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THE DYNAMICS OF UNSTEADY DETONATION WITH DIFFUSION [*]

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Here we consider an unsteady detonation with diffusion included. This introduces an interaction between the reaction length scales and diffusion length scales. Detailed kinetics introduce multiple length scales as shown though the spatial eigenvalue analysis of hydrogen-oxygen system[1]; the smallest length scale is $\sim 10^{-7}\ m$ and the largest $\sim 10^{-2}\ m$; away from equilibrium, the breadth can be larger. In this paper, we consider a simpler set of model equations, similar to the inviscid reactive compressible fluid equations, but include diffusion (in the form of thermal/energy, momentum, and mass diffusion). We will seek to reveal how the complex dynamics already discovered in one-step systems[2] in the inviscid limit changes with the addition of diffusion.

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The governing equations are:

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

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

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

$$\frac{\partial}{\partial t}(\rho Y_B) + \frac{\partial}{\partial x}(\rho u Y_B + j_B^m) = \rho r, \tag{4}$$

where the constitutive and rate laws and the transport definitions are given by:

$$p = \rho R T, \tag{5}$$

$$e = c_v T - q Y_B = \frac{p}{\rho(\gamma - 1)} - q Y_B, \tag{6}$$

$$r = H(p - p_s) a (1 - Y_B)\, e^{-\frac{E}{p/\rho}}, \tag{7}$$

$$j_B^m = -\rho \mathcal{D} \frac{\partial Y_B}{\partial x}, \tag{8}$$

$$\tau = \frac{4}{3}\mu \frac{\partial u}{\partial x}, \tag{9}$$

$$j^q = -k \frac{\partial T}{\partial x} + \rho \mathcal{D} q \frac{\partial Y_B}{\partial x}. \tag{10}$$

Constant specific heats, c_v and c_p, thermal conductivity, k, viscosity, μ, and mass diffusion coefficient, $\mathcal{D}$, were chosen to simplify the problem still futher. Selecting the diffusion coefficient, $\mathcal{D} = 10^{-4}\ m^2/s$, thermal conductivity, $k = 10^{-1}\ W/m/K$, and viscosity, $\mu = 10^{-4}\ Ns/m^2$, yield the Lewis, Le, Prandtl, Pr, and Schmidt, Sc, numbers evaluated at the ambient density, $\rho_o = 1\ kg/m^3$, to be unity. These parameters are within an order of magnitude of those of gases at a slightly elevated temperature. Simple dimensional analysis of the diffusion and advection parameters ($U = 1000\ m/s$ was chosen as a typical velocity scale) gives rise to an approximate length scale of mass diffusion, $\mathcal{D}/U = 10^{-7}\ m$, and likewise for momentum and energy diffusion $\mu/\rho_o/U = 10^{-7}\ m$, and $k/\rho_o/c_p/U = 10^{-7}\ m$.

In the inviscid detonation, the rate constant, a, does not affect the stability properties, it merely introduces a length/time scale into the system. The activation energy, E, controls the stability of the system. To study the effect of diffusion on the system, the rate constant, a, must be fixed, since there is an interaction between the length scales of diffusion and those of the chemistry. A range for the reaction half length, $L_{1/2}$, (i.e. the distance between the inviscid shock and the location of $Y_B = 1/2$) of 100 nm to 100 μm yields a rate constant within the bounds of $1.14452336 \times 10^8\ 1/s \leq a \leq 1.14452336 \times 10^{11}\ 1/s$. This overlaps the range in which nearly-inviscid behavior would be expected as the reaction length scale is three orders of magnitude larger than that of the diffusion for $a = 1.14452336 \times 10^8\ 1/s$. For a rate constant of $a = 1.14452336 \times 10^{11}\ 1/s$ the scales of diffusion and reaction are comparable. To make direct comparisons with the results of Henrick *et. al.*[2], the ratio of specific heats was chosen to be $\gamma = 6/5$. In that work, the problem examined was dimensionless. For this work these parameters are chosen with SI units: $p_o = 101325\ Pa$, $\rho_o = 1\ kg/m^3$, $q = 5066250\ m^2/s^2$, and $2533125\ m^2/s^2 \leq E \leq 2918160\ m^2/s^2$. With this heat release, D_{CJ} for the inviscid problem is,

$$D_{CJ} = \sqrt{\gamma \frac{p_o}{\rho_o} + \frac{q\left(\gamma^2 - 1\right)}{2}} + \sqrt{\frac{q\left(\gamma^2 - 1\right)}{2}} \approx 2167.56\ m/s. \tag{11}$$

