Role of gasdynamic wave fluctuations in shock induced ignition and transition to detonation: the hotspot cascade mechanism

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1 Introduction

The last stage of the deflagration-to-detonation transition (DDT) is complex due to the simultaneous role of compressible turbulent transport and auto-ignition phenomena [1–3]. In the present study, we focus solely on the gasdynamic effects, which may generate hotspots and facilitate the transition to detonation. We hence address the question of the role of mechanical fluctuations of different wave strengths and frequencies on the DDT process in the absence of diffusive (laminar or turbulent) phenomena. The problem we address is the classical shock induced ignition problem of a piston driven shock wave into a reactive medium and its subsequent transition to detonation. At time zero, a piston acquires a finite velocity, driving a shock into the initially quiescent reactive gas. The ensuing exothermicity triggered by the lead shock couples with the dynamics of the gas and eventually forms a detonation wave. In the absence of fluctuations, this problem is relatively well understood, as a significant effort has been devoted to clarify the coupling between gasdynamics and reactive phenomena in simple chemical models (one, two and three steps) in numerical simulations and analysis exploiting certain limiting conditions using asymptotic methods [4–8]. Previous work has identified that the most critical phenomenon in the acceleration process is the Zeldovich-Lee gradient mechanism, captured analytically in the work of Short and Sharpe [6, 7] of ignition in arbitrary gradients of induction delay. In the problem of shock induced ignition, the gradient set-up by the leading shock always gives rise to a subsonic fast flame, which may accelerate if the induction time gradient was smaller. In the present study, we allow the piston to have a non-constant speed. Its modulation at arbitrary frequencies and amplitudes drives a series of non-linear gas dynamic disturbances. We study their effect on the ignition process and transition to detonation. Note that the 1D problem solved is also equivalent to a shock induced ignition behind a reflected shock, the disturbances accounting for non-ideal effects such as gasdynamic waves generated at the boundaries by shear layers or flow-boundary layer interactions; see, for example the work of Khokhlov [9].

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2 Problem Formulation

We address a purely one-dimensional problem of shock-induced ignition. Before time zero, a homogeneous gas with zero speed occupies the half domain and the piston is at rest. At time zero, the piston is allowed to have a finite speed given by $u_p = u_0 + A \sin 2\pi f t$, where u_p is piston speed and t is system time. u_0, A and f are the variables for which we study the effect on ignition. The piston then drives a main leading shock and a series of N-waves that interact with the lead shock, creating further perturbations. The gas we study is stoichiometric hydrogen-oxygen initially at 300K. The mean piston speed was chosen such that the post shock state in the absence of sinusoidal perturbations (A = 0) is 1100K and 1 atm. This state corresponds to the transition limit between strong and mild ignition observed experimentally by Meyer and Oppenheim [10].

Four fluctuation frequencies are considered over 4 orders of magnitude, as we wish to study perturbation frequencies higher than those associated to the exothermic time, slower than the induction delay time and intermediate to this two characteristic times of the chemical reactions. For reference, the ignition delay time t_i and exothermic time t_e at the reference post shock state condition are 33μs and 2μs as computed from 0D calculations using Cantera [11] and the chemical mechanism of Li et al. [12]. The forcing frequencies f considered were 4.35 kHz, 45.35 kHz, 453.5 kHz and 4535 kHz. The four levels of forcing A/u_0 investigated were 0.05, 0.1, 0.15 and 0.2.

This reactive one dimensional problem was modeled by the reactive Euler equations coupled to the multi-specie mixture evolution using the reaction rate and thermodynamic database provided by Li et al. [12]. In order to avoid the necessity of moving grids in the numerical solution in order to accommodate the non-steady motion of the piston in the Eulerian frame of reference, the mathematical model solved was formulated in Lagrangian coordinates (ϕ, t). In the Lagrangian frame of reference, boundary conditions at mass label ϕ =0 at the piston face are simply prescribed.

A custom numerical code was developed to integrate governing equations by a time splitting algorithm for each discretized mass element, separating gasdynamic compression or expansion from the reactive dynamics. The ordinary differential equations describing the chemical evolution at constant volume for each mass element are solved using CANTERA using their reactor method implemented in C++. After each fractional step of the chemistry, which updated the chemical composition, pressure and temperature in each mass element, the gasdynamic evolution was solved using Riemann solver at each mass element interface. The HLL flux solver was used. A second order central difference scheme has been adopted to reasonably improve the resolution. The CFL number was set to 0.7 for all the related simulations. Several numerical test problems have been run to validate the hydrodynamic and chemical evolution [13]. Notably, the method has been shown to propagate a ZND stable detonation at the correct speed and wave-shape.

