Multidimensional Detonation Solutions from Reactive Navier-Stokes Equations

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This study will describe multi-dimensional detonation wave solutions of the compressible reactive Navier-Stokes equations. As discussed in detail by Fickett and Davis [1], a steady one-dimensional detonation with a spatially resolved reaction zone structure is known as a ZND wave, named after Zeldovich, von Neumann, and Döring. In experiments [2] and calculations with simplified models [3], [4], [5], [6], it has been observed and predicted that these ZND waves are unstable. In the experiments, detonation in a tube with walls coated with a thin layer of soot etches detailed regular patterns on the tube walls, indicating the existence of cellular detonation wave structure. For inviscid cases, a normal mode linear stability analysis, in one dimension by Lee and Stewart [3] and in two dimensions by Short and Stewart [4], demonstrates the fundamental instability of the one-dimensional ZND structure to longitudinal and transverse disturbances. Both theoretical and numerical structure of one and two-dimensional detonations has been investigated by Bourlioux, et al. [7], [8]. Grismer and Powers [9] have shown numerically that detonations which are guaranteed stable in one dimension can be unstable when the geometry is relaxed to include two-dimensional effects. Most calculations are done with compressible reactive Euler equations, and two-dimensional cell size is often predicted to be dependent on grid resolution, which indicates numerical viscosity is playing a determining role in predicting the physics. To remedy this, we reintroduce in this study the usually-neglected physical mechanisms of mass, momentum, and energy diffusion to the conservation equations. It can be shown, as done by Lindström [10], that at low grid resolutions the solutions of both reactive Euler equations and reactive Navier-Stokes equations are similar, because the numerical diffusion dominates over physical diffusion. However, as we increase the grid resolution, the numerical diffusion decreases, and physical diffusion becomes important for the accurate solution of reactive Navier-Stokes equations. Hence, neglecting physical diffusion at high grid resolution gives rise to non-physical structures in the solutions.

When solving reactive Navier-Stokes equations, physical diffusion gives rise to smooth solutions, and there is no need to take extraordinary measures, such as embodied in Roe and Flux Corrected Transport (FCT) schemes, in performing spatial discretization. Instead, we use a simple finite difference scheme with second order central differences to model spatial gradients. Use of the central difference approximation for convective terms in the reactive Navier-Stokes equations causes oscillations to develop at the detonation front if the grid resolution is too coarse. However, the grid resolution can be made fine enough so that these oscillations disappear. Increasing the grid resolution makes the computations very expensive. Here, we exploit the simplicity of the spatial discretization to develop an efficient method to advance the solution in time. We use an implicit method based on the Beam-Warming algorithm. This algorithm uses an Alternating Direction Implicit (ADI) technique based on a linearized trapezoidal time stepping method which is second order accurate in time. The implicit time stepping technique allows use of much larger time steps relative to typical explicit schemes, which have limitations due to convection, diffusion and reaction time scales. Use of larger time steps comes at the expense of a matrix inversion, necessary at every time step. For general systems, this can be prohibitively expensive; however, for reactive Navier-Stokes equations with central difference approximation for spatial gradients and use of the ADI technique, we only need to invert block tridiagonal matrices composed of small blocks. It is much less expensive to invert these block tridiagonal systems than general systems. Overall we save computational time by using this method without any loss of accuracy.

As described in Ref. [11] model equations are as follows, employing essentially the same non-dimensionalization as that of Ref. [8], with extensions made to account for the diffusion coefficients:

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

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u} + P - \boldsymbol{\tau}) = 0, \tag{2}$$

$$\frac{\partial}{\partial t}\left(\rho\left(e + \frac{1}{2}\mathbf{u}\cdot\mathbf{u}\right)\right) + \nabla \cdot \left(\rho \mathbf{u}\left(e + \frac{1}{2}\mathbf{u}\cdot\mathbf{u}\right) + P\mathbf{u} - \boldsymbol{\tau}\cdot\mathbf{u} + \mathbf{q}\right) = 0, \tag{3}$$

$$\frac{\partial}{\partial t}(\rho\lambda) + \nabla \cdot (\rho \mathbf{u}\lambda + \mathbf{j}) = \omega, \tag{4}$$

$$\omega = K\rho(1-\lambda)\exp(-E/T), \tag{5}$$

$$e = \frac{1}{\gamma - 1}\frac{P}{\rho} - \lambda q_\circ, \tag{6}$$

$$P = \rho T, \tag{7}$$

$$\boldsymbol{\tau} = \mu\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T - \frac{2}{3}(\nabla\cdot\mathbf{u})\mathbf{I}\right), \tag{8}$$

$$\mathbf{q} = -k\nabla T, \tag{9}$$

$$\mathbf{j} = -\mathcal{D}\nabla\rho\lambda. \tag{10}$$

The dependent variables in Eqs. (1-10), ρ, $\mathbf{u}$, P, T, $\boldsymbol{\tau}$, e, $\mathbf{q}$, λ, $\mathbf{j}$, and ω, are the density, velocity vector, pressure, temperature, viscous stress tensor, internal energy per unit mass, heat flux vector, reaction progress variable, mass diffusion flux vector, and reaction source term, respectively. Parameters in Eqs. (5-10), K, E, q_o, γ, μ, k, $\mathcal{D}$, are dimensionless reaction kinetics constant, activation energy, chemical heat release, ratio of specific heats, and coefficients for viscosity, heat conduction and species diffusion, respectively.

