Effect of cellular instabilities on the blast initiation of weakly unstable detonations

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1 Introduction

Detailed experiments and numerical simulations of the detonation wave structure revealed two main classes of detonation waves.[1,2] For weakly unstable cellular detonations, the structure can be modeled and studied by solving the reacting inviscid Euler equations for compressible flow, while for highly unstable detonations, transport phenomena appear to play a more significant role. Weakly unstable detonations are now amenable to detailed direct numerical simulation (DNS). In the present paper, we are interested in determining how the presence of a cellular structure affects the initiation and propagation mechanism of weakly unstable detonation waves. To address this question, we are performing DNS of direct (or blast) initiation[3,4] by solving the unsteady reactive Euler equations in one and two space dimensions.

We first perform one-dimensional simulations in order to determine the critical energy required to initiate a one-dimensional wave devoid of cellular instabilities. In the two-dimensional simulations, we add perturbations in the shape or in the distribution of the energy source in order to trigger a cellular structure on the front of the decaying reactive blast wave. We then compare the critical source energies required for the establishment of a 1D and 2D self-sustained cellular detonations. Such computations have also a direct bearing on experiments aimed at measuring the critical initiation energies of detonations, as it is well known that a fine cellular structure is established on the blast wave surface originating from high explosives, when the front is still highly overdriven.[5]

2 Numerical Set-up

The reactive Euler equations are solved by a Godunov-type method using adaptive mesh refinement in one and two space dimensions.[2] An idealized one step reaction and perfect gas behaviour are assumed. The gas parameters studied are typical for weakly unstable detonations ($Q/RT_o = 50$, $E_a/RT_o = 27$, $\gamma = 1.2$) and give rise to a single mode of oscillation in 1D and well-behaved cellular structures in 2D.[2] The direct initiation problem is set-up in the planar geometry. A thin slab of high pressure gas is placed near a wall, with a nominal thickness of $L = \Delta_{1/2}$ (the half reaction length of the steady wave) and density equal to the unreacted gas. The energy per surface area of the source is given by the internal energy of the slab gas, i.e., $E = pL/(\gamma - 1)$. The dimension of the source L was chosen small enough such that the source pressure (p) was sufficiently high to drive a blast wave which is initially much stronger than the detonation shock in the gas; this is characteristic of direct initiation of gaseous detonations by high explosive sources.[5] Two types of perturbations are used in the two-dimensional simulations. In the first type, the shape of the high energy core is modulated with a sinusoidal perturbation with amplitude a. In the second, the amplitude of the source energy is discontinuously perturbed by

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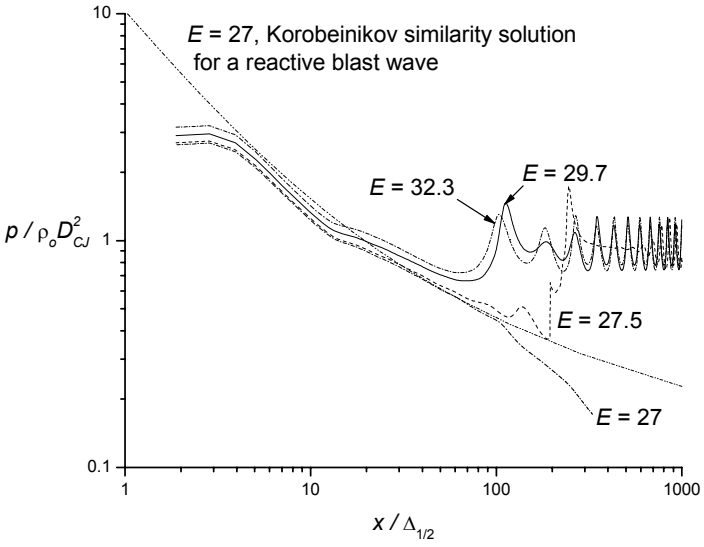

Figure 1 Shock pressure evolution in 1D

a factor j, yielding a piece-wise distribution of source energy per unit area in the transverse direction alternating between $(1+j)E$ and $(1-j)E$. Both types of perturbation conserve the average energy per surface area of the total source energy E and yield essentially an initial modulation of the strength of the blast wave with a characteristic wavelength. Both the strength and the wavelength of the perturbations in the y-direction were varied in order to generate cellular structures and transverse waves with a given strength and wavelength. The numerical simulations were performed with a maximum resolution of 64 grid points/$\Delta_{1/2}$, which ensures grid convergence for the numerical method used.[2]