Calculations were done at the inviscid CJ condition using a stable activation energy and a rate constant of $a = 1.14452336 \times 10^{10}\ 1/s$; this gives an one order of magnitude diffference between the length scales of reaction and diffusion. The inviscid ZND solution is used to initialize the calculation. The diffusion reduces the magnitude of the density as the wave propogates, see Figure 1. The diffusion also smoothes the structure of the wave, though there is still a strong peak as seen in Figure 2. However, the maximum magnitude of the pressure remains nearly the same as the inviscid case, see Figure 3. When unstable activation energies are chosen we expect results similar to those in Figure 4, as taken from Henrick *et. al.*[2]. In the figure, a dimensionless activation energy was chosen of $E = 26$, while the dimensionless heat release was chosen $q = 50$. The dimensionless rate constant was, $a \approx 36$, thus the non-dimensional time of $t = 300$ in dimensional terms is 1 μs; the dimensionless speed, $D_{CJ} \approx 6.805$ is equivalent to $D_{CJ} = 2167.56\ m/s$. The unsteady dynamics of an one-dimensional detonation including diffusion are calculated using a combination of fifth order WENO with Lax-Friedrichs for the hyperbolic terms, high order central differences for diffusive terms and a third order Runge-Kutta scheme for temporal integration.

In the full paper, it is anticipated that diffusion will delay the onset of instability of the system when the length scales of the chemistry and diffusion overlap. Further the nonlinear nature of the model system, including the possibilities of limit cycles and bifurcations, will be explored. Also a detailed kinetic model of ozone will be studied using the wavelet adaptive multilevel representation (WAMR)[5], which can be compared with the work of Aslam and Powers[3,4]. With the detailed kinetic model the rate constant, a, and the activation energy, E are intrinsic, thus the bifurication parameter is the overdrive of the denotation.

References

[1] Powers, J. M., and Paolucci, S., "Accurate Spatial Resolution Estimates for Reactive Supersonic Flow with Detailed Chemistry," *AIAA Journal*, Vol. 43, No. 5, 2005, pp. 1088-1099.

[2] Henrick, A. K., Aslam, T. D., and Powers, J. M., "Simulations of Pulsating One-Dimensional Detonations with True Fifth Order Accuracy," *Journal of Computational Physics*, Vol. 213, No. 1, 2006, pp. 311-329.

[3] Aslam, T. D., and Powers, J. M., "Shock-Fitted Calculation of Unsteady Detonation in Ozone," AIAA Paper 2008-1036, 2008.

[4] Aslam, T. D., and Powers, J. M., "The Dynamics of Unsteady Detonation in Ozone," AIAA Paper 2009-0632, 2009.

[5] Singh, S., Rastigejev, Y., Paolucci, S., and Powers, J. M., "Viscous Detonation in $H_2 - O_2 - Ar$ Using Intrinsic Low-Dimensional Manifolds and Wavelet Adaptive Multilevel Representation," *Combustion Theory and Modelling*, Vol. 5, No. 2, 2001, pp. 163-184.

