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

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

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

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

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

Equations were transformed to a steady moving reference frame.

Constitutive Relations

$$P = \rho R T,$$

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

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

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

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

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

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

Case Examined

Let us examine this one-step kinetic model with:

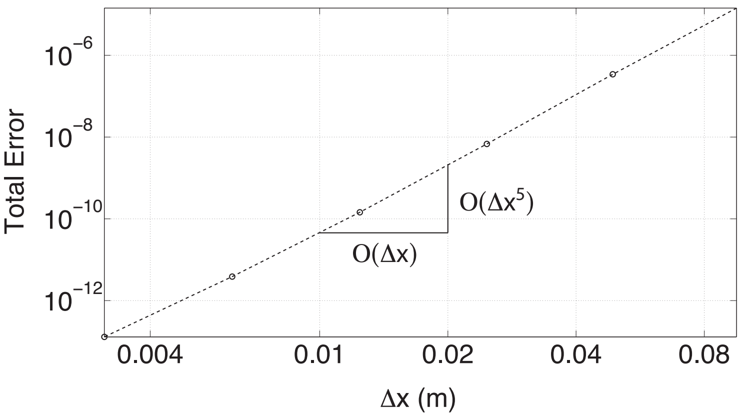
- a fixed reaction length, $L_{1/2} = 10^{-6}\ m$, which is similar to that of H_2-O_2.
- a fixed diffusion length, $L_{\mu} = 10^{-7}\ m$; mass, momentum, and energy diffusing at the same rate.
- an ambient pressure, $P_o = 101325\ Pa$, ambient density, $\rho_o = 1\ kg/m^3$, heat release $q = 5066250\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

Numerical Method

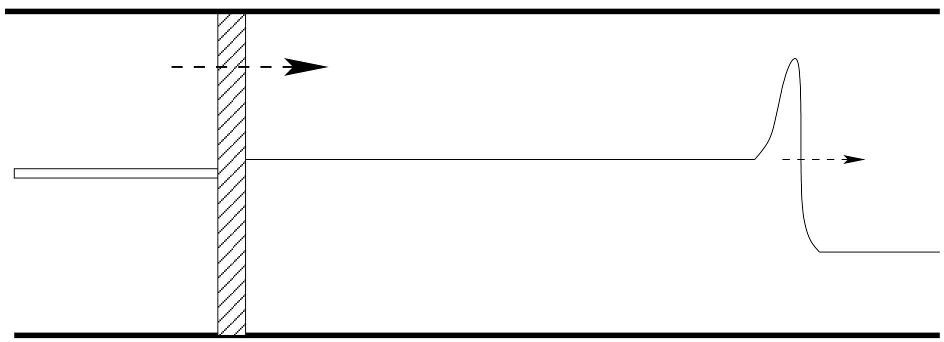
- Finite difference, uniform grid
  $\left(\Delta x = 2.50 \times 10^{-8} m, N = 8001, L = 0.2\, mm\right)$.
- Computation time = 192 hours for $10\ \mu s$ on an AMD $2.4\ GHz$ with $512\ kB$ cache.
- A point-wise method of lines aproach was used.
- Advective terms were calculated using a combination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