Equations (1-3) express conservation principles for mass, momenta, and energy, respectively. Equation (4) is an evolution equation for species mass fraction. A single, first-order, irreversible, exothermic reaction is employed, $A \rightarrow B$. The reaction progress variable λ ranges from zero before reaction to unity at complete reaction. Species mass fractions, Y_i are related to the reaction progress variable by the formulæ, $Y_A = 1 - \lambda$, $Y_B = \lambda$. Equation (5) defines the reaction source term of Eq. (4) according to the Arrhenius depletion model. Equations (6-7) are caloric and thermal equations of state, respectively. Equation (8) defines the viscous stress as a linear function of the strain rate for an isotropic material which obeys Stokes' assumption. Equations (9-10) express the heat flux and mass diffusion flux by Fourier's and Fick's Laws, respectively. Heat flux due to concentration gradients is neglected along with Dufour and Soret effects and μ, k and $\mathcal{D}$ are assumed to be constant.

In our numerical study, we consider a two-dimensional detonation wave propagating in an infinite width rectangular channel. The initial state is taken to be the steady solution of the one-dimensional reactive Euler equations. The initial one-dimensional profile is spatially perturbed in the transverse direction. The perturbation is sinusoidal with a wavelength equal to that predicted by Short and Stewart [4] for a case in which only one unstable mode was found in their linear stability analysis. Since periodic perturbations are used, periodic boundary conditions are imposed in the direction transverse to the direction of wave propagation. So as to minimize the size of the computational domain, we study detonation wave solutions in a frame which is stationary with respect to the steady wave speed predicted by steady inviscid analysis. The boundary conditions imposed at left and right side of the computational domain are fixed and are the same as the left and right states of the initial inviscid ZND wave.

Shown in Figs. 1 and 2 are the detonation wave solutions for the reactive Euler equations and reactive Navier-Stokes equations. Parameter values utilized are $K = 3000$, $E = q_\circ = 50$, $\gamma = 1.2$, $\mu = 0.01$, $k = 0.06$, and $\mathcal{D} = 0.01$. It is found that the results are similar at a coarse grid resolution for both reactive Euler equations and reactive Navier-Stokes equations (Figs. 1a and 2a). For higher grid resolutions we predict that the solutions of reactive Euler equations and reactive Navier-Stokes equations are very different (Figs. 1b-1c and 2b-2c). The reactive Navier-Stokes equations have multiple physical length scales associated with them: a relatively large length scale (approximate dimensional

value 11 μm) associated with the reaction zone and a relatively small diffusion length scale which is of the order of 2 μm. We note that while the diffusion length is similar to that found in experiments, the reaction zone length has been made artificially short in order to make the two lengths comparable. For a coarse grid size, the diffusion length scale is completely unresolved and the numerical diffusion dominates over the physical diffusion making the reactive Euler and reactive Navier-Stokes solutions appear similar. But for finer grid sizes as the diffusion length scales are resolved, the reactive Euler and reactive Navier-Stokes solutions begin to differ. Hence as we go to higher resolutions, both the diffusion and reaction length scales are resolved simultaneously, and the solution of the reactive Navier-Stokes equations converge. The reactive Navier-Stokes equations were solved using the Beam-Warming algorithm which is computationally faster due to the relaxed stability restrictions.

Our numerical study of reactive Navier-Stokes equations has shown the importance of the physical diffusion terms for accurately resolving fine scale structures. At fine grid resolutions, when the numerical diffusion becomes negligible, we predict non-physical structures appearing in the solution of reactive Euler equations. Hence it became necessary to solve the full reactive Navier-Stokes equations for complete detonation wave solutions. We have also shown that the grid size should be small enough to resolve both length scales associated with chemistry and physical diffusion. Due to the requirement of small grid sizes, we used simple central differences to approximate spatial gradients as the oscillations are minimal for very high resolutions. Finally an efficient Alternating Direction Implicit scheme of Beam-Warming was used to advance in time. This reduced the computational time by up to five times, relative to Roe's method conventionally used for detonation solutions, while preserving accuracy. Subsequently, such elaborate and computationally expensive upwind schemes are not necessary.

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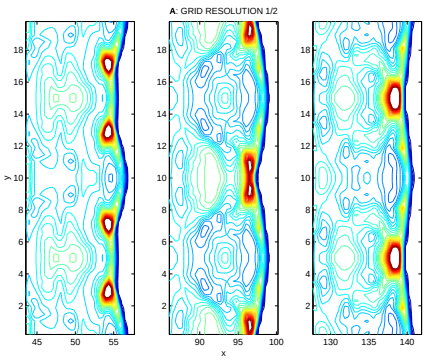

Figure 1: Isochoric lines for the solutions of reactive Euler equations at times $t = 40$, 80, and 120.

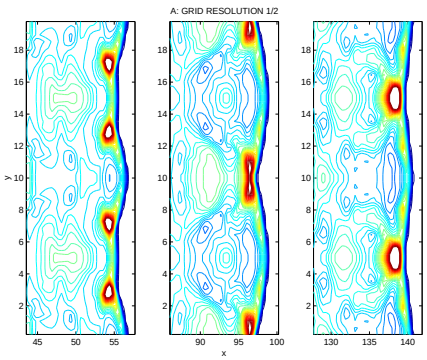

Figure 2: Isochoric lines for the solutions of reactive N-S equations at times $t = 40$, 80, and 120.