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Title: THE DYNAMICS OF UNSTEADY DETONATION WITH DIFFUSION

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Title:
The Dynamics of Unsteady Detonation with Diffusion

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Abstract:
The dynamics of one-dimensional detonations using a one-step irreversible Arrhenius kinetic model with the inclusion of momentum, energy and mass diffusion were investigated. A high-order spatio-temporal integration of the underlying compressible, reactive Navier-Stokes equations are constructed. A series of calculations in which activation energy is varied, holding the length scales of diffusion and reaction constant, were carried out. As in the inviscid case, as the activation energy is increased, the system goes through period-doubling phenomena and eventually undergoes a transition to chaos. Within the chaotic regime there still remain regions of stable limit cycles. An approximation to Feigenbaum's constant, the rate at which bifurcation points converge, is obtained. The addition of diffusion significantly influences the dynamics of the system in the region of instability, delaying the onset of the instability.

The Dynamics of Unsteady Detonation with Diffusion

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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 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 shock-fitting technique.

One-Dimensional Unsteady Compressible Reactive Navier-Stokes Equations

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

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

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

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

Equations were transformed to a steady moving reference frame.

Constitutive Relations

$$P = \rho R T,$$

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

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

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

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

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

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:

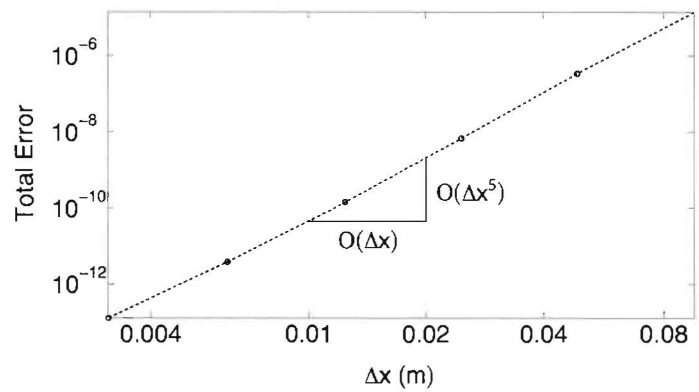
- a fixed reaction length, $L_{1/2} = 10^{-6}\ m$, which is similar to that of H_2-O_2.
- a fixed diffusion length, $L_\mu = 10^{-7}\ m$; mass, momentum, and energy diffusing at the same rate.
- an ambient pressure, $P_o = 101325\ Pa$, ambient density, $\rho_o = 1\ kg/m^3$, heat release $q = 5066250\ m^2/s^2$, and $\gamma = 6/5$.

Numerical Method

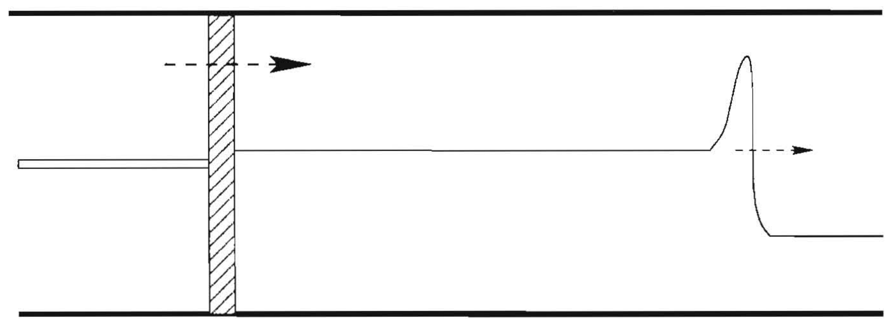
- Finite difference, uniform grid $(\Delta x = 2.50 \times 10^{-8} m, N = 8001, L = 0.2\, mm)$.
- Computation time = 192 hours for $10\ \mu s$ on an AMD $2.4\ GHz$ with $512\ kB$ cache.
- A point-wise method of lines aproach was used.
- Advective terms were calculated using a combination of fifth order 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.