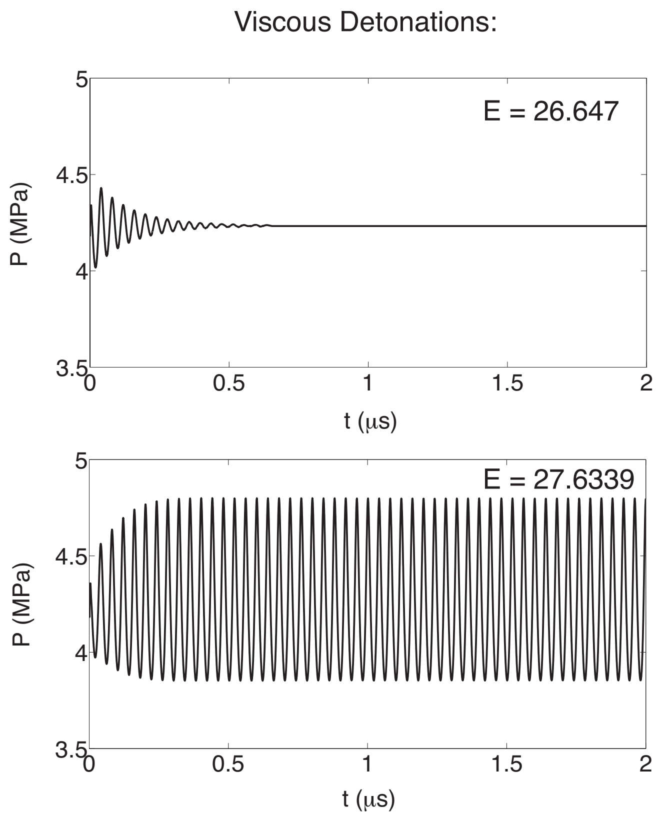


Method



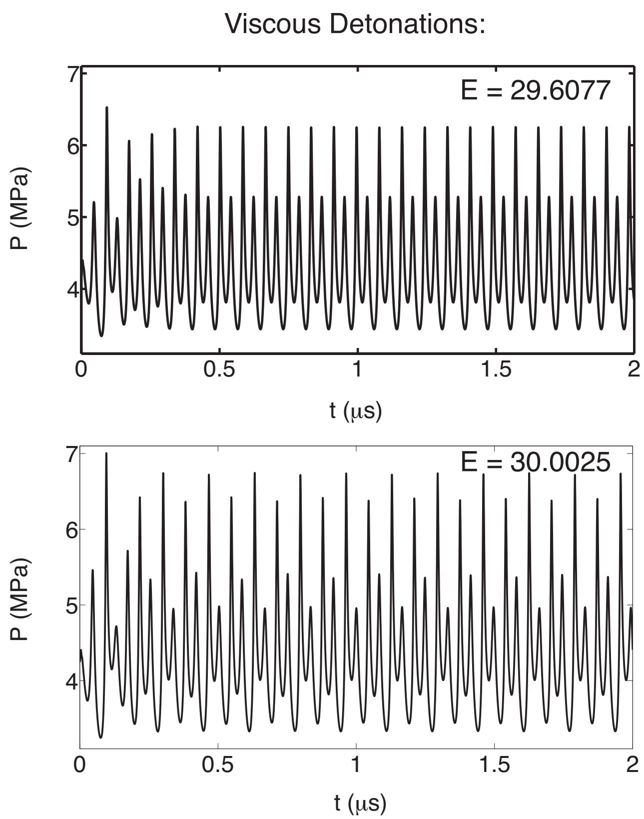
- Initialized with inviscid ZND solution.
- Moving frame travels at the CJ velocity.
- Integrated in time for long time behavior.

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 $\delta_\infty \approx 4.669201.$