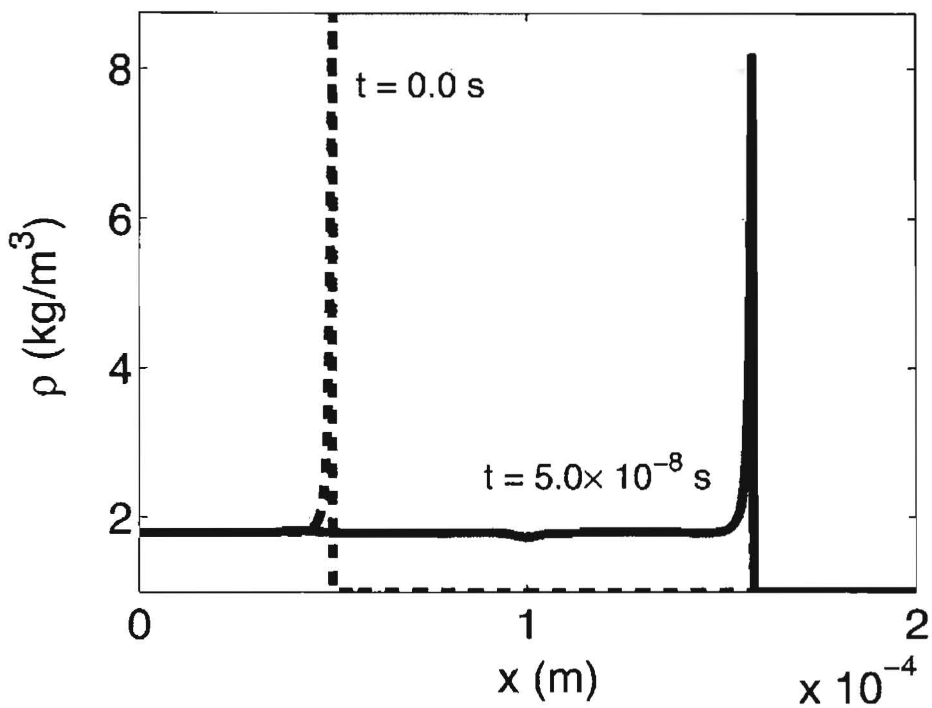

Figure 1: Profile of density vs. distance for a stable detonation.

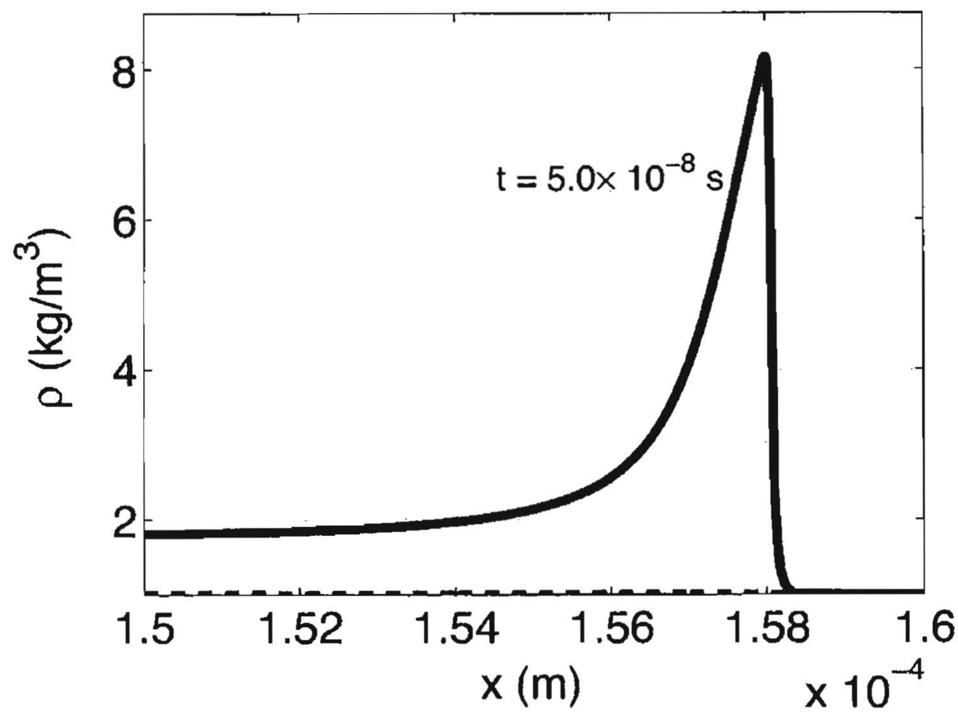

Figure 2: Maginified view of density near peak magnitude.

