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?
• 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.
- 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


- 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.

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

\[ P = \rho RT, \]

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

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

\[ \dot{j}_B^m = -\rho D \frac{\partial Y_B}{\partial x}, \]

\[ \tau = \frac{4}{3} \frac{\partial u}{\partial x}, \]

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

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 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 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 achieved 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 \( \delta_\infty \approx 4.669201 \).

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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 similarities 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:

Period-5

Period-6

Period-3

Period-3 Chaotic
Bifurcation Diagram

(a) Inviscid model with shock-fitting algorithm

(b) Diffusive model
Effect of Diminishing 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.