3 Results

Figure 1 shows the dynamics of the lead shock pressure as a function of distance for the conditions close to criticality in 1D. The figure illustrates well the characteristic dynamics of the initiation process from a strong blast wave.[3-5] On scales comparable with that of the source $x \sim L$, while the shock pressure is much larger than the detonation pressure and the chemical energy addition is negligible, the dynamics are characterized by the relaxation towards a self-similar non-reactive blast wave. At larger scales $x > 30L$, the influence of the chemical energy addition is felt on the blast motion and the blast strength is well approximated by the quasi self-similar solution derived by Korobeinikov to account for the chemical energy addition and departure from Taylor-Sedov blast waves.[6] It is during this interval that the chemical reaction zone either remains coupled with the shock front to form a self-sustained detonation or decouples into a shock-fast flame complex.[4] Detailed investigation of the flowfield revealed very similar events to those described by Eckett et al. for ideal self-similar blast waves devoid of the early relaxation effects associated with the finite dimension energy source.[4] For the gas parameters used, we find that the critical non-dimensional energy of the source $\tilde{E}_* = \left(E_* / \rho_o D_{CJ}^2 \Delta_{1/2}\right)$ required for initiation is bracketed between 27 and 27.5. Larger source energies yield blast waves decaying to a self-sustained detonation wave, while lower source energies yield decoupling between the blast and chemical reactions. Note that strictly speaking, re-initiation will occur even for the sub-critical waves via DDT on very long time scales due to the irreversible nature of the chemical reaction. This is however outside the range of interest of the blast initiation problem where we are interested in the coupling between the lead shock decay and the chemical reaction induced by the decaying shock.[4]

The results of the multi-dimensional simulations are shown in Table 1 for a wavelength of the perturbation corresponding to the natural cell size in the system ($\lambda = 20$) obtained in a channel of width 10. For these conditions, we find that more energy is required for the establishment of a detonation from a perturbed blast wave than from an unperturbed one. Careful examination of the results of Table 1 indicates that the critical energy also increases with the strength

Table 1 Critical initiation energies for 1D and 2D perturbed blast waves

	1D	2D			
		$a / \Delta_{1/2} = 0.1$	$a / \Delta_{1/2} = 1$	$j = 0.01$	$j = 0.05$
$\tilde{E}$	27-27.5	30-35	35-40	29.1-29.7	30.7-31.3

of the perturbation, both when the shape or the amplitude of the energy source are perturbed.

Figure 2 shows the development of the cellular structure on the front of the reactive decaying blast wave, obtained for a source energy of $\tilde{E} = 35$ and a shape modulation of $a / \Delta_{1/2} = 1$. Note that for the same energy, a one-dimensional reactive blast wave decays to a self-sustained detonation. The temperature flowfield shown is easily interpreted in that the shocked yet un-reacted gas, which is cooler than the burned products, can be easily identified, hence giving a direct indication of the reaction zone structure of the reactive blast wave. The given perturbation gives rise to a cellular structure of the reacting blast wave from the very start, sustained by the same mechanism as self-sustained cellular detonations, i.e. the imbalance of exothermicity behind the Mach shock and weaker incident shock. In the second frame of Figure 2, the average shock speed is close to the ideal CJ wave and the reactive blast wave resembles very closely the structure of the self-sustained wave.[2] The main difference is the highly transient nature of this wave, due to the strong expansion wave responsible for the blast wave decay. For this strength of energy source and strength of the expansion wave, the reactive blast wave further decays and does not permit a self-sustained detonation to be established. These dynamics are illustrated in subsequent frames of Figure 2. Due to the blast decay, the lead shocks are continuously weakened by rear expansions and the gases accumulate unreacted behind the front for progressively longer times. Due to the original cellular instability established at earlier times, the unreacted gas accumulates primarily behind the weaker portions of the front and gives rise to the well known un-reacted pocket structure usually observed in self-sustained highly unstable detonations.[2] As the wave further decays, the reaction zone further decouples from the leading shock fronts and the whole system decays to a shock followed by a much slower fast flame.

4 Discussion

The results of the numerical simulations indicate that in all the cases studied, a perturbed blast wave always requires more energy to initiate a detonation than an unperturbed 1D blast wave. This surprising result is not evident at first glance, in view of the significant non-linearities involved in the coupling between the unsteady gas dynamics and exothermicity during the decay of cellular blast waves. In fact, one could argue that the periodic pulsations of the lead front above the average strength and the supplementary shock heating by transverse shocks may provide a mechanism for promoting the sustenance of the wave (e.g., Ref 7). However, it seems that such mechanisms are inefficient in the initiation process studied here.