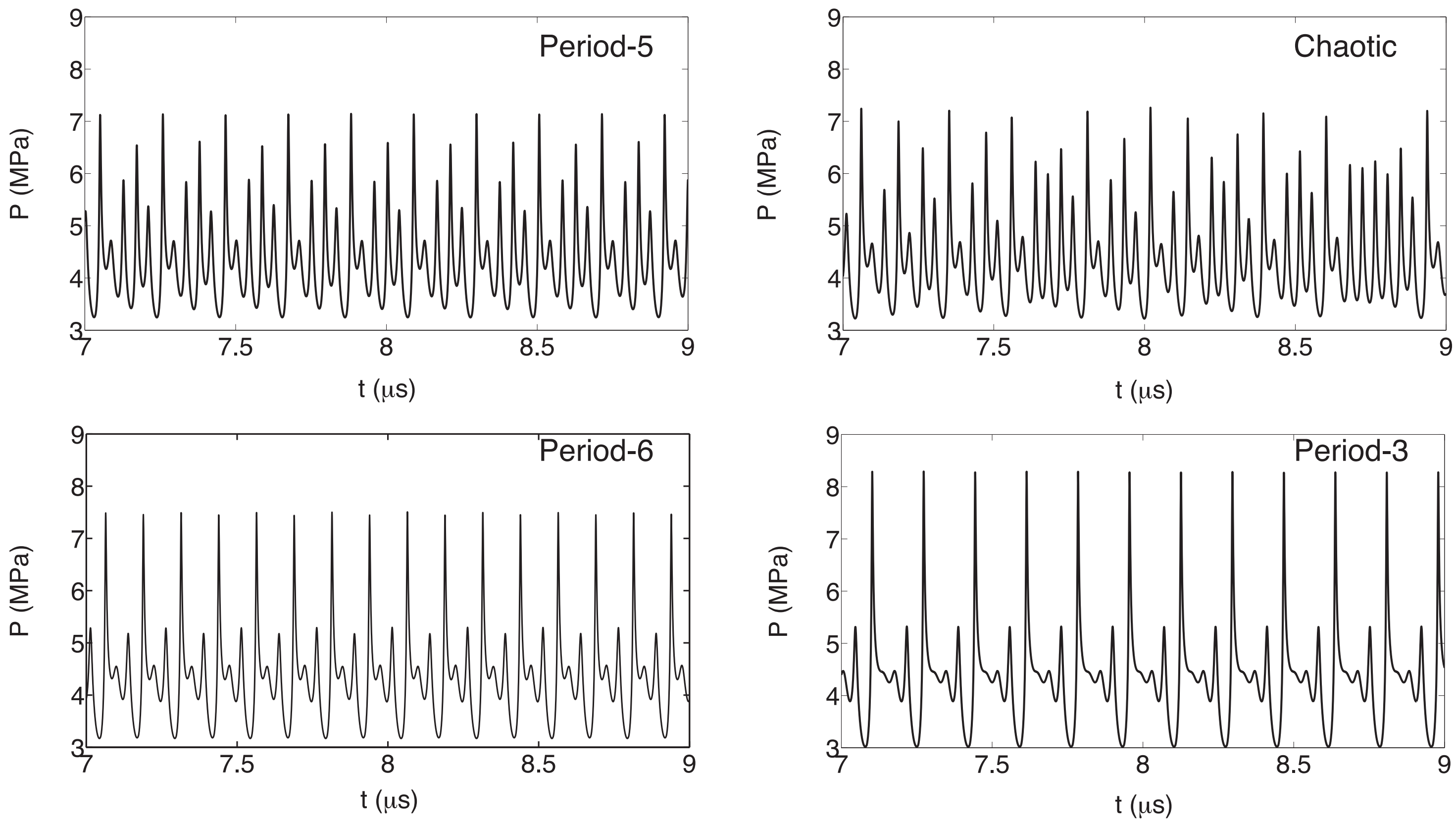
	Inviscid	Inviscid	Viscous	Viscous
n	E_n	δ_n	E_n	δ_n
0	25.2650	-	27.1404	-
1	27.1875	3.86	29.3116	3.793
2	27.6850	4.26	29.8840	4.639
3	27.8017	4.66	30.0074	4.657
4	27.82675	-	30.0339	-

Effect of Diffusion in the Chaotic Regime

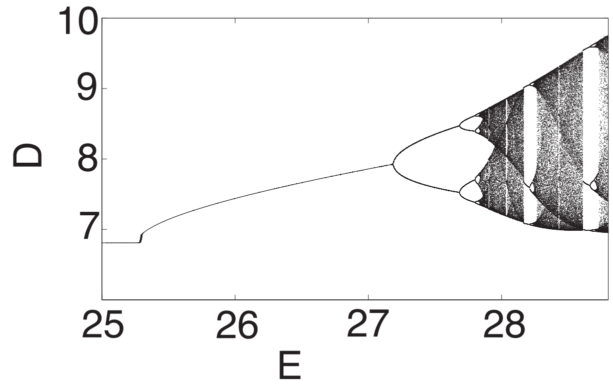
- The period-doubling behavior and transition to chaos predicted in both the viscous and inviscid limit have striking similarilities to that of the logistic map.
- Within this chaotic region, there exist pockets of order.
- Periods of 5, 6, and 3 are found within this chaotic region.

