Numerical Study of Unsteady Pathological Detonations

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Introduction

As pointed out by G.I. Taylor [1], the existence of a steady detonation wave depends on the ability to match the transient solution for the unsteady expansion of the detonation products to the steady boundary condition of the reaction zone, i.e. Chapman-Jouguet (C-J) plane. This matching can only take place when the flow velocity at the C-J plane is sonic relative to the shock front. This may not always be possible, e.g. imploding detonations [2].

Non-ideal effects, such as the curvature or friction can be incorporated in the conservation equations as source terms. Under these non-ideal conditions, a steady detonation solution can still be found using the so-called generalized C-J criterion [3]. The detonation solution is obtained when the competing effects of heat release, flow divergence (i.e. curvature) and friction lead to a vanishing effective heat release rate at the sonic plane.

The source terms can readily be incorporated in a numerical simulation of the transient development of a detonation. Previous studies [4] have demonstrated that the resulting detonation wave may be either stable or unstable (pulsating) depending on the parameters of the flow (i.e. the activation energy). But most importantly, it was shown that the asymptotic solution, if it exists, corresponds to the stable solution obtained using the generalized C-J criterion. Moreover, when an unstable solution is obtained, it oscillates around a mean value corresponding to that obtained based on the generalized C-J criterion.

In the previous study, the chemical reactions have always been modeled as an irreversible single-step Arrhenius rate law. A one-step rate can not simulate endothermic reactions, which could in turn lead to pathological detonations. The pathological detonation solution is found when the endothermic and exothermic chemical energy release rates cancel one another at the sonic plane. The remaining (mainly endothermic) reactions occurring beyond the sonic plane do not affect the detonation wave propagation. This results in an effectively higher energy release that drives the detonation above its equilibrium C-J velocity value. Steady-state ZND calculations with this kinetic model confirm the existence of pathological detonations [5].

Thus so far, no transient analysis has been carried out to see if the steady pathological detonation can be realized under different initial conditions. The present paper investigates the transient development of a 1D-detonation wave subjected to a two-step chemical rate and establishes the conditions for its approach to a steady-state solution.

Steady-state properties

In previous studies [6] [7], steady-state calculations of pathological detonations have been carried out for the H_2-Cl_2 mixture using detailed chemistry. In the present work, a simpler model that reproduces qualitatively the behavior of pathological detonations is used. Following Fickett and Davis [5], the simplest chemical reaction scheme leading to a pathological detonation is a model where an irreversible exothermic reaction changing molecule A into molecule B is followed by an irreversible endothermic reaction changing the molecule B into molecule C:

$$A \rightarrow B \quad \text{(Exothermic)}$$
$$B \rightarrow C \quad \text{(Endothermic)}$$

with :

$$\lambda_1 = 1 - x_A \qquad\qquad \lambda_2 = x_C$$

$$\frac{d\lambda_1}{dt} = k_1(1-\lambda_1)\exp\left(\frac{-Ea_1}{RT}\right) \qquad\qquad \frac{d\lambda_2}{dt} = k_2(\lambda_1-\lambda_2)\exp\left(\frac{-Ea_2}{RT}\right)$$

where x_A and x_C respectively stand for the mass fractions of molecules A and C. The generalized C-J criterion can be represented by the following two equations:

$$u = c_f \quad \text{and} \quad \dot{\lambda}_1 Q_1 + \dot{\lambda}_2 Q_2 = 0$$

Values of Q_1=50 and Q_2=-10 and a polytropic equation of state with γ=1.2 are used throughout. For the steady calculations, the actual values of the activation energies Ea_1 (exothermic) and Ea_2 (endothermic) are not important. Only their difference has an effect of the steady detonation solution. The steady ZND detonation profiles were first obtained and shown on Fig. 1. These steady pathological detonation results agree with the steady-state ZND theory [5]. Different flow patterns behind the sonic depend on the rear boundary condition of a prescribed piston velocity. For piston velocities below the so-called weak value, the chemical reactions proceed until the weak detonation state is reached. A receding expansion wave then connects this weak state to the piston surface. For piston velocity equal to the weak value, a constant state region extends from the piston surface to the weak point. For piston velocities above the weak value, but below the strong one, the chemical reactions also proceed down to the weak point. However, a receding shock wave then connects the weak point to the constant state region downstream of the shock. For piston velocity equal to the strong value, two solutions are possible. Either a slope discontinuity is observed at the sonic point and the pressure then smoothly rises up to the strong value, or the reactions proceed down to the weak point, and then a shock wave connects the weak state with the strong one. For piston velocities above the strong value, an overdriven detonation is obtained. For overdriven detonation, no sonic point is embedded in the reaction zone; the detonation is no longer pathological.

Transient pathological detonation

An unsteady 1D Lagrangian detonation code is now used to study the transient development of pathological detonations. The one-dimensional reactive Euler equations are numerically solved using a combination of second-order two-step explicit MacCormack scheme [8] and FCT scheme of Boris and Book[9]. This code has been used previously in the study reported in Ref. [4].

