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Title: THE DYNAMICS OF DETONATION WITH WENO AND
NAVIER-STOKES SHOCK-CAPTURING

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THE DYNAMICS OF DETONATION WITH WENO AND NAVIER-STOKES SHOCK-CAPTURING *

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We consider an unsteady one-dimensional detonation with diffusion and simple one-step kinetics. The advective terms from the Navier-Stokes equations are calculated using a combination of a fifth order WENO scheme and Lax- Friedrichs. The diffusive terms are treated with sixth order central differences. The diffusive effects remove the discontinuities from the system by smoothing the shock. It is shown that the bifurcation path to chaos, well-established for the inviscid analog of the same equations, is significantly modulated by the presence of physically realistic mass, momentum, and energy diffusion. Moreover, when physical diffusion is captured with an appropriately fine grid, a fifth order central difference of advective terms works as well as a WENO method in capturing the detonation dynamics.

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The Dynamics of Detonation with WENO and Navier-Stokes Shock-Capturing

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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, operator splitting, and turbulence modeling, all of which filter small scale physical dynamics?
 - Do we really need WENO methods if the problem demands resolved diffusive length scales?
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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 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.
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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.
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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.
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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 are transformed to a steady moving reference frame.

Constitutive Relations

$$P = \rho RT,$$

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

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

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

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

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

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

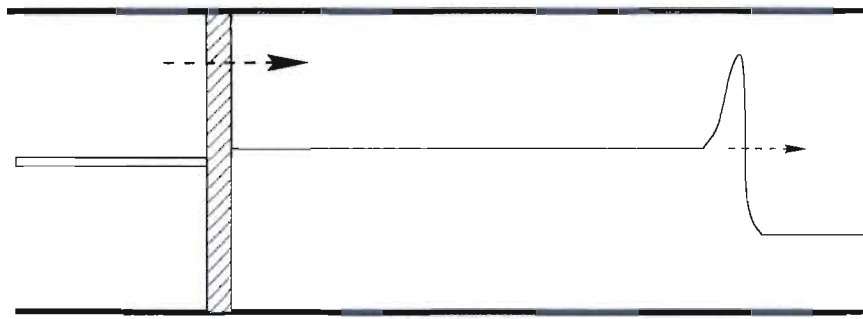
Let us examine this one-step kinetic model with:

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

Numerical Method

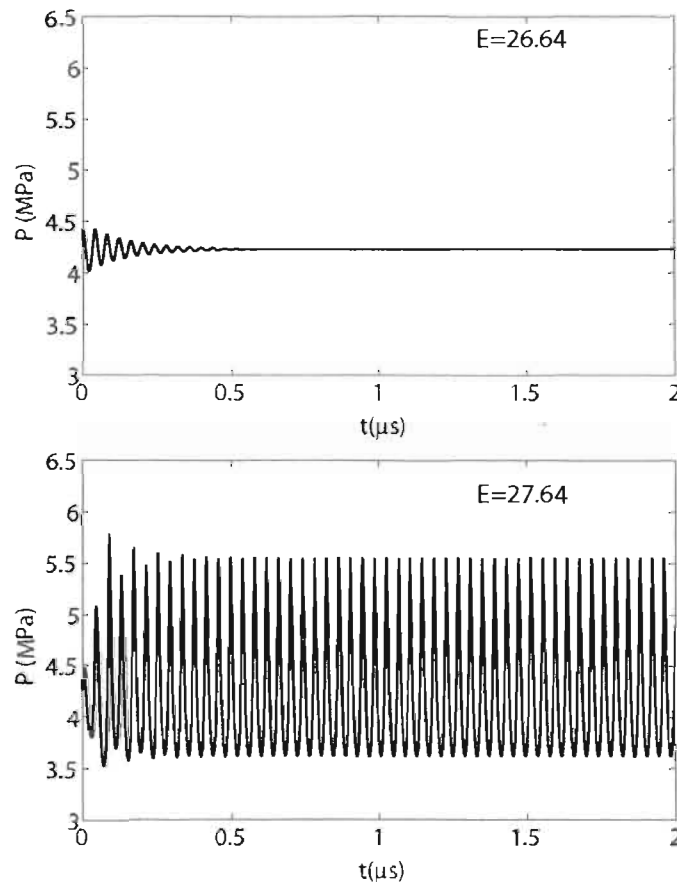
- Finite difference, uniform grid
($\Delta x = 2.50 \times 10^{-8} m$, $N = 8001$, $L = 0.2 \text{ mm}$) .
- Computation time = 192 hours for $10 \mu s$ on an AMD 2.4 GHz with 512 kB cache.
- A point-wise method of lines approach was used.
- Advective terms were calculated using a combination of fifth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



