Mean Structure of Unstable Pathological Detonations

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1 Introduction

Pathological detonations can arise in reactive systems where exothermic and endothermic reactions are present simultaneously.[1-3] A fluid element traversing the steady wave structure of a pathological detonation is accelerated as the chemical reactions release heat (while subsonic) or absorb heat from it (while supersonic). Within this reaction zone, there exist a location where the flow moves at the local sound speed away from the leading shock, which is known as the *sonic point*. Upstream from the sonic point, the exothermic reactions release heat faster than the endothermic reactions absorb heat, hence the subsonic flow (relative to the leading shock) is accelerated; downstream from the sonic, the endothermic reactions predominate so that the supersonic flow is further accelerated due to heat removal until reaching the chemical equilibrium (i.e., complete reaction); the overall rate of heat releases vanishes as the flow passing through the sonic point. Due to the predominance of exothermicity in the subsonic reaction zone, the amount of heat release that supports the shock front to propagate is greater than total amount of heat release at the CJ equilibrium state. Hence, a pathological detonation wave propagates at a velocity that is greater than the CJ velocity. There exists a unique (or *eigenvalue*) solution for this velocity that permits the rates of exothermic and endothermic reactions to be balanced in the flow upon reaching the sonic point, and this solution can be determined by iterating upon the propagation velocity and successively solving for the one-dimensional, steady ZND structure.

In most real detonation systems, detonation waves exhibit a multidimensional, unsteady structure while experiencing intense instabilities. The exothermic and endothermic processes are not only chemical reactions, but also dissipative processes (e.g., frictional effects) and the relaxation of mechanical and thermal fluctuations due to the instabilities towards equilibria. It remains unclear whether a one-dimensional, steady wave structure where only chemical reactions are incorporated can accurately predict

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the location of the effective sonic surface in a spatio-temporally unstable pathological detonation wave. In other words, the physical significance of the relaxation processes on the hydrodynamic thickness of unstable detonations has not yet been well demonstrated using the available theoretical tools based on the ZND solution.

In this study, stable and unstable pathological detonations are computationally simulated. Via performing the averaging analysis that has been explored for detonation studies over the past decade [4-6], a time- and density-weighted mean wave structure can be obtained for these simulated pathological detonations. The objective of this study it to compare these mean structures with their corresponding ZND predictions, and examine whether the interplay between the chemical reactions and the relaxation processes has significant effects on the reaction zone dynamics, hence, the wave propagation behavior. These effects can be further illustrated by evaluating the fluctuations in flow quantities based on the averaged simulation results. An advantage of using a pathological detonation system to study the effects of the relaxation processes on detonation hydrodynamic thickness is that a sonic point can be clearly identified, and thus, a well-defined hydrodynamic thickness (i.e., distance from the leading shock to the sonic point) can be determined in the ZND solution and very likely in the mean structures as well.

2 Problem description

The pathological detonation system considered in the study is governed by the one- or two-dimensional reactive Euler equations. Two consecutive irreversible reactions $\mathrm{A} \rightarrow \mathrm{B} \rightarrow \mathrm{C}$ with Arrhenius (temperature-dependent) reaction rates are considered in this model. Reactions $\mathrm{A} \rightarrow \mathrm{B}$ and $\mathrm{B} \rightarrow \mathrm{C}$ are exothermic and endothermic, respectively. The reactive system consists of an inviscid, calorically perfect gas (i.e., with a constant ratio of specific heat γ). The governing equations (for one-dimensional space) in a lab-fixed reference frame with flow and state variables non-dimensionalized with respect to the pre-shock, initial state are as follows,

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{U})}{\partial x} = \mathbf{S}(\mathbf{U}) \tag{1}$$

where the conserved variable **U**, the convective fluxes **F**, and reactive source term **S** are, respectively,

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho e \\ \rho Z_{1,2} \end{pmatrix} \quad \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (\rho e + p)u \\ \rho Z_{1,2} u \end{pmatrix} \quad \mathbf{S} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \rho \Omega_{1,2} \end{pmatrix} \tag{2}$$