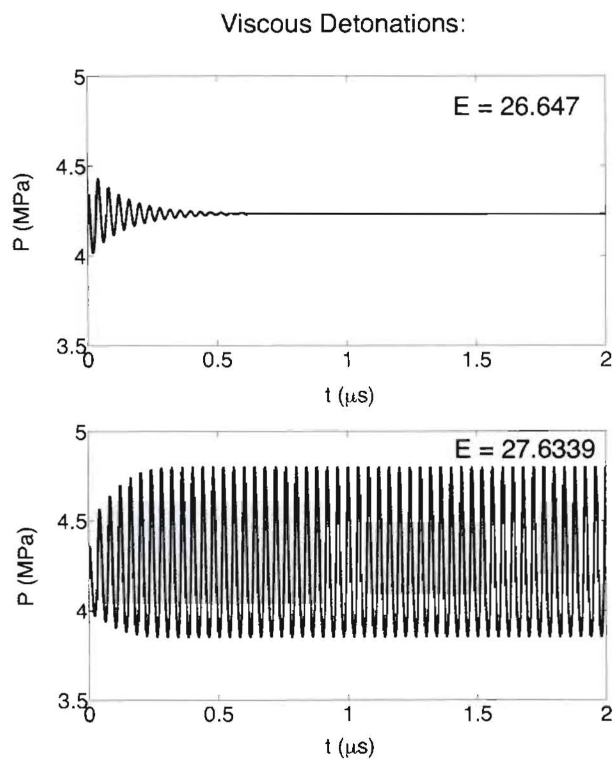


Method



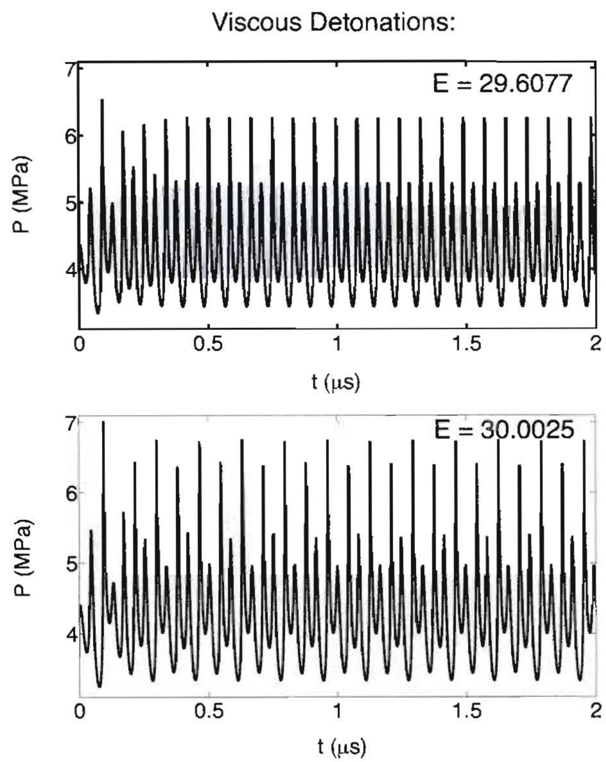
- Initialized with inviscid ZND solution.
- Moving frame travels at the CJ velocity.
- Integrated in time for long time behavior.

Effect of Diffusion on Limit Cycle Behavior



- Lee and Stewart revealed for $E < 25.26$ the steady ZND wave is linearly stable.
- For the inviscid case Henrick *et al.* found the stability limit at $E_0 = 25.265 \pm 0.005$.
- In the viscous case $E = 26.647$ is still stable; however, above $E_0 \approx 27.1404$ 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.
- For the inviscid case the period-doubling began at $E_1 \approx 27.2$.
- In the viscous case the beginning of this period doubling is delayed to $E_1 \approx 29.3116$.

Effect of Diffusion on Transition to Chaos

- In the inviscid limit, the point where bifurcation points accumulate is found to be $E_\infty \approx 27.8324$.
- For the viscous case, $L_\mu/L_{1/2} = 1/10$, the accumulation point is delayed until $E_\infty \approx 30.0411$.
- For $E > 30.0411$, a region exists with many relative maxima in the detonation pressure; it is likely the system is in the chaotic regime.