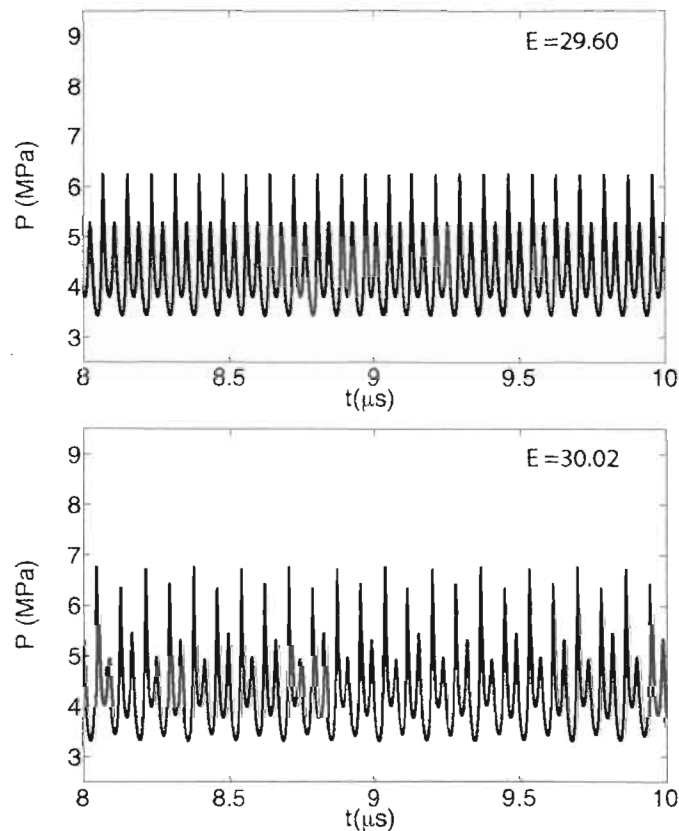
- Initialized with inviscid ZND solution.
- Moving frame travels at the CJ velocity.
- Integrated in time for long time behavior.

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 $E = 26.66$ 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.
- 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 $E_1 \approx 29.32$.

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 $E_{\infty} \approx 30.0327$.
- 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

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

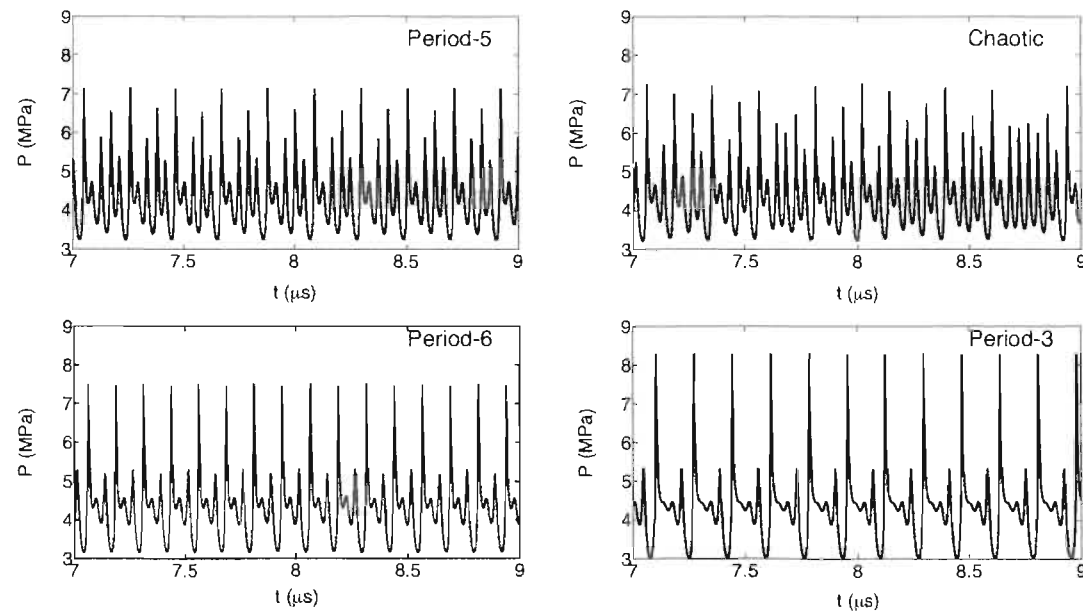
Feigenbaum predicted $\delta_{\infty} \approx 4.669201$.