In such a reaction scheme, Z_1 and Z_2 are the reaction progress variables (1 for unreacted and 0 for completely reacted) monitoring the exothermic and endothermic reactions, respectively, and can be related to the mass fractions of species A, B, and C, i.e., Y_A, Y_B, and Y_C, as $Y_\mathrm{A} = Z_1$, $Y_\mathrm{B} = Z_2 - Z_1$, and $Y_\mathrm{C} = 1 - Z_2$. The dimensionless specific total energy e for a homogeneous system is thus defined as $e = p/(\gamma - 1)\rho + u^2/2 + Z_1 Q_1 + Z_2 Q_2$ where Q_1 and Q_2 are the dimensionless specific heat release for the exothermic and endothermic (with a negative Q_2) reactions, respectively. In Eq. 2, Ω_1 and Ω_2 are the rates of exothermic and endothermic reactions in forms as follows,

$$\Omega_1 = -kZ_1\text{Exp}(-E_{\text{a}1}/T) \quad \text{and} \quad \Omega_2 = k(Z_1 - Z_2)\text{Exp}(-E_{\text{a}2}/T)$$

where E_{a} is the dimensionless activation energy and k is the pre-exponential factor that is arbitrarily chosen to be the same for both reactions.

In this current abstract, with $Q_1 = 100$, $Q_2 = -75$, and $\gamma = 1.2$, one-dimensional simulations have been performed for three cases of different propagation behaviors: 1) steady propagation with $E_{\text{a}1} = 20$ and $E_{\text{a}2} = 50$; 2) periodically pulsating propagation with $E_{\text{a}1} = 21$ and $E_{\text{a}2} = 20$; 3) highly chaotic pulsation with $E_{\text{a}1} = 27$ and $E_{\text{a}2} = 20$. The parameters for the above-mentioned cases are selected according to the analysis and simulation results shown in [7,8]. In all cases, a rightward-propagating detonation wave was initiated by a high pressure (5 times the CJ pressure) placed near the left end of the computational domain. The value of k was chosen so that the half-reaction-zone length in the eigenvalue ZND solution equals unity.

3 Numerical methodology and averaging analysis

The simulation code used to solve the reactive Euler equations was based upon a uniform Cartesian grid. This code used the MUSCL-Hancock TVD Gudonov-type finite-volume scheme with an exact Riemann solver and the van Leer non-smooth slope limiter. The reaction process was solved using a second-order, two-stage explicit Runge-Kutta method. The Strang splitting method was used in order to maintain second-order accuracy.

In order to obtain the mean detonation structure, density-weighted (Favre), temporal averaging was performed to the simulation data. The averaging method used in this study, similar to that first used by Sow *et al.* [5], is based on a reference frame moving at the instantaneous propagation velocity of the leading shock V_{ins}. In this moving reference frame, the spatial coordinates and particle velocity are transformed as $x' = x - \int_0^t V_{\text{ins}}(\tau)\text{d}\tau$ and $u' = u - V_{\text{ins}}(t)$, respectively. A simple temporal averaging, i.e., Reynolds averaging, procedure is applied to density and pressure as follows,

$$\bar{\rho}(x') = \frac{1}{t_2 - t_1}\int_{t_1}^{t_2} \rho(x', t)\text{d}t \quad \text{and} \quad \rho = \bar{\rho} + \rho^{\circ} \qquad \bar{p}(x') = \frac{1}{t_2 - t_1}\int_{t_1}^{t_2} p(x', t)\text{d}t \quad \text{and} \quad p = \bar{p} + p^{\circ}$$

where t_1 and t_2 indicate the starting and ending time of the period over which ρ and p are averaged. The bar "$-$" and superscript "$\circ$" indicate temporally averaged variables and their fluctuating quantities, respectively. Favre averaging (i.e., density-weighted) averaging is then applied to particle velocity and reaction progress variables as follows,

$$\overline{u'} = \frac{\overline{\rho u'}}{\bar{\rho}} \quad \text{and} \quad u' = u^* + u'' \qquad \overline{Z_{1,2}} = \frac{\overline{\rho Z_{1,2}}}{\bar{\rho}} \quad \text{and} \quad Z_{1,2} = Z_{1,2}{}^* + Z_{1,2}{}''$$

where superscripts "$*$" and "$''$" indicate Favre-averaged variables and their corresponding quantities, respectively. The averaged structure of the wave is therefore governed by the one-dimensional, steady Favre-averaged Euler equations as follows,

$$\frac{\partial}{\partial x'}(\bar{\rho}u^*) = 0 \tag{3}$$

$$\frac{\partial}{\partial x'}\left(\bar{\rho}u^{*2} + \bar{p} + \overline{\rho u''^2}\right) = -\overline{\rho \dot{V}_{\mathrm{ins}}} \tag{4}$$

$$\frac{\partial}{\partial x'}\left(\bar{\rho}e^* u^* + \overline{\rho e'' u''} + \overline{pu}\right) = -\overline{\rho u \dot{V}_{\mathrm{ins}}} \tag{5}$$

In Eqs. (4) and (5), terms $\overline{\rho \dot{V}_{\mathrm{ins}}}$ and $\overline{\rho u \dot{V}_{\mathrm{ins}}}$ represent the inertial (pseudo-) force and the work done by it due to the transformation to a reference frame moving at V_{ins}. Note that these two terms are zero for a steady wave propagation.