Table of 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 $\delta_\infty \approx 4.669201.$

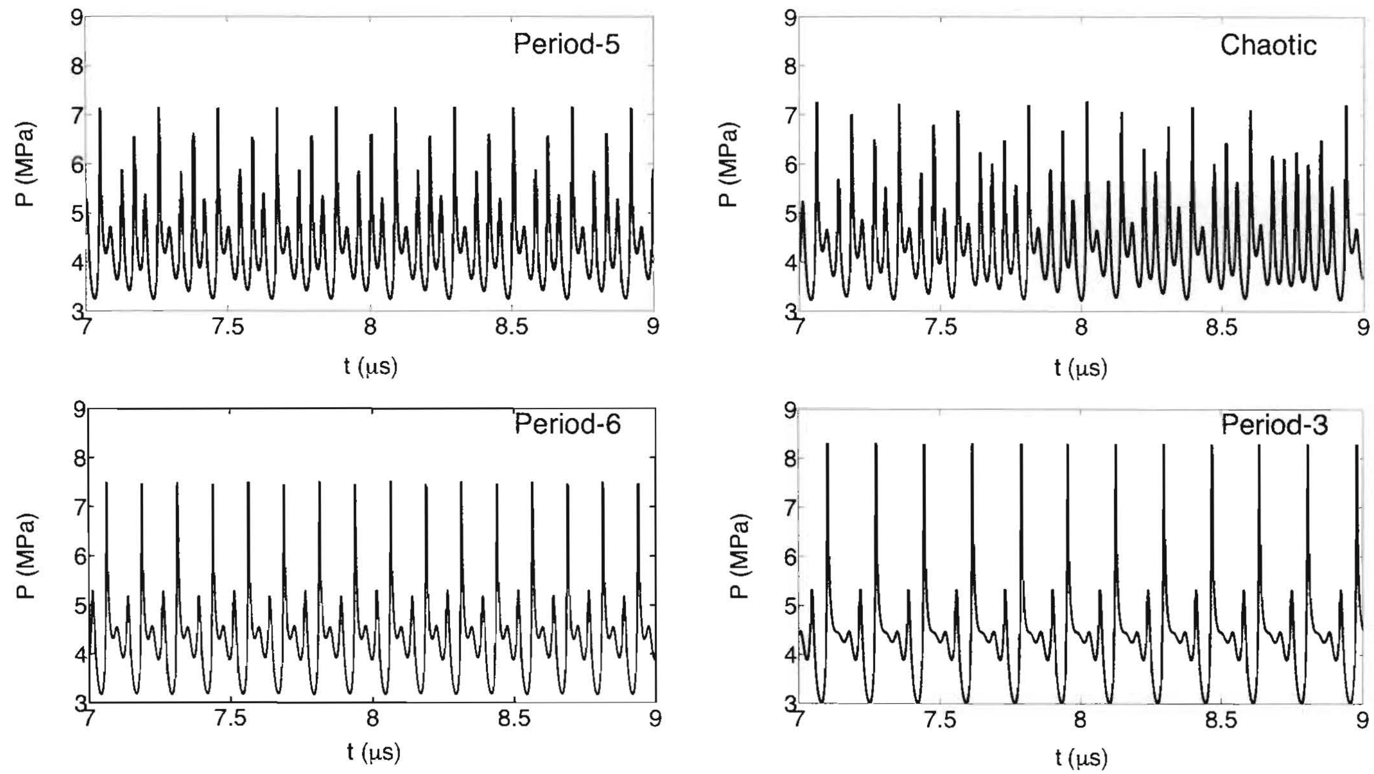
	Inviscid	Inviscid	Viscous	Viscous
n	E_n	δ_n	E_n	δ_n
0	25.2650	-	27.1404	-
1	27.1875	3.86	29.3116	3.793
2	27.6850	4.26	29.8840	4.639
3	27.8017	4.66	30.0074	4.657
4	27.82675	-	30.0339	-

Effect of Diffusion in the Chaotic Regime

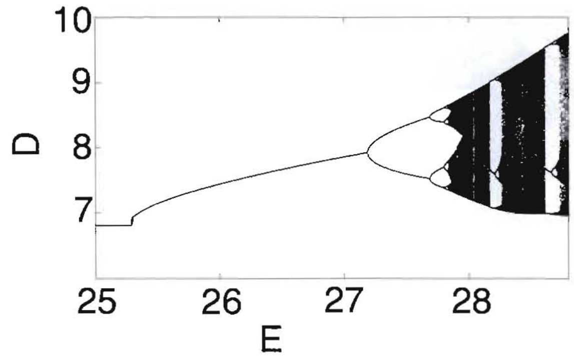
- The period-doubling behavior and transition to chaos predicted in both the viscous and inviscid limit have striking similarilities to that of the logistic map.
- Within this chaotic region, there exist pockets of order.
- Periods of 5, 6, and 3 are found within this chaotic region.