	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	-	-	-

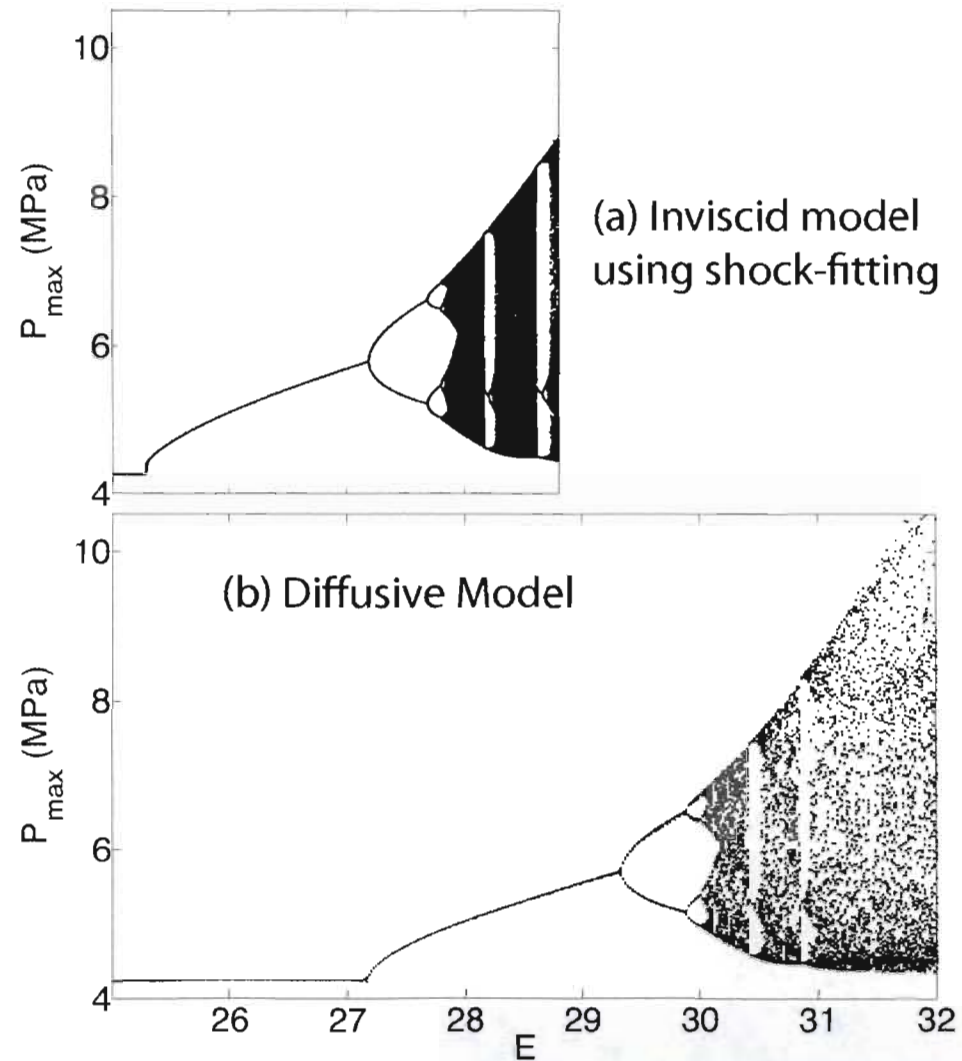
Chaos and Order

- 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:

