Verified Calculation of Nonlinear Dynamics of Viscous Detonation

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1 Introduction

It is a common notion in detonation theory that the effects of diffusion can be neglected in comparison to those of reaction and advection [1]- [8]. However, there are indications that such an assumption can be problematic. For example, using grid sizes around $10^{-6}\ m$ for their three-dimensional simulations of unsteady H_2-air detonations, Tsuboi *et al.* [8] report wave dynamics that show strong sensitivity to the fineness of the grid. While apparent convergence of some structures was reported, they also note with regard to some particulars of the detonation structure "The present results cannot resolve such cross-hatchings in the ribbon because of a lack of grid resolution." The presence of reaction dynamics and steep gradients at micron length scales suggest that physical diffusion has an important role to play. Indeed, Powers [9] showed that two-dimensional detonation patterns are strongly grid-dependent for simulations of reactive Euler equations, but relax to a grid-independent dissipative structure for a comparable reactive Navier-Stokes calculation. This suggests numerical diffusion is playing a significant role in the inviscid limit and that one should consider the introduction of physical diffusion to properly capture the dynamics.

Consideration of the reaction-advection length scales admitted by an inviscid detonation explains why such fine scales are necessary. Powers and Paolucci [10] performed a spatial eigenvalue analysis on a detailed kinetic H_2-air model and showed for inviscid detonations that the length scales for a steady Chapman-Jouguet (CJ) detonation can span five orders of magnitude near equilibrium, with the smallest length scale for an ambient mixture at atmospheric pressure being $10^{-7}\ m$ and the largest being $10^{-2}\ m$; away from equilibrium the breadth of scales can be even larger. These fine reaction scales are a manifestation of an averaged representation of the molecular collision model in which the fundamental length scale is the mean free path [11]. The choice of a one-step kinetic model induces a single reaction scale, in contrast to the multiple reaction scales of detailed kinetic models. This allows for the effects of the interplay between chemistry and transport phenomena on detonations be more easily studied. Such a model has been studied extensively; the stability and non-linear dynamics are well understood in the inviscid limit [12]- [18]. The goal of this paper is to predict the effects of diffusion on the long-time dynamics of a detonation described by simple one-step kinetics. The plan of the paper is as follows. First the mathematical model is discussed. This is followed by a description of the computational method and verification of the stated method. The model is used to predict the viscous analog of the period-doubling phenomena predicted in the inviscid limit [15, 17, 18]. The convergence of the period-doubling bifurcation points is shown to be in agreement with the general theory of Feigenbaum, [19, 20] and diffusion is seen to have a generally stabilizing effect on detonation dynamics.

2 Mathematical Model

The model equations adopted here are the one-dimensional unsteady compressible reactive Navier-Stokes equations with one-step kinetics:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left(\rho u\right) = 0, \tag{1}$$

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

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$$\frac{\partial}{\partial t}\left(\rho\left(e+\frac{u^2}{2}\right)\right)+\frac{\partial}{\partial x}\left(\rho u\left(e+\frac{u^2}{2}\right)+j^q+(P-\tau)\,u\right)=0, \tag{3}$$

$$\frac{\partial}{\partial t}\left(\rho\lambda\right)+\frac{\partial}{\partial x}\left(\rho u\lambda+j^m_\lambda\right)=\rho r, \tag{4}$$

where the independent variables are time, t, and the spatial coordinate, x. In Eqs. (1-4), ρ is the mass density, u the particle velocity, P the pressure, τ the diffusive viscous stress, e the specific internal energy, j^q the diffusive heat flux, λ the reaction progress variable, j^m_λ the diffusive mass flux, and r the reaction rate. The equations were transformed to a frame of reference moving at a constant velocity, D. The constitutive relations chosen for mass, momentum, and energy diffusion are

$$j^m_\lambda=-\rho\mathcal{D}\frac{\partial\lambda}{\partial x}, \tag{5}$$

$$\tau=\frac{4}{3}\mu\frac{\partial u}{\partial x}, \tag{6}$$

$$j^q=-k\frac{\partial T}{\partial x}+\rho\mathcal{D}q\frac{\partial\lambda}{\partial x}, \tag{7}$$

