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Computational study of non-ideal and mildly-unstable detonation waves

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ABSTRACT

This paper deals with some salient features of numerical detonation modeling, whose shock dynamics exhibits mildly oscillations behavior. The study is based on the integration of the hyperbolic equations with source terms, using a fifth-order Weighted Essentially Non-Oscillatory (WENO) scheme for the convective flux and a third-order Runge–Kutta scheme for time advancement. Strang's splitting technique is used for the integration of the source terms. The computations are performed for both stable and mildly unstable detonation waves. The study shows that the rate of convergence depends on the smoothness of the solution and that in presence of strong detonation waves, the accuracy is much lower than commonly believed. To improve the computation accuracy, a simple algorithm for shock detection is proposed along with a chemical activator for weak activation energies. A mesh refinement is also employed to achieve high resolution computations. It is found that a resolution of 66 points per half reaction zone is required to correctly capture the main structure of the detonation front and the associated flow instabilities. Examples are carried out to show that the proposed model yield accurate results. In particular, as the friction and the heat losses increase, the mean detonation velocity decreases and a series of period-doubling self sustained oscillations appears. It is also found that non-adiabatic conditions play a crucial role on the dynamics of the shock front, by enhancing the fluctuations. This aspect should be properly accounted for when dealing with multi-dimensional detonations.

1. Introduction

A detonation wave is a supersonic combustion where a leading shock is strongly coupled with a reaction zone, in which a chemical decomposition occurs until the fresh mixture is completely converted into products. The strong coupling between the shock and the reaction zone makes the detonation wave self-similar. The minimum self-sustained detonation velocity is the ideal Chapman–Jouguet (CJ) detonation speed. The inner structure of the detonation wave can be determined from the ZND (Zel'dovich, von Neumann, Döring) model, which relies on the steady one-dimensional Euler reactive formalism. For CJ detonations, the end of the reaction zone is characterized by the sonic condition in the reference frame attached to the shock [1,2].

In the past, several authors have studied the dynamics of ideal one-dimensional detonations using a single-step Arrhenius model [3–6] by numerical means. These studies indicated that the activation energy (E_a) is the main parameter which controls the onset of the longitudinal instability for constant heat of reaction and specific heat ratio. For activation energies below a critical threshold $E_{a,c}$, the linear stability analysis shows the existence of a stable steady detonation structure. Above $E_{a,c}$, oscillatory modes emerge [7,4] making the detonation weakly then mildly unstable up to becoming chaotic through the Feigenbaum double-period scenario.

Moreover, with scale reduction the propagation of detonations is affected by the confinement effect, in contrast to the ideal case [8,2, Chap. 7]. The detonation velocity is therefore lower than the theoretical value due to the presence of solid walls. Following the pioneering work of Zel'dovich [8] which considers the momentum loss as the main mechanism responsible for the velocity deficit, Zhang and Lee [9] and later Dionne et al. [10] showed that the onset of the instability is not only triggered by E_a but that drag forces are also important. Indeed, their numerical results indicated that the wall friction tends to enhance the natural detonation instabilities. They also pointed out that the stability limit is reduced in frictional detonations.

Furthermore, defining the sonic locus is a key issue in detonation. For steady state solutions, the generalized CJ criterion [2,11,12] can be used to determine the subsonic reaction zone. In unsteady detonations, Kasimov and Stewart [3] defined the sonic locus as a separatrix of the family of forward characteristics. Another important aspect in detonation problems is the dynamics of the leading shock which can be seen as a signature

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of different non-stationary events appearing in the subsonic reactive zone.

From a numerical view point, Romick et al. [13] have indicated that a shock-capturing method retrieves the main features of the detonation front dynamics with much finer resolution compared to the shock-fitting technique [14]. In the case of weakly and mildly unstable detonations, Bourlioux et al. [15] used a shock-tracking technique. However, the issue of numerical convergence remains when an "explosion within explosion occurs", and when secondary fronts form within the reaction zone and overtake the leading shock [16]. When using a shock-capturing technique, a criterion for determining the shock location is required. For example, Colella [17] for inert strong shocks and later Quirk [18] for detonation waves, used an empirical shock indicator based on the local relative pressure jump. Although, their criterion is well designed, it seems to be problem dependent. Recently, Yee et al. [19] used a minmod-like shock indicator. Their paper presents a state-of-art review of split and unsplit strategies. Spurious numerical solutions are reported when under-resolved computations are performed, as deflagration takes place within the numerical shock layer. Several numerical schemes are compared, as well as the extension to chemistry of the well-balanced strategy, which was primarily designed to deal with specific issues associated with stiff geometric source terms [20]. Lately, Menikoff and Shaw [21] proposed a shock sensor based on the Hugoniot jump conditions for condensed phase-detonations, which is independent of the numerical dissipation. As the numerical scheme is entropy-positive, the shock sensor is based on the relative position of the thermodynamic states within the shock numerical layer as compared to the Hugoniot curve. This criterion is however dependent on the state upstream of the shock. Thus no burning occurs within the numerical shock width [22]. Activation of chemistry thereby occurs only after the shock passage, which is in accordance with the ZND theory. This is also a common prescription to ensure the correct detonation speed [23], even for underresolved resolution of the reaction zone. Timmes et al. [24] show that the strength of the cellular features, which depend on the detonation instabilities are resolution-dependent. Papatheodore and Messer [23] also point out that the numerical prohibition of burning within the numerical shock can affect the capabilities of the numerical method to capture the associated flow instabilities.