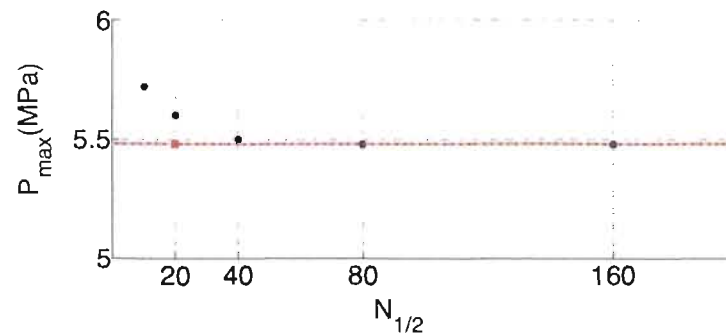


Bifurcation Diagram

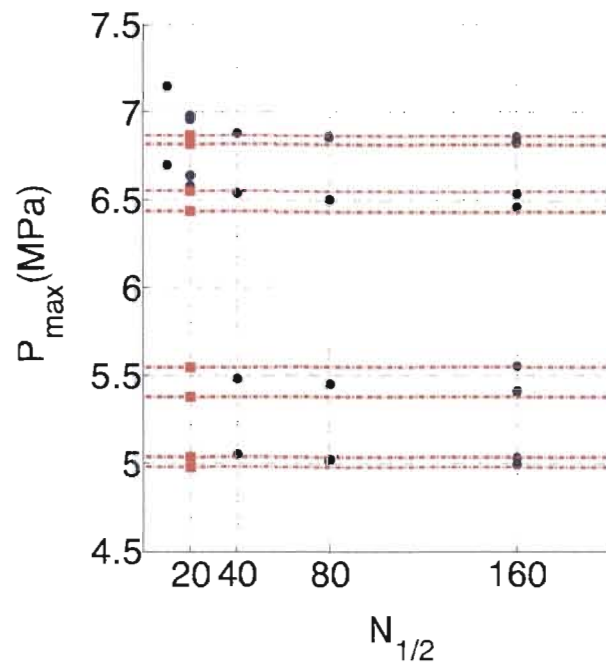


WENO5M Shock-Capturing (Inviscid)

- 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 ($P_{max} = 5.48 \text{ MPa}$).
- 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%

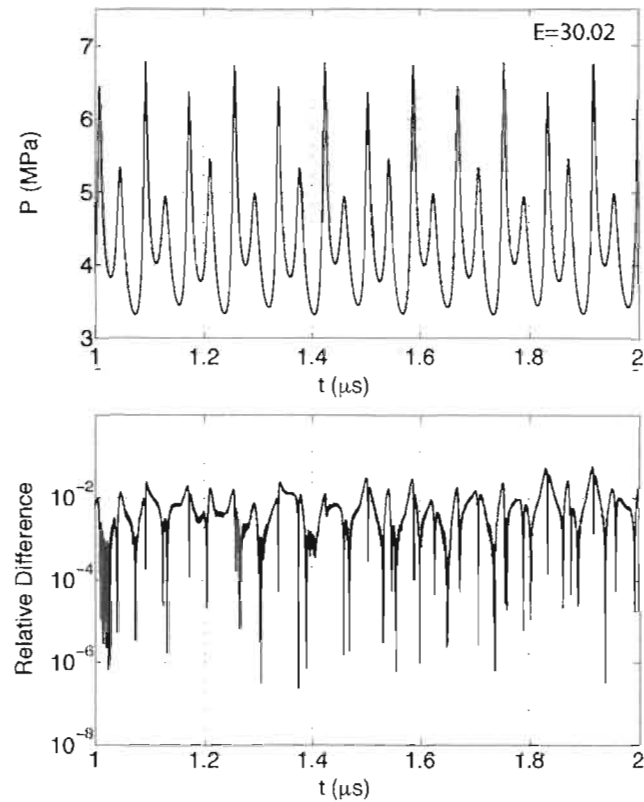


WENO5M Shock-Capturing (Inviscid)