Chaos and Order

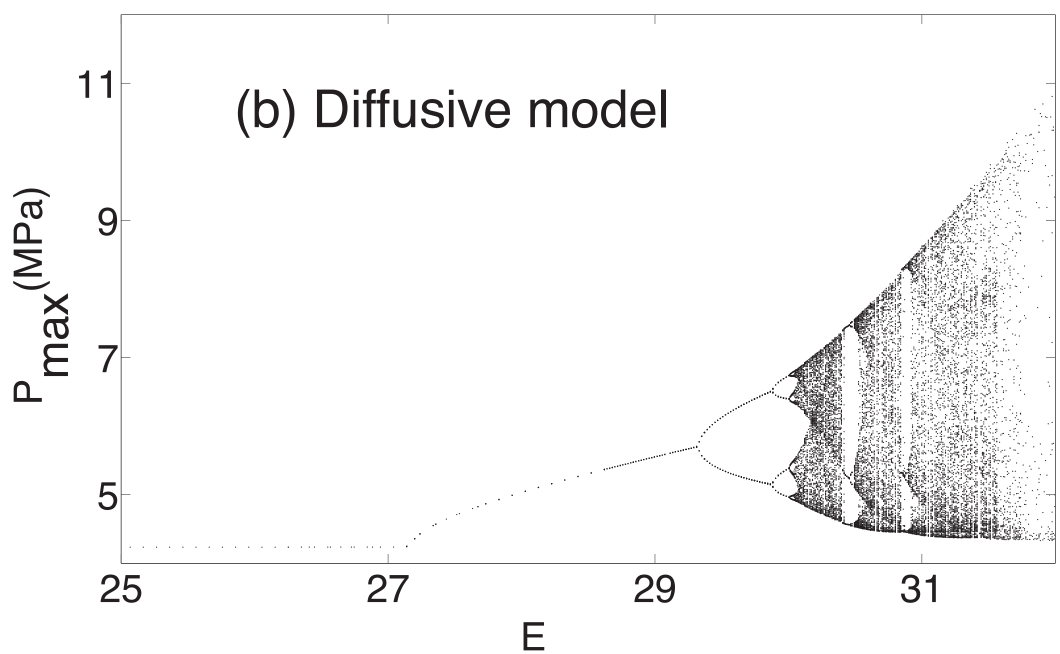
Viscous Detonations:



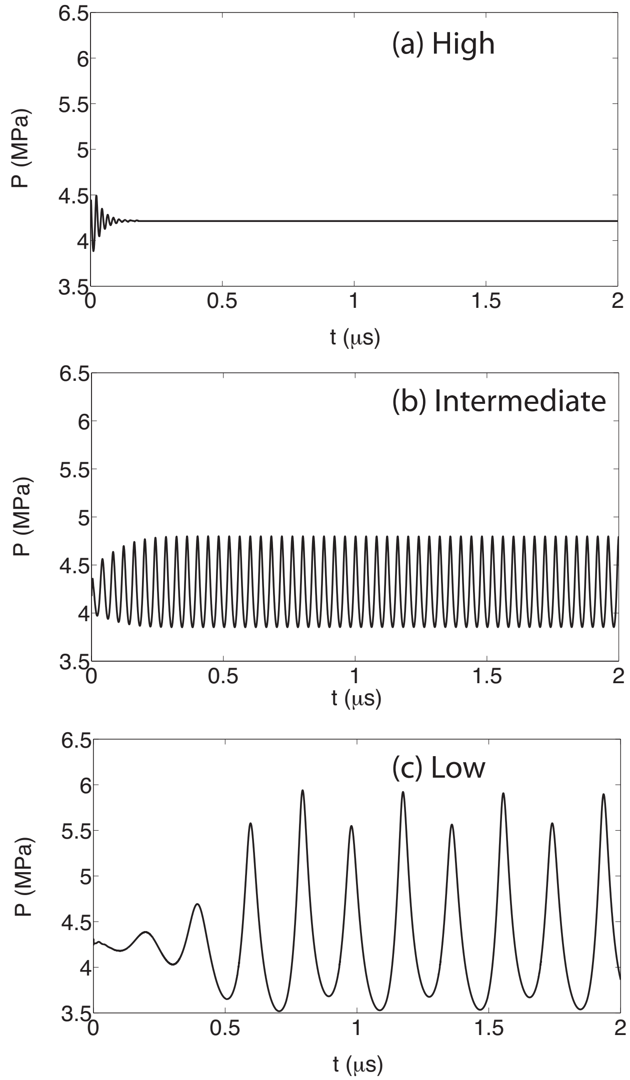
Bifurcation Diagram



(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.