Collision Modes of Constant-Speed Planar Auto-Ignition Waves

Laurence Bonneau, Vincent Robin, Ashwin Chinnayya,
Institut PPRIME - UPR 3346 - CNRS - ISAE-ENSMA - Université de Poitiers, France

1 Introduction

The transition from subsonic deflagration to supersonic detonation [1] has been the subject of numerous studies due to its importance in propulsion systems [2] and industrial safety. This phenomenon is the result of several mechanisms, including flame folding, interactions between shock waves and flame, and turbulence (see review papers [3, 4]), and remains an active area of research [5–8]. The initiation of detonation can occur through three main pathways. First, strong ignition is triggered by a sufficiently strong shock wave that induces rapid chemical reactions. Second, the detonation arises from weak ignition, driven by the Zel'dovich gradient mechanism [9], in which self-ignition waves emerge in non-uniform temperature or composition fields [10]. Third, the deflagration-to-detonation transition (DDT) occurs when a propagating flame accelerates due to turbulence and confinement effects, generating precursor shocks that eventually couple with the reaction front [11]. Although DDT is a complex process involving multiple interacting mechanisms, one key feature is the interaction between reactive fronts, which can play a crucial role in triggering detonation. Thus, this study investigates flame collisions [12] in a highly simplified configuration, yet the scenario remains representative of the dynamics observed in DDT. The canonical numerical configuration considered involves two subsonic planar auto-ignition waves, propagating at constant velocity, that collide at a prescribed angle. Previous work [12] showed that the transition to detonation occurs only for acute collision angles, but only one transition scenario was analyzed. In this extended study, the collision parameters—namely the collision angle α, the reactive front propagation velocity S_n, and the density ratio d between fresh reactants and outer-layer gases—have been systematically varied. As a result, additional transition modes have been identified, which are presented in the following sections, after a description of the numerical setup.

2 Computational Framework and Canonical Numerical Setup

The numerical simulations solve the compressible reactive Euler equations using a high-resolution HLLC Riemann solver and a third-order Runge-Kutta integration scheme. The chemistry is modeled by a single-step Arrhenius reaction, calibrated to match realistic ignition delay times of hydrogen-air mixture at an initial pressure of 16 atm. The time evolution of the temperature profiles obtained with homogeneous reactor simulations are presented in Figure 1-left.

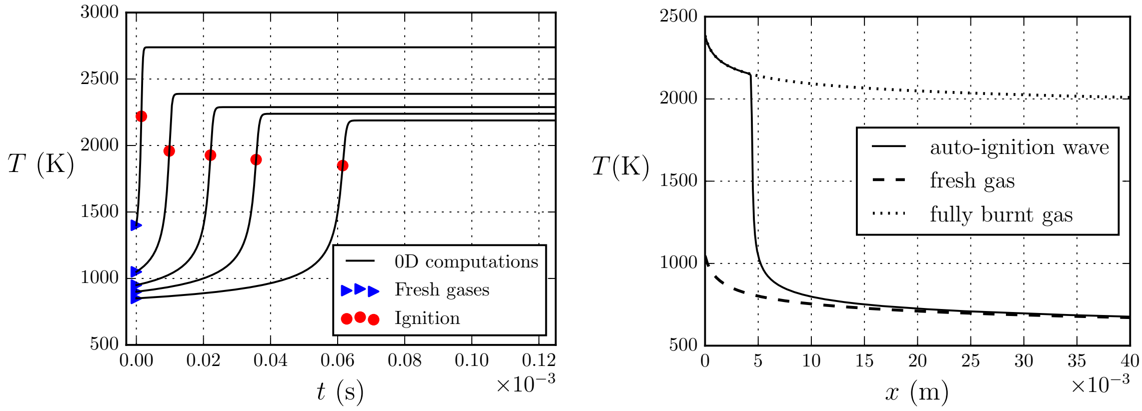

Figure 1: Left: Time evolution of the temperature (solid lines) for different values of fresh gas temperature T_u (blue triangles) obtained from 0-D computations. Right : Initial fresh gas temperature profile (dashed line), given by Eq. 1, leading to a constant speed auto-ignition wave. Corresponding fully burnt gas (dotted line). The solid line is an instantaneous profile. These figures are from reference [12]