where $\mathcal{D}$ is the mass diffusion coefficient, μ the dynamic viscosity, k the thermal conductivity, T the temperature, and q the heat release. A calorically perfect ideal gas model is adopted. The reaction rate r is given by:

$$r=H(P-P_s)a\,(1-\lambda)\,e^{-\frac{\tilde{E}}{P/\rho}}. \tag{8}$$

Here a is the reaction rate, $\tilde{E}$ the activation energy, and $H(P-P_s)$ is a Heaviside function which suppresses reaction when $P<P_s$, where P_s is a selected pressure. The ambient pressure and density are taken to be P_o and ρ_o, respectively.

3 Computational Method and Verification

A temporally explicit point-wise method of lines approach is used, which allows separate temporal and spatial discretizations. It also allows for the easy inclusion of source terms. The advective terms were calculated using a combination of a fifth order WENO scheme and Lax-Friedrichs discretization [21]; the diffusive terms are treated with sixth order central differences. Temporal integration is done using a third order Runge-Kutta scheme.

The exercise of demonstrating the harmony of the discrete solution with the foundational mathematics is known as verification [22]. The method of manufactured solutions [23] was used to verify the code. In this method, a solution form is assumed, and special source terms are added to the governing equations in such a fashion that the assumed solution satisfies the modified equations. A periodic form for the solution was assumed

$$\rho\,(x,t)=a_1+b_1\cos\left[\pi(x-t)\right], \tag{9}$$

$$u\,(x,t)=a_2+b_2\cos\left[\pi(x-t)\right], \tag{10}$$

$$p\,(x,t)=a_3+b_3\cos\left[\pi(x+t)\right], \tag{11}$$

$$\lambda\,(x,t)=a_4+b_4\cos\left[\pi(x+t)\right], \tag{12}$$

with a domain $x\in[-1,1]$. The coefficients are taken to be $a_1=a_2=a_3=a_4=1$ and $b_2=b_3=b_4=1/10, b_4=1$. The initial conditions are those given by Eqs. (9-12) at $t=0$. Figure 1 shows fifth order asymptotic convergence of the error of the discrete approximation as the spatial grid is refined. The ordinate is the sum of all variables' L_1 errors normalized by the maximum value of the variable. It is noted that for convergence of the reactive Navier-Stokes equations, the presence of the Heaviside step function in the reaction rate term may preclude a full fifth order convergence rate.

4 Results

Next simulations of the reactive Navier-Stokes equations are presented. All calculations were performed in a single processor environment on an AMD 2.4 GHz processor with 512 kB cache. The simulation is initialized with

the inviscid Zel'dovich-von Neumann-Döring (ZND) solution in a moving frame traveling at the CJ speed. Each simulation is integrated in time to determine the long time behavior. For a calculation of $2.5\ \mu s$ the computational time required was two days. Some calculations took as long as nine days for full relaxation. By selecting the diffusion coefficient, $\mathcal{D} = 10^{-4}\ m^2/s$, thermal conductivity, $k = 10^{-1}\ W/m/K$, and viscosity, $\mu = 10^{-4}\ Ns/m^2$ the Lewis, Le, Prandtl, Pr, and Schmidt, Sc numbers evaluated at the ambient density, $\rho_o = 1\ kg/m^3$, are unity. In the inviscid detonation, the activation energy controls the stability of the system; the rate constant merely introduces a length/time scale into the system, the half reaction length, $L_{1/2}$, (the distance between the inviscid shock and the location at which $\lambda = 1/2$). If $L_{1/2}$ is fixed, the effect of diffusion on the system can be studied. With these parameters, all of the diffusion length scales are the same and is denoted by $L_\mu = 10^{-7}\ m$. The parameters in the governing equations are $P_o = 101325\ Pa$, $P_s = 200000\ Pa$, $\rho_o = 1\ kg/m^3$, $q = 5066250\ m^2/s^2$, $\gamma = 6/5$, and $\tilde{E} \in [2533125, 3232400]\ m^2/s^2$. To compare directly with previous work in the inviscid limit, the activation energies will be presented in dimensionless form, $E = \tilde{E}/\left(1.01325 \times 10^5\ m^2/s^2\right)$, thus $E \in [25, 32]$. Unless otherwise stated, the calculations presented are for a ratio of $L_\mu/L_{1/2} = 1/10$.