Taking the expressions for average specific total energy $e^* = \bar{p}/\bar{\rho}(\gamma - 1) + u^{*2}/2 + Q_1\bar{Z}_1 + Q_2\bar{Z}_2$ and averaged speed of sound $c^* = \sqrt{\gamma\bar{p}/\bar{\rho}}$ into Eqs. (3) to (5), after some algebraic manipulation, one obtains the so-called *master equation* as follows,

$$\frac{\mathrm{d}u^*}{\mathrm{d}x} = \frac{\phi_{\mathrm{I}} + \phi_{\mathrm{M}} + \phi_{\mathrm{T}} + \phi_{\mathrm{R1}} + \phi_{\mathrm{R2}}}{\bar{\rho}\left(c^{*2} - u^{*2}\right)}$$

The master equation describes how a fluid element traversing through a Favre-averaged wave structure is accelerated by the thermicity due to inertial force (ϕ_{I}), mechanical fluctuations (ϕ_{M}), thermal fluctuations (ϕ_{T}) and exo- and endothermic reactions (ϕ_{R1} and ϕ_{R2}). The detailed derivation of the master equation and expressions of the thermicity terms can be found in [5].

4 Results and Discussion

The history of the instantaneous propagation velocity V_{ins} for the cases with 1) $E_{\mathrm{a1}} = 20$ and $E_{\mathrm{a2}} = 50$, 2) $E_{\mathrm{a1}} = 21$ and $E_{\mathrm{a2}} = 20$, and 3) $E_{\mathrm{a1}} = 27$ and $E_{\mathrm{a2}} = 20$ are plotted as (blue curves) functions of the leading shock position x_{s} in Fig. 1(a), (b), and (c), respectively. As shown in Fig. 1(a), after a short initiation process, V_{ins} reaches a steady value of $1.678V_{\mathrm{CJ}}$ that agrees with the eigenvalue velocity V_{eigen} (black dashed line) predicted by the ZND model. For the cases with $E_{\mathrm{a1}} = 21$ and $E_{\mathrm{a2}} = 20$ shown in Fig. 1(b), the resulting V_{ins} starts to periodically oscillate with an increasing amplitude after the initiation process. An averaged velocity V_{avg} in agreement with the eigenvalue solution is obtained after V_{ins} settles into a steady oscillation with a fixed amplitude (i.e., after $x_{\mathrm{s}} \approx 3000$). The case with $E_{\mathrm{a1}} = 27$ and $E_{\mathrm{a2}} = 20$ results in a highly chaotic wave propagation as shown in Fig. 1(c). The V_{avg} measured over a long distance (i.e., from $x_{\mathrm{s}} \approx 1000$ to 4000) approximately equals to V_{CJ}, but significantly lower than its corresponding eigenvalue solution $V_{\mathrm{eigen}} = 1.079V_{\mathrm{CJ}}$.

Via performing the averaging procedure described in Sec. 2, mean wave structures have been obtained for the two unstable cases, i.e., periodic pulsation with $E_{\mathrm{a1}} = 21$ and $E_{\mathrm{a2}} = 20$ and highly chaotic propagation with $E_{\mathrm{a1}} = 27$ and $E_{\mathrm{a2}} = 20$, and shown in Fig. 2. The averaged pressure profile (blue curve) and the location of the averaged sonic point (open blue circle) for the case of periodic pulsation, as shown in Fig. 2(a), very closely match that the ZND predictions (black dashed curve and solid black circle, respectively). Hence, for this case, the hydrodynamic thickness l_{h} of the mean structure agrees well with that predicted by the ZND model. In Fig. 2(c), as indicated by the black curve that represents the overall amount of heat release by the reactions (i.e., $Q_1\bar{Z}_1$+$Q_2\bar{Z}_2$) in the mean structure for the periodic pulsating case, an "overshoot" in exothermicity upon reaching the sonic point contributes to the super-CJ propagation speed of this pathological detonation wave.