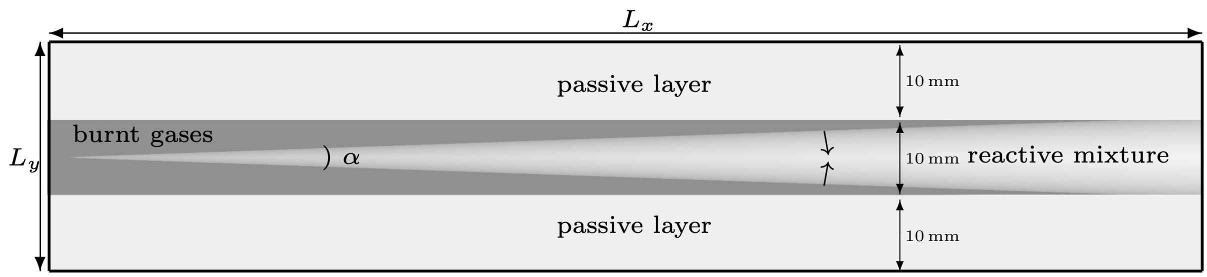

Figure 2: Initial reactive front shape corresponding to a pair of plane auto-ignition waves colliding with the angle α and propagating towards the reactive mixture initially at constant speed.

The core concept of this canonical configuration is to define a perfectly controlled initial condition to maintain a constant low-Mach propagation velocity of auto-ignition fronts. Thus, the fresh gas temperature profile follows a specific profile, see Figure 1-right, that was first defined in a 1D planar case, as proposed in [12]:

$$T_u(x_n) = a/\log\left[(x_n - x_{mr})/(S_n b) + \tau_{mr}/b\right]. \tag{1}$$

Where x_n is the direction normal to the reactive front, x_{mr} is the location of the first ignited point, τ_{mr} the corresponding ignition delay of the most-reactive mixture, S_n is the auto-ignition wave velocity and $a = 8196.2\,\mathrm{K}$ and $b = 3.9830 \times 10^{-9}\,\mathrm{s}$ the coefficient used to express the ignition delay times as a function of fresh gas temperature: $\tau(T_u) = b\exp(a/T_u)$. Unlike traditional approaches where the temperature gradient induces spontaneous acceleration, this method ensures controlled propagation. This previous study showed that the initial movement of the reactive front induced a compression wave, slightly modifying the propagation velocity imposed by the initial profile. However, the results demonstrated that after the passage of this wave, the propagation velocity, although slightly higher, remained constant. Thus, this 1D profile was then used to define the 2D computational domain, which consists of two colliding auto-ignition fronts propagating at a constant velocity, see Figure 2. To mitigate boundary effects, the domain is surrounded by inert layers that isolate the reactive zone from the computational edges. The boundaries are fully transmissive, preventing artificial wave reflections.

The previous study [12] considers multiple collision angles α, ranging from planar ($\alpha = \pi$), then a moderate angle ($\alpha = 2\pi/3$), to sharply acute cases ($\alpha = \pi/45$)) and even $\alpha \to 0$. The objective of this study was to demonstrate that the key parameter for triggering a transition is not the front velocity, but rather the collision point speed, defined as follows: $S_x = S_n/\sin(\alpha/2)$. When the collision point velocity is largely subsonic, no DDT occurs. However, when it becomes supersonic, a DDT appears, even if the fronts themselves remain largely subsonic, and a detonation overtakes the auto-ignition fronts. Only one case of DDT was presented in this initial study [12]. An additional parameter was introduced in this follow-up study: the confinement degree d of the reactive zone, defined as the ratio of the fresh gas density to the inert outer layer density. This parameter influences the efficiency of compression wave reflection on the outer layer. Although the full parametric study is still in progress, we present here the main collision modes that have been identified.

3 Collision Modes

3.1 Quasi-stationary collision structures

For an obtuse collision angle and a low front velocity ($\alpha = 2\pi/3$, S_n =$50\,\mathrm{m\,s^{-1}}$, $d \approx 1.5$), the collision point velocity remains largely subsonic, resulting in a quasi-stationary structure of the reactive fronts and a nearly constant propagation velocity, see the case $\alpha = 2\pi/3$ in [12].