4.1 Effect of diffusion on the bifurcation behavior

In the inviscid case, linear stability analysis by [13] revealed that for $E < 25.26$, the steady ZND wave is linearly stable and is otherwise linearly unstable. This stability boundary is labeled as E_0. The stability limit was numerically found for the inviscid case, by [18], at $E_0 = 25.265 \pm 0.005$, which is in excellent agreement with the prediction of linear stability analysis. For a case above the inviscid stability limit, $E = 26.647$, the viscous ZND detonation predicted by steady theory is stable. A period-1 limit cycle is realized above $E_0 \approx 27.1404$, for the viscous case.

A period-doubling behavior and transition to chaos for unstable detonations are found to be remarkably similar to that predicted by the simple logistic map [24, 25]. The activation energy at which the behavior switches from a period-2^{n-1} to a period-2^n solution is denoted as E_n, for $n \geq 1$. As predicted by [15, 17, 18] transition to a period-2 oscillation occurs at $E_1 \approx 27.2$ in the inviscid case. For the viscous case, this initial period-doubling effect is delayed to $E_1 \approx 29.3116$. Bifurcation points for the inviscid and viscous models are listed in Table 1 along with approximations for Feigenbaum's constant, δ_∞ :

$$\delta_\infty = \lim_{n\to\infty} \delta_n = \lim_{n\to\infty} \frac{E_n - E_{n-1}}{E_{n+1} - E_n}. \tag{13}$$

Table 1: Numerically determined bifurcation points for inviscid and viscous detonation, and approximations to Feigenbaum's constant

	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	-

A bifurcation diagram was constructed by sampling over 300 points with $E \in [25, 32]$. The late time behavior of relative maxima in P versus activation energy is shown in Fig. 2(b). It shows period-doubling bifurcations up to roughly $E_\infty \approx 30.0411$. It is likely that in the dense portions of the bifurcation diagram that the system is in the chaotic regime. As in the inviscid limit, within this chaotic regime there exist pockets of order, with periods of 5, 3, and 6. In the diffusive case there is no true discontinuity, thus the shock speed cannot be predicted as in the inviscid limit, shown in Fig. 2(a).

4.2 Effect of diminishing diffusion

By increasing the reaction length scale, $L_{1/2}$, the relative effect of diffusion decreases. Figure 3 shows solutions for $E = 27.6339$, for the ratios $L_\mu/L_{1/2}$ of (a) $1/5$, (b) $1/10$, and (c) $1/50$. The system undergoes transition from

a stable detonation to a period-1 limit cycle, to a period-2 limit cycle. The amplitude of the pulsations increase with (a) relaxing to a $P \approx 4.213\ MPa$, (b) having a relative maximum of $P_{max} \approx 4.799\ MPa$ and (c) having relative maxima of $P_{max} \approx 5.578\ MPa$ and $P_{max} \approx 5.895\ MPa$. The pulsation frequency also decrease with decreasing diffusion. In the $L_\mu/L_{1/2} = 1/50$ case the period-2 behavior of the inviscid case has been recovered.

5 Conclusions

Investigation of the one-step kinetic model of one-dimensional unsteady detonation with mass, momentum, and energy diffusion has shown that the dynamics are significantly influenced in the region of instability or near instability relative to its inviscid counterpart. As in the inviscid limit, bifurcation and transition to chaos is predicted and shows 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. As physical diffusion is reduced, the behavior of the system trends towards the inviscid limit. If the dynamics of unstable and marginally stable denotations are to be captured, physical diffusion needs to be included and needs to dominate numerical diffusion. It is likely that these results will extend to detailed kinetic systems and that detonation cell pattern formation will be influenced by the magnitude of the physical diffusion [9].