Chaos and Order

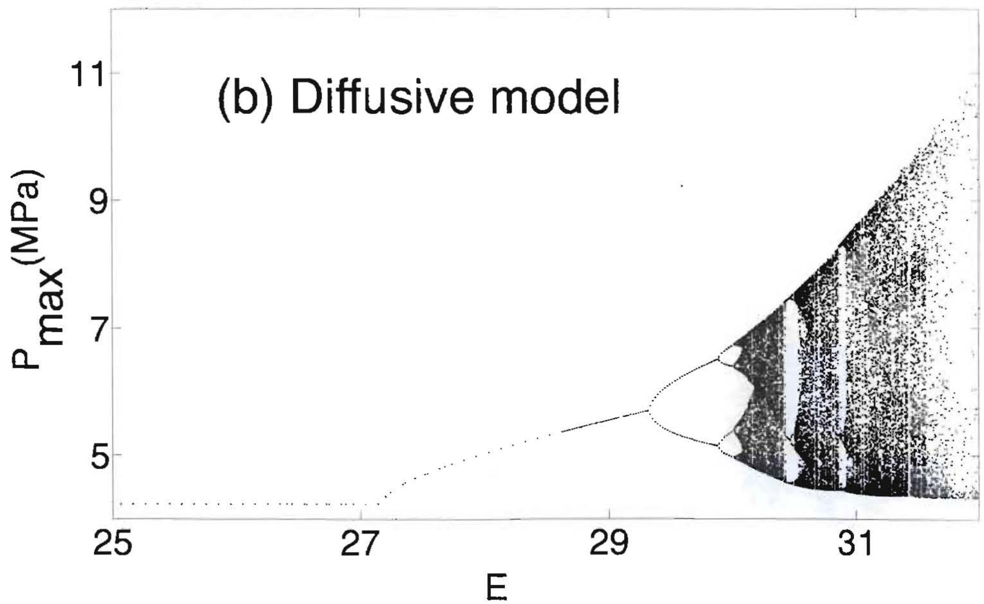
Viscous Detonations:



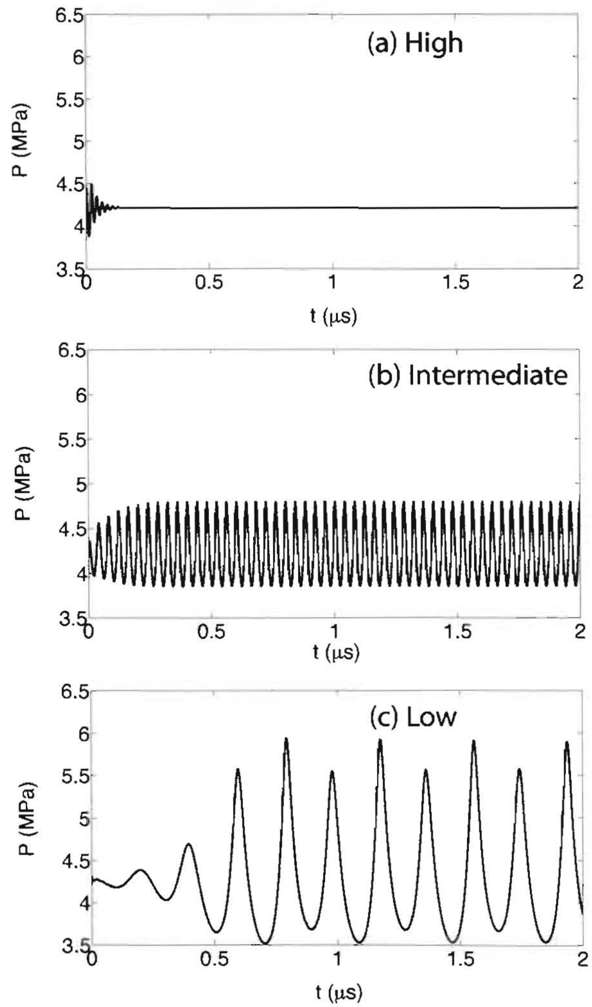
Bifurcation Diagram



(a) Inviscid model with shock-fitting algorithm



Effect of Diminshing Viscosity ($E = 27.6339$)



- 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.

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.