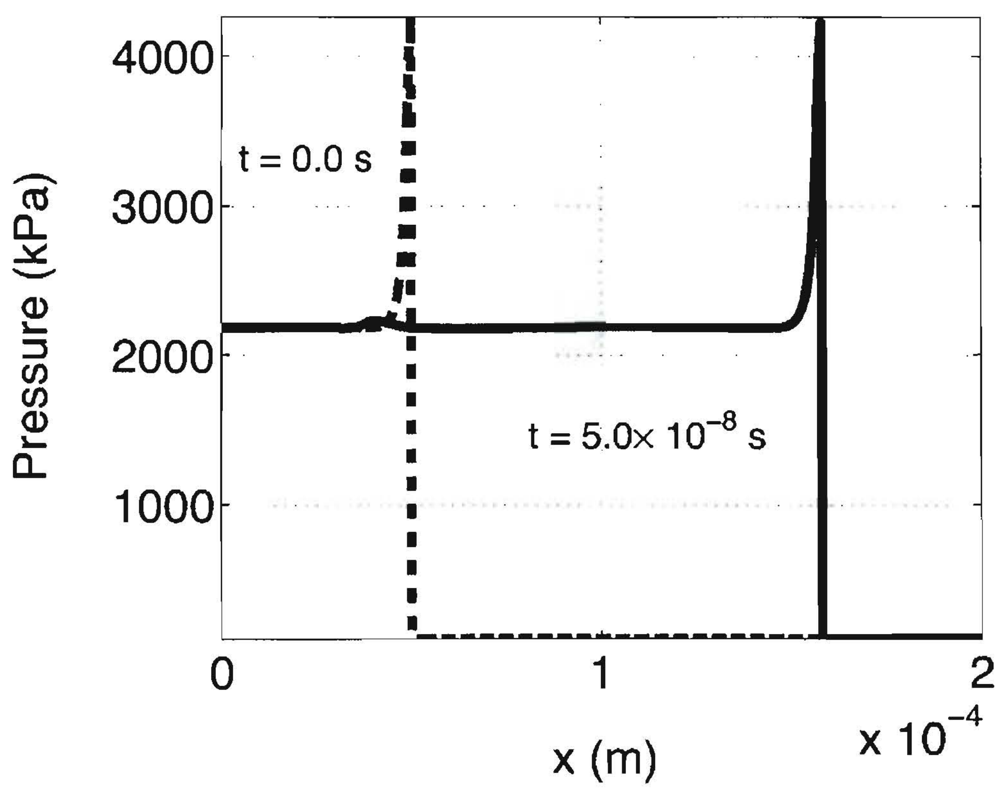

Figure 3: Profile of pressure vs. distance for a stable detonation.

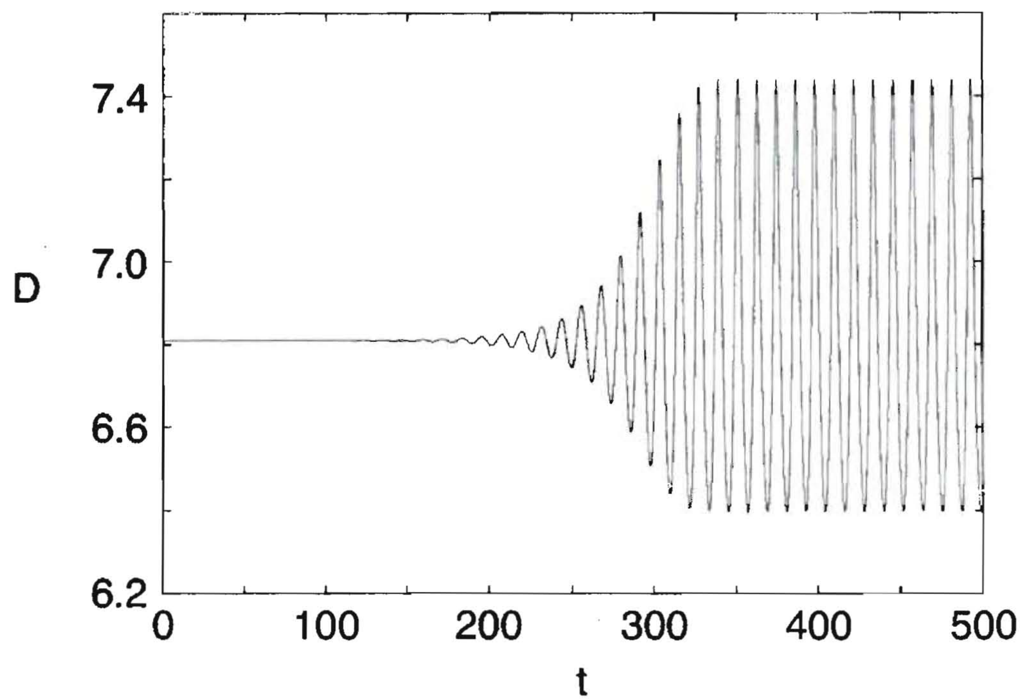

Figure 4: From reference 2: Numerically generated detonation velocity, D vs. t, for $E = 26$, $q = 50$, and $\gamma = 1.2$.