3 Results and Discussion

Figure 1 shows the evolution of temperature in the absence of fluctuations. Prior to the first ignition, the gas decomposition is thermally neutral. After the first ignition along the piston path (corresponding to the fluid partcile first shocked) at $t = 33\mu$s, a rapid acceleration of the ignition front is observed, following the transient process described in detail by Sharpe and Maflahi [8, 14] for a simpler two step chain-branching model mimicking the ignition. This consists of pressure waves propagating forward and compressing the gas in the induction zone. This results in shorter ignition delays, which contribute stronger amplification of

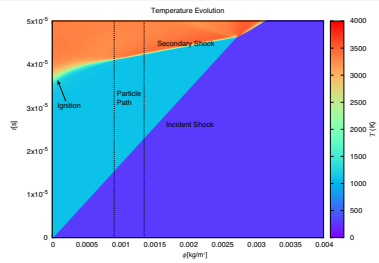

Figure 1: Temperature evolution $T(\phi, t)$: non-fluctuated

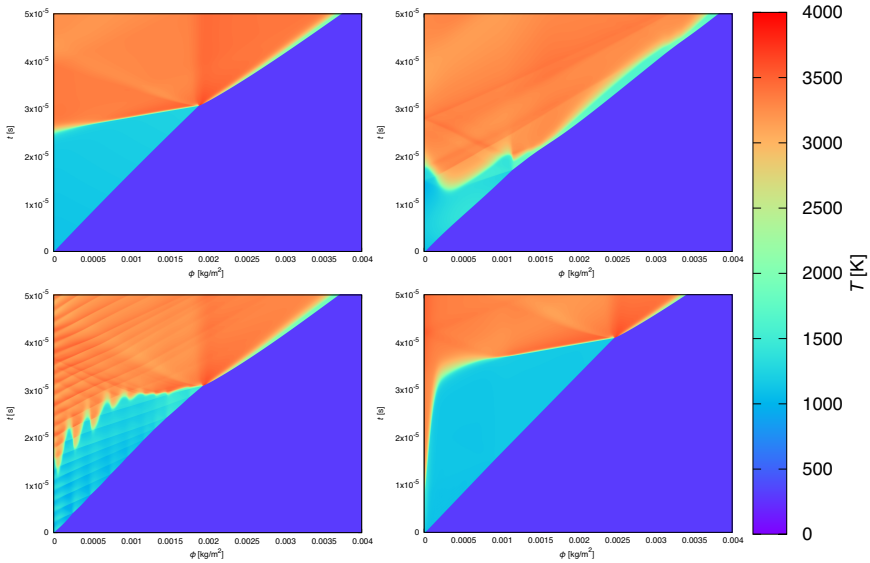

Figure 2: Temperature evolution $T(\phi, t)$ $A/u_0 = 0.2$: top left, f = 4.535 kHz; top right, f = 45.35 kHz; bottom left f = 453.5 kHz; bottom right f = 4535 kHz.

forward facing compression waves. This rapid amplification occurs on the exothermic time scale of energy deposition of t_e = 2μs. Following this initial rapid accelaration, a weak detonation is formed consisting of a leading internal shock bringing the gas to ignition, and an ignition front converting the gases to products [15]. When the shock leading the weak detonation reaches the leading shock first driven by the piston, a detonation wave is formed. We thus recover the classical *strong* shock initiation behavior in the limit of short reaction time compared to induction time, characteristic of all ignition processes at typical fuels.

The results obtained in the presence of forced gasdynamic waves show different behaviors, depending on the frequency of forcing. Fig. 2 shows the temperature evolution for the four frequencies investigated for A/u_0 = 0.20. At a low frequency of f = 4.535 kHz corresponding to a modulation with period longer than the nominal ignition delay, the ideal ignition illustrated in Fig. 1 in the absence of perturbations is recovered, although the ignition time and detonation formation time are shortened due to the supplementary heating of the gas by compressive motion (see Fig. 3).