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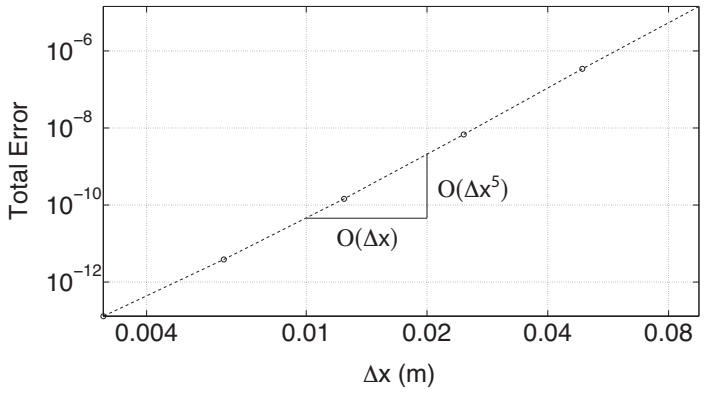

Figure 1: The normalized L_1 error versus Δx for a manufactured solution.

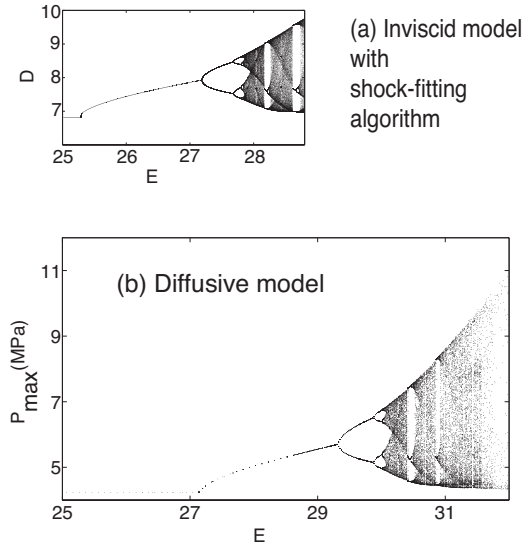

Figure 2: Comparison of numerically generated bifurcation diagrams: (a) inviscid detonation from Henrick *et al.*, (b) viscous detonation with $L_\mu/L_{1/2} = 1/10$.

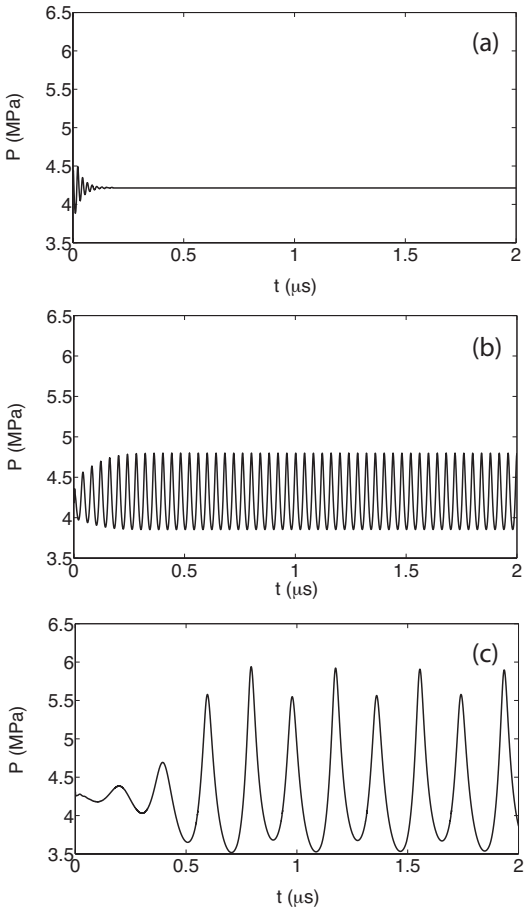

Figure 3: P versus t for viscous detonation with $E = 27.6339$ and (a) $L_\mu/L_{1/2} = 1/5$, stable, (b) $L_\mu/L_{1/2} = 1/10$, period-1, (c) $L_\mu/L_{1/2} = 1/50$, period-2.