The first set of calculations simulates a blast wave initiation by driving a piston at a high velocity during a period of time sufficient to initiate the detonations and stopping it right after. For low exothermic activation energy, the initially overdriven detonation asymptotically decays towards a steady value (Fig.2). This steady value is found to correspond to the steady pathological state based on the generalized C-J criterion. For high value of the exothermic activation energy, the detonation is unstable, and oscillates around a mean value (Fig. 3). No steady solution exists, as it becomes impossible to match the steady reaction zone with the unsteady flow downstream. However, the average velocity of the pulsating detonation is found to correspond to the pathological velocity based on the generalized C-J criterion. The stability limit is found to depend mainly on the exothermic activation energy.

In the second series of calculations, the detonation is initiated by a piston driven at various constant velocities throughout. When too low a value of the piston velocity is selected, it was found that no detonation was initiated. The profile is that of a non-reactive shock wave. For sufficiently large values of the piston velocity, a detonation can be initiated. Similar to the blast initiation results, both unstable (Fig.4) and stable (Fig.5) detonations can be generated, depending on the exothermic activation energy. Piston travelling at velocities equal or below the strong value, do not affect the shock front propagation. The pressure profiles for steady piston-supported detonations can readily be compared with the steady ZND predictions (Fig.6).

For both strong and overdriven piston velocities, the detonation states and profiles are in good agreement with the steady-state theory. For the strong piston, the second case discussed in the steady section is observed, i.e. a shock wave connects the weak and strong solutions. For piston velocities between the weak and the strong values, the steady-ZND theory states that a shock wave should be observed downstream of the reaction zone. However, the present profile does not indicate a definitive shock, but rather a smooth compression wave. According to the steady-state theory, the shock wave recedes from the reaction zone. Pistons propagating at the weak velocity and below were found to be unable to initiate a detonation. Detonations with low constant velocity piston have to be started by initially overdriving the piston for a certain time, before bringing it back to the desired velocity. Nevertheless, the obtained profiles correspond to the steady-state predictions.

Conclusion

It may be concluded that pathological detonations can be realized from arbitrary initial conditions when a two-step chemical rate law is introduced. Similar to the C-J case, both stable and unstable (pulsating) pathological detonations can be observed depending on the value of the exothermic activation energy. For low exothermic activation energy, a stable detonation corresponding to the predicted ZND value is obtained. For high exothermic activation energy, the pathological detonation is unstable with oscillatory behavior. It becomes impossible to match a steady reaction zone with the unsteady flow downstream. Nevertheless, the average properties of the unstable detonations are also found to correspond to the steady ZND predictions.

The transient solution recovers the steady ZND results for various cases of the piston velocity. The present study thus confirms the validity of the generalized C-J criterion when endothermic and exothermic reactions compete to drive the flow towards the sonic point.

References

[1] G.I. Taylor, The dynamics of the combustion products behind plane and spherical detonation fronts in explosives, Proc. Roy. Soc. Ser. A 200:235-247, 1950.

[2] B.H.K. Lee, Non-uniform propagation of imploding shocks and detonations, AIAA Journal 5:1997-2003, 1967.

[3] J.B. Bdzil, Steady-state two-dimensional detonation, J. Fluid. Mech., 108:195-226, 1981

[4] J.H.S. Lee, F. Zhang, Friction-induced oscillatory behaviour of one-dimensional detonations, Proc. R. Soc. Lond. A, 446:87-105, 1994

[5] W. Fickett, W.C. Davis, *Detonation*, University of California Press, 1979

[6] H. Guénoche, P. Le Diuzet, C. Sèdes, Influence of the Heat-Release Function on the Detonation States. Presented at the 7th ICOGER, Gottingen, Germany, p. 387-407, 1981

[7] J.P. Dionne, R. Duquette, A. Yoshinaka, J.H.S. Lee, Pathological Detonations in H_2-Cl_2, to be presented at the 17th ICDERS, 1999.

[8] R.W. MacCormack, The effect of viscosity in hypervelocity impact cratering, AIAA paper 69-354, 1969

[9] J.P. Boris, D.L. Book, Flux-Corrected Transport I, SHASTA, a Fluid transport algorithm that works, Journal of Computational physics, 11:38-69, 1973

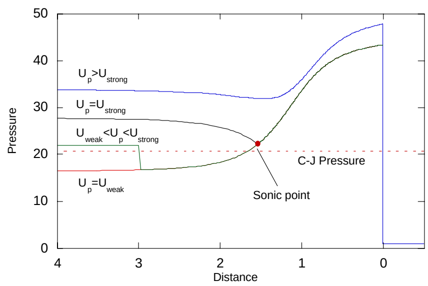

Figure 1: Steady ZND pressure profiles for different piston velocities (Ea_1=22, Ea_2=35)

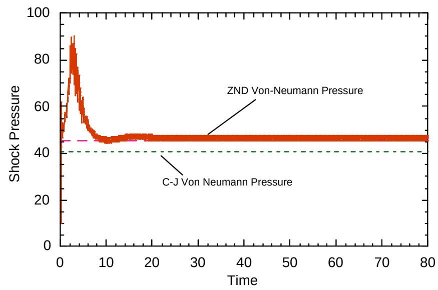

Figure 2: Stable pathological detonation with blast initiation (Ea_1=22, Ea_2=35)