By increasing the fluctuation frequency to $f = 45.35$kHz(Fig.2 top right), the first ignition delay has been shortened to $t = 1.3 \times 10^{-5}$s. This frequency corresponds to a perturbation period shorter that the nominal induction time by a factor of 1.49. The first ignition was started from a large hotspot. The mechanism for

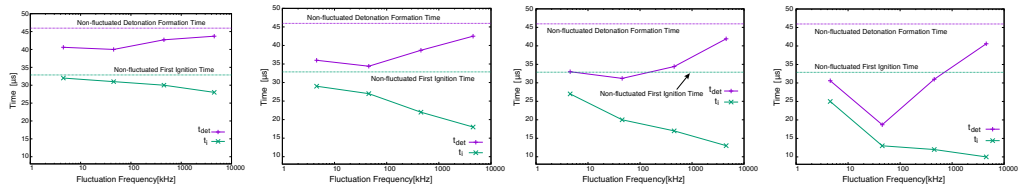

Figure 3: First ignition delay and detonation formation time plot with fluctuation frequency: top left, $A = 5\%u_0$; top right, $A = 10\%u_0$; bottom left $A = 15\%u_0$; bottom right $A = 20\%u_0$

this hot spot formation is through the strengthening of the leading shock by the forward facing pressure wave originating at the piston during the compression phase of the oscillation. The scale of such hotspot is dictated by the fluctuation frequency. The first ignition splits into two reaction fronts, propagating both forward and backward. The forward propagating reaction front did not couple with the shock it drives owing the induction time gradients not being in phase with the acoustics. However, a second hotspot was generated when the lead shock wave caught up with the leading shock, creating a strong entropy wave along the particle path (ϕ = 1.15×10^{-3}kg/m^2). The ignition from the second hot spot eventually resulted in a detonation forming at approximately $t = 18\mu$s.

When the fluctuation frequency was increased to $f = 453.5$kHz, more hotspots appeared and ignited individually, as shown in Fig.2 bottom left. This fluctuation frequency corresponds to a fluctuation period shorter by a factor of 15 as compared to the nominal induction delay time, but larger than the main exothermic time. At this high frequency, a system of N waves has had time to develop in the gas (see below), as clearly discernible as forward facing striations. The sequence of hot-spots formed in the induction zone correspond to entropy waves generated along particle paths when the sequence of N waves shocklets arrive at the leading shock. During this process, the lead shock is slowly amplified. It is only after the sixth generation of such hotspots the lead shock gives rise to an ignition front in phase with the acoustics, resulting in strong shock amplification and detonation formation.

In the limit of a frequency higher than the exothermic time, the hot-spots created lose their ability to contribute to a fast detonation formation. The last case with frequency of f = 4535 kHz, shown in Fig.2 bottom right shows that the modulation of very high frequency leads to a very localized gas heating, as the train of N waves is attenuated extremely fast (see below). The first ignition started very early at $t = 10\mu s$ but a detonation does not form until $t = 40\mu s$. Once the first ignition is operated and negligible gas-dynamic evolution is obtained due to out of phase energy release with the acoustics, the rest of the gas evolves as in the non-perturbed nominal case. This high frequency regime captures what is known as *mild* ignition in the literature [16], where single hotspot is observed, without directly contributing to the bulk of the ignition process.

Figure 3 shows the variation of ignition delay and detonation formation time with frequency of the perturbations, as compared with the nominal non-perturbed ignition process. While an increase in frequency of the forcing leads systematically to a lower ignition delay, the time of detonation formation is non-monotonous. The minimum in the detonation formation time is observed for the cases where the cascade of hotspots give rise to an ignition wave in phase with the acoustics. This case generates the most efficient amplification of shock waves by the classical Zeldovich-Lee mechanism. Here, however, the fast flame takes the form as a sequence of punctuated hot-spots, each one helping set-up a more favorable gradient for the next one. Since this cascade of hotspots has never been observed before, we label it the *hotspot cascade* mechanism.

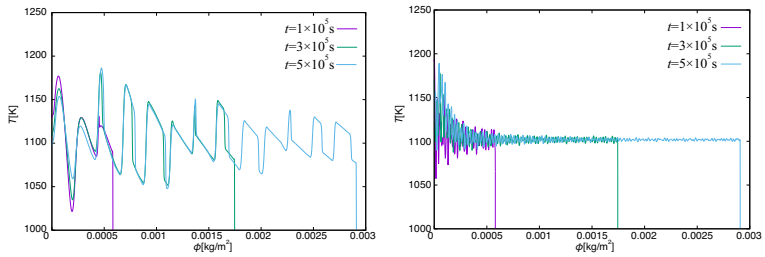

Figure 4: Temperature plot for inert shock simulation with a fluctuated piston $A = 5\%u_0$: left, $f = 453.5$kHz; right, $f = 4535$kHz