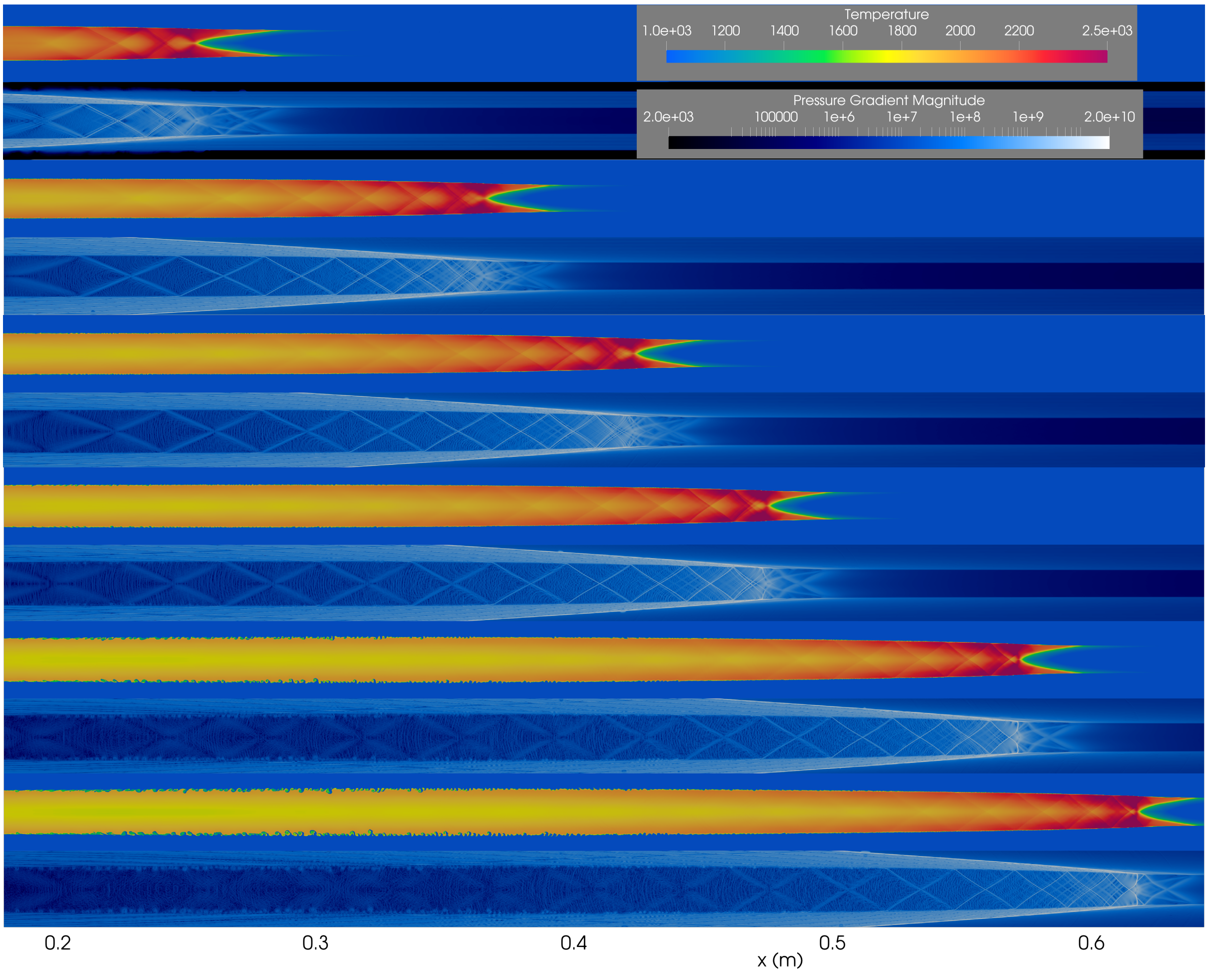

Figure 3: Supersonic quasi-stationary structure: collision point pulling a train of shock waves. Temperature field in K and pressure gradient field in Pa/m

In the opposite case ($\alpha = \pi/45$, S_n =80 $\mathrm{m\,s^{-1}}$, $d \approx 60$), where the collision point velocity is exceeding that of a detonation, a quasi-stationary structure and a nearly constant propagation velocity are also observed (see the results in Figure 3). These results show that the auto-ignition fronts pull a train of shock waves, with the leading precursor shock located in the burned gases just beyond the impact point of the two reactive fronts. Although this is not a detonation, cellular structures very similar to those observed in detonations are observed.

3.2 Plane precursor Shock in Fresh Gas

For an acute angle of $\alpha = \pi/45$, a front propagation velocity of $S_n = 50$m/s and a confinement degree of 1.5, a hot spot appears within the fresh gas cone, acting as the precursor to the DDT (see [12]).

