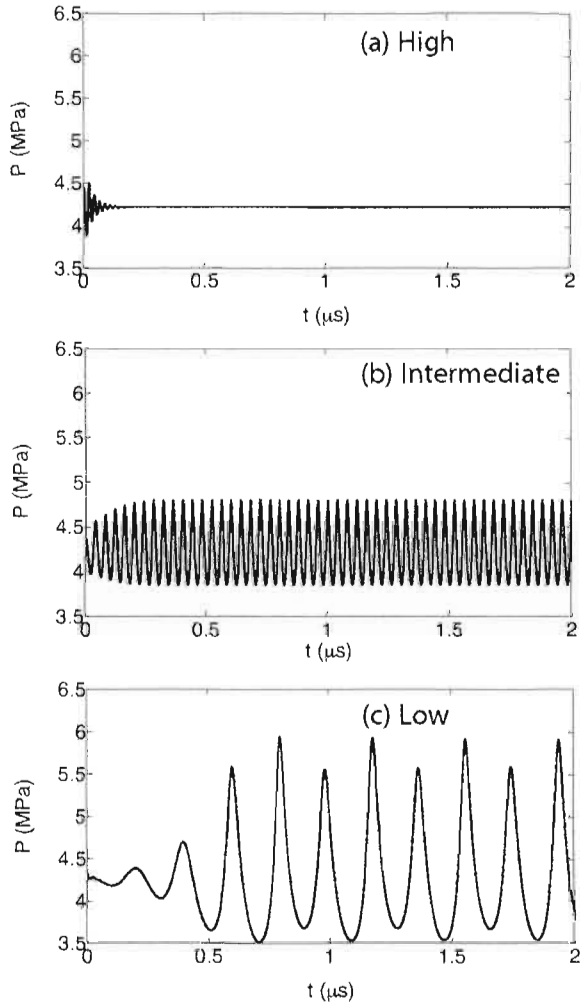
Viscous Detonations:



Bifurcation Diagram (Viscous)



Effect of Diminshing Viscosity ($E = 27.64$)



- The system undergoes transition from a stable detonation to a period-1 limit cycle, to a period-2 limit cycle.
- The amplitude of pulsations increases.
- The frequency decreases.

Convergence Rate

- Theoretical convergence rate in space is 5^{th}, however due to the Heaviside function acting as a weak 1^{st} order error, the true convergence rate is below the theoretical value.
- Here are two representative points in pressure for two different activation energies.

$\Delta x\ (m)$	$P_{29.0}\ (MPa)$	$r_{c_{29.0}}$	$P_{29.5}\ (MPa)$	$r_{c_{29.5}}$
3.33×10^{-8}	4.1998	-	5.8825	-
1.66×10^{-8}	3.7527	3.74	4.8461	3.61
1.11×10^{-8}	3.7165	-	4.7540	-

Conclusions

- Dynamics of one-dimensional detonations are influenced significantly by mass, momentum, energy diffusion in the region of instability.
- In general, the effect of diffusion is stabilizing.
- Bifurcation and transition to chaos show similarities to the logistic map.
- For physically motivated reaction and diffusion length scales not unlike those for H_2-air detonations, the addition of diffusion delays the onset of instability.

Conclusions-Continued

- As physical diffusion is reduced, the behavior of the system trends towards the inviscid limit.
- If the dynamics of marginally stable or unstable detonations are to be captured, physical diffusion needs to be included and dominate numerical diffusion or an LES filter.
- Results will likely extend to detailed kinetic systems.
- Detonation cell pattern formation will also likely be influenced by the magnitude of the physical diffusion.