To reconcile the discrepancy between our results and the generally expected outcome of our numerical experiments, we analyzed the flow fields in great detail. We found that indeed the localized pulsations of the cell structure, transverse wave collisions with the wall and transverse shocks alone all give rise to local accelerations of the reaction rate with respect to the average. However, these same cellular pulsations of the shocks also gave rise to colder gases reacting at rates lower than average and accumulating as un-reacted pockets. Since the leading shock strength and its decay rate is a consequence of the rate at which the gas burns behind it and energy is released, than the pockets of colder gases also play a role in delaying the global exothermic rates and the sustenance of the shocks. Inspection of the flow fields indeed indicates that the initiation of a self-sustained detonation wave is not only a local phenomenon requiring localized regions of enhanced exothermicity, but also involves time scales associated with the slower exothermic rates of the colder gases in the cell cycles. It thus appears that a much broader interval of time scales is relevant to the initiation process other than just the triple shock collisions at the front.

This interpretation is consistent with the results obtained by Radulescu et al.[2] regarding the average structure of self-supported cellular detonation waves. They found that a self-sustained cellular detonation is hydrodynamically much thicker than predicted by the one-dimensional model, although both waves propagate, on average, at approximately the same speed. This result was explained by considering the Arrhenius dependence of the reaction rate on the local shock strengths of the cellular detonation coupled with the hydrodynamics. Since the leading shock strength pulsates, the pulsations below average upset the pulsations above average and make the net exothermicity slower than the equivalent steady wave. We also verified these conclusions for the present unsteady waves, and found the average exothermic region behind the cellular blast wave is always thicker than the equivalent one-dimensional wave.

It is interesting to note that the reverse trend was obtained by Jones et al.[7] in numerical simulations of the detonation diffraction problem. They found that a smoothed front detonation quenches more easily than a detonation with a cellular structure and concluded that the cellular structure enhances the detonability of the wave. However, the computational resources available limited them to low resolutions of only ~20 grid points per detonation cell or ~1 grid point per induction zone thickness of a self-sustained wave. This is approximately two orders of magnitude less than in the present study and the question arises if they truly obtained a grid converged conclusion. For example, we also performed simulations with decreasing resolution in our initiation studies, and found that as the resolution decreases, the cellular detonations are more easily established. Inspection of the flow fields revealed that this effect was associated with the unphysical rapid burnout of the pocket gases behind the front at lower resolutions, due to the very large numerical dissipation.[2] It would thus be worthwhile to repeat the simulations of Jones et al. with the improved computational capabilities of today and verify whether their conclusions remain valid.

5 Conclusions

The results of our numerical experiments indicate that it can be more difficult to initiate inviscid detonations in the presence of multi-dimensional perturbations and cellular instabilities.

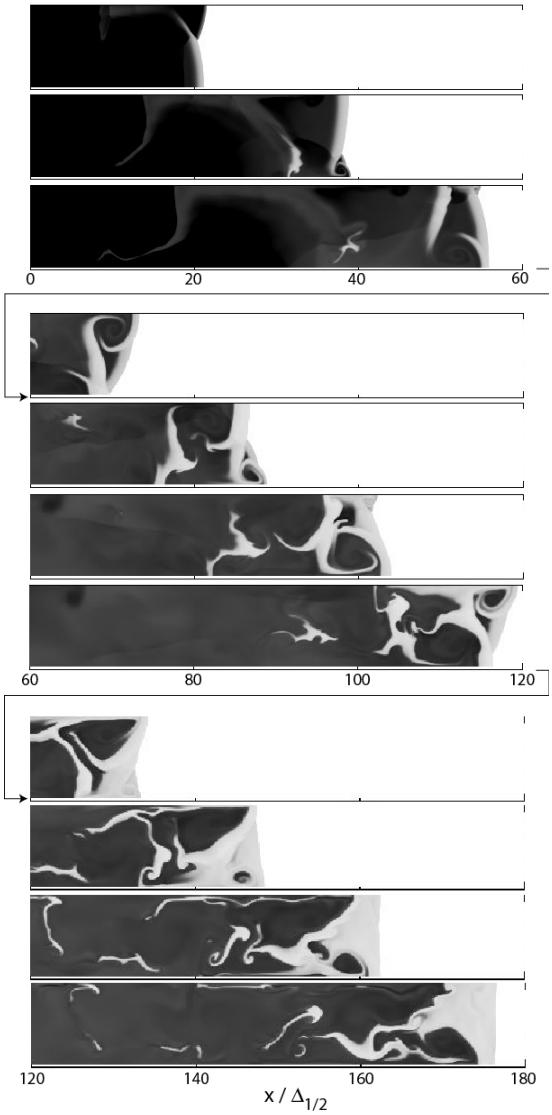

Figure 2 Temperature field evolution for $\widetilde{E} = 35$, $a = \Delta_{1/2}$

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