Moreover, the use of higher order schemes for the hyperbolic part is much more suitable to properly capture the period of the shock oscillation, while a second-order scheme can be sufficient to retrieve the peak pressure. As shown in Hwang et al. [6], higher-order ENO schemes (higher than three) are able to predict the oscillation period more accurately for a given mesh spacing compared to second-order schemes. The former schemes achieve better convergence behavior. Yet, they indicate that higher-order schemes can achieve the correct peak pressure with a relatively coarse mesh. Indeed, in detonation computations, it seems important to resolve as accurately as possible the reaction zone, which contains a wide variety of smooth fine scales, which has been one of the scopes of the design of the WENO schemes [33]. Indeed, the fluctuations of the leading shock give rise to a train of characteristic as well as entropy waves. In turn, they modify the state sensitive reaction-rate and the reaction zone behaves like a non-linear oscillator [26]. For example, during the deceleration of the leading shock, a reaction front and a pressure buildup will arise and will then overtake the leading shock. It is thus desirable not to smooth out the peak overpressure, as would do any TVD scheme, in order to capture the time dynamics of this leading shock. In another context, the space–time diagram and the corresponding shock to detonation transition have been shown by Xu et al. [27] to be more accurately captured with a fifth-order WENO numerical scheme compared to a second-order scheme. In this study, we use the usual Strang splitting to couple the integration of the hyperbolic operator with that of the chemistry, as recalled by Yee et al. [19]. Moreover, the latter authors, based on extensive numerical studies between fifth and second-order schemes have concluded that the less dissipative scheme, the better for very coarse grid, in particular as for the shock location. This is of particular interest for our study. Thus the use of high-order numerical schemes is recommended, when dealing with detonation instabilities.

We then focus on the inherent numerical resolution needed in order to capture this increase of instabilities. More specifically, we investigate the dynamics of the von-Neumann spike, which is the post-shock state characterized by a local extremum in the flow. It is therefore the most difficult feature to capture. The effect of the mesh refinement and that of the shock indicator versus the activation energy are studied. The objective is to highlight the numerical features needed to apply the non-linear analysis of Ng et al. [4] to the post-shock state and to determine the mean sonic locus [25] which accounts for the presence of the fluctuations in the reaction zone, in the case where the detonation non-ideality comes from the momentum and heat losses.

This paper is organized as follows. The governing equations as well as the post-processing procedure leading to the definition of the mean detonation structure and the sonic locus are presented in Section 2. The numerical procedure is given in Section 3. Results and discussions are presented in Section 4. The main conclusions are drawn in Section 5.

2. Governing equations

The flow is governed by the one-dimensional unsteady reactive Euler equations with friction and heat loss (Zel'dovich model). The system is cast into the following conservative form

$$U_\tau + F_\chi = S \tag{1}$$

where $U = (\rho, \rho v, \rho E, \rho Y)$ is the conservative vector, $F = (\rho v, \rho v^2 + p, \rho E v + p v, \rho Y v)$ the convective flux, and $S = (0, f, \dot{q}_{th} + v f, \dot{\omega})$ are the source terms. τ and χ are the coordinates in the laboratory frame. ρ, v, p and E denotes density, velocity, total energy $E = e + v^2/2$, respectively. $e = p/(\gamma - 1)\rho + Yq$ is the internal energy, Y the reactant mass fraction, q the heat of reaction, and γ the polytropic coefficient. $f = -c_f \rho |v| v/2d$ is the drag force, c_f the skin friction. The heat loss is $\dot{q}_{th} = -h_c(T - T_w)/2d$, where $h_c = \rho c_p |v| c_f/2$ is obtained via the Reynolds analogy [11]. c_p, T, T_w and d are the heat capacity, the static temperature, the wall temperature and the diameter of the tube, respectively. A simple Arrhenius exothermic source term $\dot{\omega} = -\mathcal{A}\rho Y \exp(-E_a/RT)$ is used to model the chemical reaction. Both reactants and products are considered as perfect gases, having the same molecular mass and specific heats. $\mathcal{A}$ and E_a denote the pre-exponential factor and the activation energy, respectively. The chemical source term is set to zero when the mass fraction goes below a threshold of 10^6. In Sow et al. [30], we show that the work of friction which is expressed by the product of friction force by the velocity implies that the only source of entropy production is due to the irreversible chemical reaction. In the present study, the thermal heat transfer should be added as another source of entropy production. This difference with the more classical formulation has been done in order to underline the extra-deficit of velocity of the detonation front and its dynamics, which are inferred by the presence of fluctuations. Indeed, the right-hand side of the mean Gibbs relation would imply only quantities with fluctuations, whereas in the other case, there will be terms relative to mean quantities, hiding the physics. When a metric ξ_χ, which will be defined in Section 3.2, is used the governing equation can be cast in the following form

$$U_\tau + \xi_\chi F_\xi = S \tag{2}$$