For the highly chaotic cases shown in Fig. 2(b), the mean profile of pressure (blue curve) significantly deviates from the ZND solution. The averaged von Neumann pressure is lower than that in the ZND profile, and the averaged sonic point seems to be located very far downstream from the leading shock. The l_{h} of the mean structure is likely greater than that of the ZND solution by an order of magnitude. As shown in Fig. 2(d), the total amount of chemical energy, i.e., $Q_1\bar{Z}_1$+$Q_2\bar{Z}_2$, is monotonically released (black curve decreases) without an overshoot in exothermicity choking the flow as predicted in the ZND solution. The hypothesized mechanism underlying such a mean structure is that the relaxation processes of the intense fluctuations in this highly chaotic case are effectively endothermic, hence, the overall exothermicity is never sufficiently strong to choke the flow until reaching the equilibrium CJ state far downstream; this mean structure thus supports a wave propagation at an average velocity that is very closed to V_{CJ}. This hypothesis can be verified via quantitatively examining the fluctuation terms in Eq. 6 and their relaxation processes.

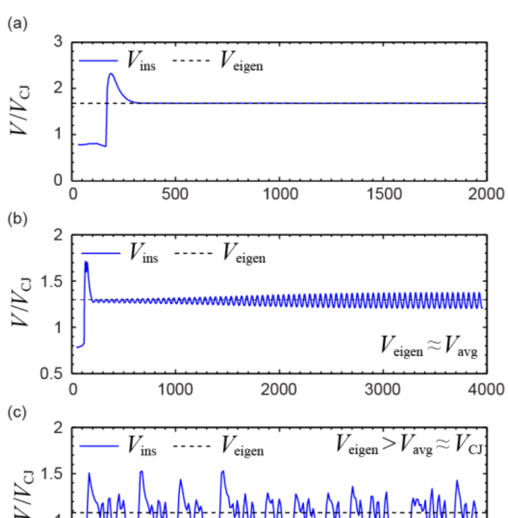

Figure 1. History of the instantaneous propagation velocity V_{ins} for the cases with (a) $E_{\mathrm{a1}} = 20$ and $E_{\mathrm{a2}} = 50$, (b)| $E_{\mathrm{a1}} = 21$ and $E_{\mathrm{a2}} = 20$, and (c) $E_{\mathrm{a1}} = 27$ and $E_{\mathrm{a2}} = 20$ are plotted as (blue curves) functions of the leading shock position and compared to their corresponding eigenvalue velocities.

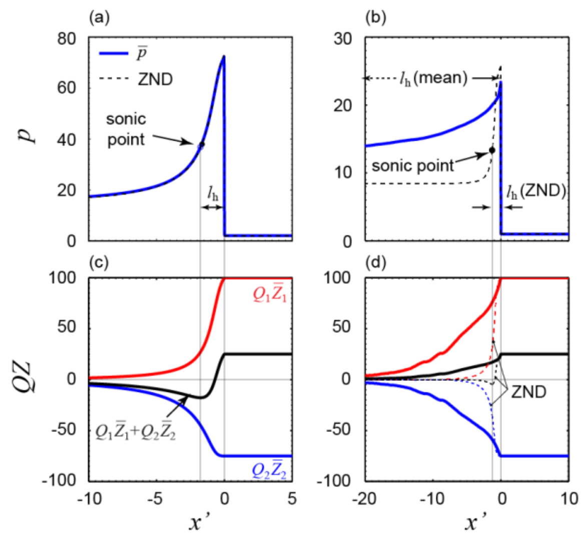

Figure 2. Mean profiles of pressure ((a) and (b)) and reaction progresses ((c) and (d)) comparing to the ZND solutions. The case with $E_{\mathrm{a1}} = 21$ and $E_{\mathrm{a2}} = 20$ is shown in (a) and (c); the case with $E_{\mathrm{a1}} = 27$ and $E_{\mathrm{a2}} = 20$ is shown in (b) and (d).

5 Conclusion

In this study, one-dimensional pathological detonations have been simulated for three different (stable, periodically pulsating, and highly chaotic) cases. The mean wave structures have been obtained via Favre averaging analysis for the two unstable cases. While the mean structure for the periodically pulsating cases agrees well with the ZND solution, that resulting from the highly chaotic case significantly differs from the ZND profile with an elongated hydrodynamic thickness. Further analysis will be performed to examine the hypothesized role played by the relaxation processes of the fluctuating quantities. In future efforts, this study will be extended to two-dimensional pathological detonation systems where transverse instabilities are present.

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