Nonlinear Dynamics of Gaseous Detonations With Losses

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1 Gaseous detonations with losses of momentum and heat

Momentum and heat losses incurred on gaseous detonation propagation due to channel walls, solid particles or other obstacles, which are often present in real systems, lead to a deficit of detonation velocity compared to its ideal value [3, 7]. In the simplest theory of one-dimensional detonation, the velocity deficit can be calculated within the framework of one-dimensional reactive Euler equations with momentum and heat-loss terms included in the equations of motion and energy. Such theory was developed originally by Zel'dovich [7] and was subsequently revisited by many researchers [1, 2, 5, 8, 9].

In the recent analysis of gaseous detonation propagating in the interstitial space of a packed bed of inert particles [5], it was found that the steady traveling wave solutions form a one-parameter family parameterized by pressure or temperature in the products when the wave velocity is below certain critical value. These solutions (termed "set-valued" in [5]) consist of the lead shock followed by an entirely subsonic flow. Understanding the stability of these solutions is of interest. The stability problem is not completely resolved also for detonations with small velocity deficits. Here we analyze these problems by means of the numerical solution of unsteady reactive Euler equations with bulk momentum and heat losses. Steady state solutions are taken as initial conditions, thus we investigate the stability of these steady-state solutions.

In conservation form, the mass, momentum, energy, and reaction equations can be written as

$$\rho_t + (\rho u)_x = 0, \tag{1}$$

$$(\rho u)_t + \left(p + \rho u^2\right)_x = -\frac{f}{\phi},\tag{2}$$

$$\left(\rho e\right)_t + \left(\rho u\left(e + p/\rho\right)\right)_x = -\frac{h}{\phi},\tag{3}$$

$$(\rho\lambda)_t + (\rho u\lambda)_x = \rho\omega,\tag{4}$$

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where ρ , u, p, λ , ω , and ϕ are the density, velocity, pressure, reaction-progress variable, reaction rate, and (constant) porosity of the medium, respectively. The total energy is given by $e = p/(\rho(\gamma - 1)) + u^2/2 - \lambda Q$ with the heat release denoted as Q. The reaction rate is taken in the standard Arrhenius form, $\omega = k(1 - \lambda) \exp(-E/RT)$, E is the activation energy. The momentum and heat loss terms are given by

$$f = c_f \rho |u| u, \quad h = c_h |u| (T - 1),$$
(5)

where the dimensionless loss coefficients c_f and c_h depend on various properties of the mixture and the matrix of the porous medium. The equations are taken dimensionless exactly as in [5] with units of pressure and density taken as their upstream values p_a and ρ_a , while that of velocity as $\sqrt{p_a/\rho_a}$. The length scale is the half-reaction length of the ideal detonation and time scale is that over the velocity scale.

2 Nonlinear stability of steady state solutions

To explore stability of the steady-state solutions with losses, we developed a numerical algorithm that combines high resolution spatial discretization, high order time integration, and shock fitting (the details can be found in [6]). In addition, the algorithm is made parallel in order to be able to compute extremely long relaxation zones that are present at very low velocities. An example of a typical $D - c_f$ dependence found following [5] is shown in Fig. 1. For this case, the ideal detonation is stable [4]. When the losses are included and the steady state solutions are taken moving down along the top branch of the $D - c_f$ dependence, these solutions become unstable and the onset of limit cycles of increasing complexity is observed. For the particular case of Fig. 1, the number of bifurcations that occur before the failure takes place appears to be finite. That is, as we move down the $D - c_f$ curve, a fews bifurcations occur, but the proximity to the turning point leads to detonation failure rather than further bifurcations. However, if we consider the case of E = 27, for which the ideal detonation is already unstable, we find that with the increase of c_f there exists a sequence of period doubling bifurcations leading to chaos before the failure occurs. The computed bifurcation diagram in the space of the maximum detonation velocity and c_f is shown in Fig. 2.

The instabilities that arise when the set-valued solutions are taken as initial conditions, are quite different in their nature from the ones that arise from the top branch. No oscillatory dynamics is observed early on. Instead, the detonation velocity begins to grow very slowly, with the fire moving toward the lead shock. The motion is very slow at early times, but the fire accelerates and produces a secondary detonation wave (or a strong compression wave) ahead in the reaction zone that eventually overtakes the lead shock. In Fig. 3, we show the evolution of detonation velocity for initial conditions at points d through h in Fig. 1. In all cases, there is a transition to the top branch, the key difference between the cases being the duration of the early transient, which is the largest for point h. After the transition, the detonation propagates in a pulsating manner with the average velocity around the steady-state value of the top branch.

Qualitatively, one could depict the transition process on the $D - c_f$ diagram as a point moving in the vertical direction at a given c_f . For example, if the initial condition corresponds to point h in Fig. 1, then the slow acceleration at early times corresponds to the point moving up through g, f, e in the set-valued region before transitioning to the top branch and eventually oscillating around point c. We attribute the slowness of the early transient to the passage through the sequence of steady-state solutions in the set-valued region, wherein the shock acceleration is extremely small. After the point exits the set-valued region, there is no longer a steady-state solution in the neighborhood, and the acceleration becomes large resulting in a rapid transition to the top branch.



Figure 1: $D - c_f$ dependence for detonation with Q = 50, E = 25, $\gamma = 1.2$, $c_h = 0.4c_f$. Points c - h correspond to $c_f = 0.012$.

This process is reminiscent of DDT, the fire being a deflagration wave in the frame of the lead shock. The fire accelerates in response to the favorable conditions that are created upstream due to the effects of compressibility and frictional heating. An example of the transition is shown in Fig. 4, where we plot the magnitude of the pressure gradient as a function of space and time.

When the $D - c_f$ dependence is a curve of the usual reverse-C shape, as is the case when heat losses are absent, the lower branch is unstable, but unlike the set-valued solutions, the branch has no neighborhood of steady solutions at a given c_f . Thus a small perturbation results in a rapid transition to the top branch (or failure). The existence of set-valued solutions on the other hand is a stabilizing factor for the low velocity solutions as then the solution that starts in the set-valued region is surrounded by other steady-state solutions. For this reason, the transition to the top branch is expected to be very slow as our simulations confirm.

It is of interest to understand how various factors such as the forms of the bulk losses and of the heat-release function, play a role in this stabilization mechanism. Multidimensionality is another factor that may play an important role in the observed dynamics. These and other related questions are being currently investigated and we hope to report on them in the near future.

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Figure 2: Bifurcation diagram for detonation with losses showing the maximum of D in the limit cycle as the friction coefficient is varied. The other parameters are Q = 50, E = 27, and $\gamma = 1.2$. D_{CJ} is the ideal velocity at these parameters.

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Figure 3: Time evolution of D for solutions starting at points d - h in Fig. 1.



Figure 4: Space-time depiction of the transition process from the set-valued to the high-velocity regime. The parameters are: $D/D_{CJ} = 0.3$ for the steady state, E = 25, Q = 50, $\gamma = 1.2$, $c_f = 0.012$, $c_h = 0.4c_f$. The computational domain of length L = 1000 with resolution of $N_{1/2} = 100$ points per half-reaction length was used.