4 N-wave decay and penetration distance

The numerical results also show that the penetration distance of the N-wave system driven by the piston plays an important role in controlling the sequence of hotspots in the cascade. In order to clarify the mechanism controlling the decay and the penetration distance of these N waves, inert piston-shock simulations have been performed. These are representative of the gasdynamic evolution in the induction zone, prior to exothermicity. Figure 4 shows the post shock temperature evolution for two different frequencies. At the lower frequency, a complicated system of gasdynamic waves is set-up between the piston and the lead shock, involving compressive and entropy waves reflected by the shock and interacting with the piston generated forward facing waves. Nevertheless, the amplitude of the system of waves decay away from the piston. The wave amplitude near the piston is larger than that closer to the leading shock. At the higher frequency, the wave train decays much faster, with gas dynamic disturbances attaining negligible amplitudes close to the lead shock. It is also interesting to note that the average temperature near the piston is also larger than away from the piston, and increases with time. Both the decay of the N-wave system and the bulk heating is due to the dissipation by the shocks forming the N-wave system. We have also derived the decay of the N-wave system using simple gasdynamic arguments. N waves with higher frequency have shocks followed by steeper pressure and speed gradients. The shock change equations thus require that the decay rate scales with the amplitude and frequency of the N-waves. This is reason that the hot gas is limited very close to the piston in the high frequency limit, with local hotspot formation exclusively near the piston.

Fluctuation-shock interaction and dissipation dominate the temperature distribution in the induction zone. The first phenomenon, in which the compression fluctuations catch up with the leading shock and intensify the leading shock strength temporally, is the main mechanism to form local hotspots in the induction zone. The local hotspots need to be big enough to accelerate the local ignition to supersonic speed. The second phenomenon is that the shock fluctuation wave dissipates the energy to the local gas. Since the dissipation rate is related to the local fluctuation frequency and the amplitude, most of the wave energy goes into heating the gas close to the piston. This mechanism prevents hot-spot formation far from the piston, which hampers the DDT process.

In mixtures characterized by a stronger ignition delay sensitivity to temperature and shorter reaction to induction time ratios, more complex phenomena can be observed at very high frequencies. An example is shown in Fig. 5 for the system C_2H_4 + $3O_2$. A first generation of hotspots can be created, with each hotspot evolving independently of the other, since their evolution occurs on a time scale shorter that the acoustic -entropy feedback of the first hotspot with the leading shock. Nevertheless, the second generation of hotspots is triggered after the lead shock is strengthened by the first hotspot, which eventually leads to

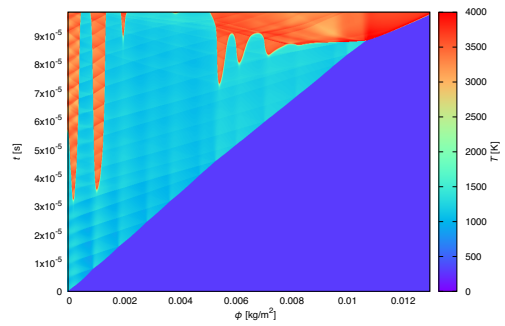

Figure 5: Temperature plot on shock induced ignition. Initial state:C_2H_4+3O_2, $p = 6.2$kPa, $T = 293$K. Incident non-fluctuated shock strength:$M = 4.5$, $A = 20\% u_0$, $f = 200$kHz

in-phase coupling with the acoustic waves and formation of a detonation.

5 Conclusion

The present study has investigated the role of forced gasdynamic perturbations in ignition phenomena. For sufficiently high frequencies of forcing, rapid initiation of detonation can be achieved when the sequence of hot-spots generated by sequential disturbances of the lead shock become in phase with the forward facing pressure waves, favoring the detonation formation by the Zeldovich-Lee mechanism. The sequence of each successive generation of hot-spot brings the forward facing fast flame more in phase with the acoustic waves. We call this the hotspot cascade gradient mechanism of initiation. We also show that large amplitude and large frequency forcing causes the driven N-wave system to decay rapidly, leading to localized heating. This corresponds to local hotspots resembling the mild ignition phenomenon observed experimentally in sensitive mixtures with long ignition delays, for which perturbations become essentially very high frequency.

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