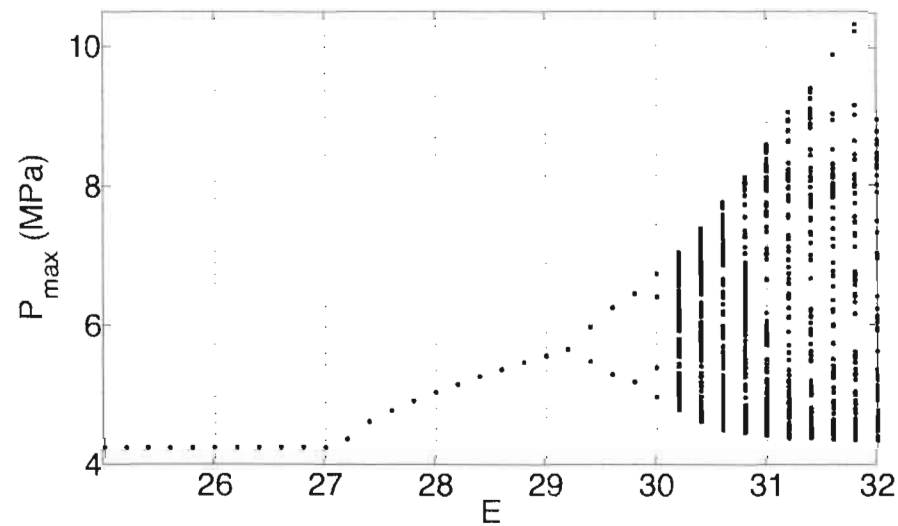
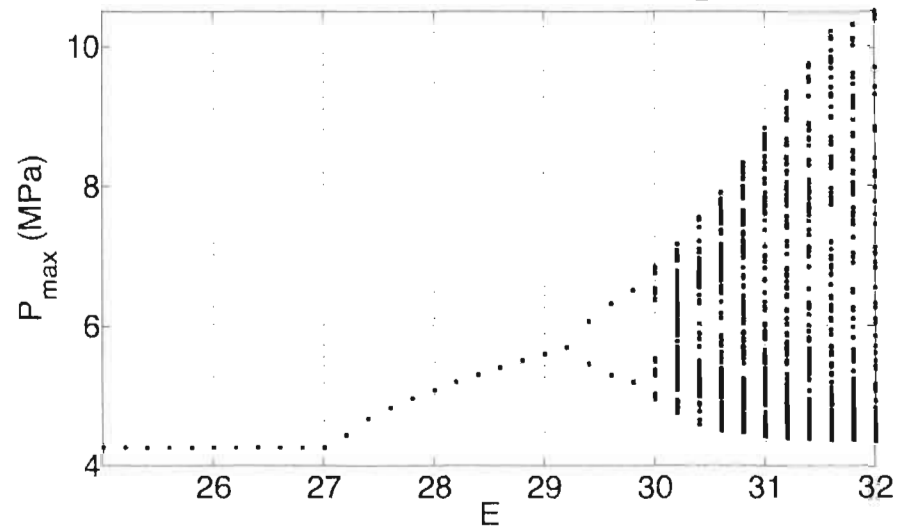
- At a higher activation energy, ($E = 27.82$), shock-fitting predicts a period-8 detonation, whereas shock-capturing using $N_{1/2} = 40$ predicts a period-4 detonation. To reconcile this difference, the resolution of the shock-capturing technique must be increased to $N_{1/2} \approx 160$.
- Numerical 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.

WENO5M & Central Differencing (Viscous)

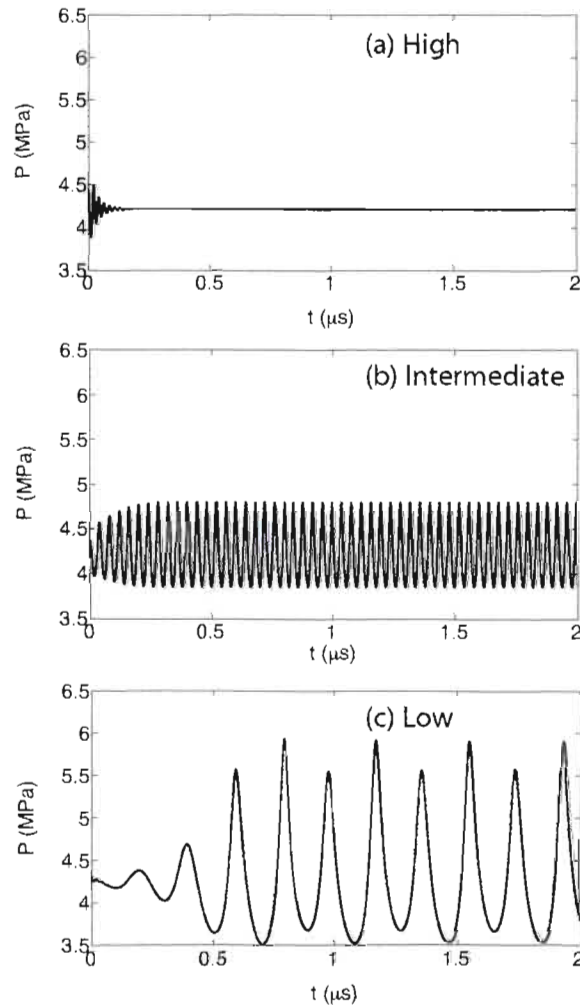


- Even when a complex behavior is predicted by the WENO scheme (period-8 detonation), the central difference predicts the same behavior.
- The values of the detonation pressure match minus a time-shift which originates at the initialization.

WENO5M & Central Differencing (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.

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

- When physical diffusion is captured with an appropriately fine grid a central difference of advective terms works as well as a WENO method in capturing the detonation dynamics.
 - 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.
-