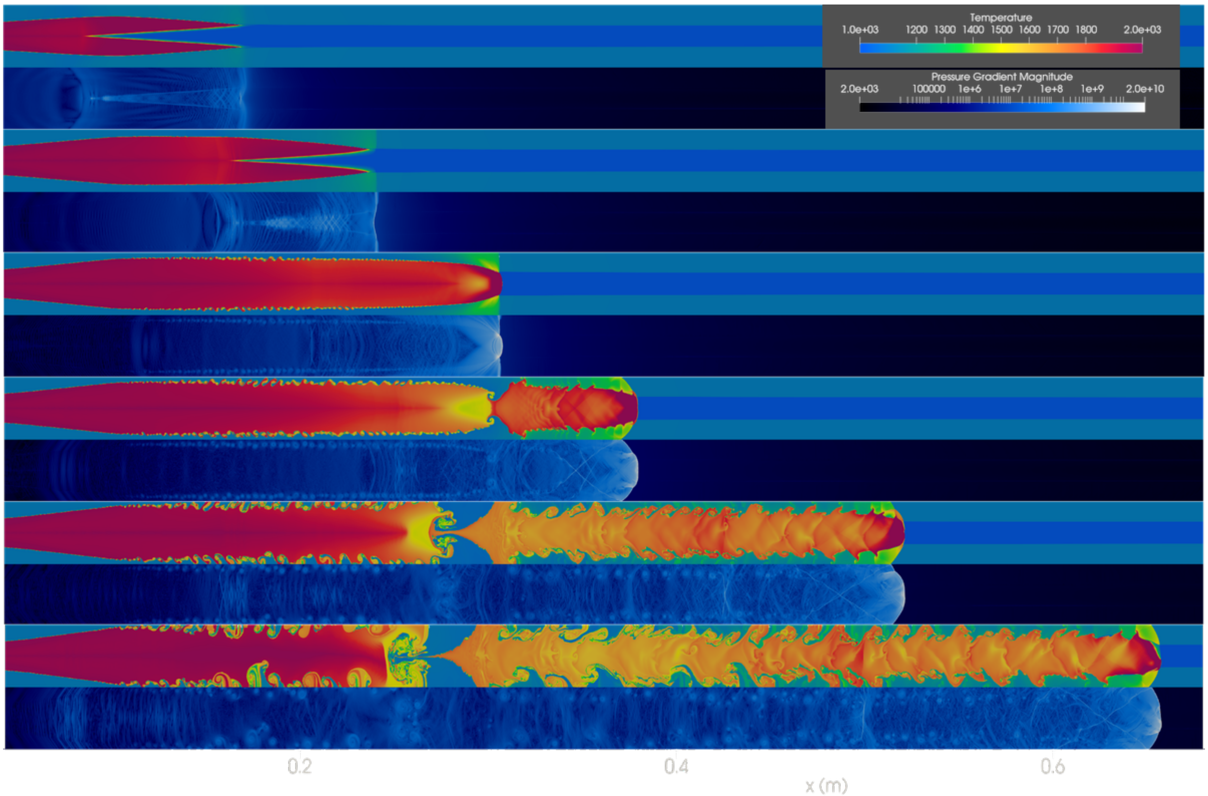

Figure 4: Plane precursor Shock of DDT at the entrance of the fresh gas cone. Temperature field in K and pressure gradient field in Pa/m

The parametric study conducted here shows that the position of the hot spot within the cone depends on the collision point velocity and of the confinement degree. Thus, the transition can occur at the entrance of the fresh gas cone, taking the form of a planar shock rather than a localized hot spot, see Figure 4 where the following set of parameters have been used: $\alpha = 3\pi/90$, S_n =50 $\mathrm{m\,s^{-1}}$, $d \approx 0.75$. In this figure, it can be observed that this planar transition leads to a large vortical structure in the burned gases. Additionally, this result shows that the confinement degree significantly influences the expansion of the burned gases.

3.3 Precursor Shock in Burnt Gas

Thus, another set of parameters ($\alpha = \pi/45$, S_n =70 $\mathrm{m\,s^{-1}}$, $d \approx 60$) can also lead to a scenario where the hot spot, acting as the precursor to the DDT, forms in the burned gases just behind the impact point, see Figure 5. The resulting shock rapidly becomes planar, and as the collision point velocity is lower than the detonation velocity, the detonation overtakes the impact point and gradually propagates through the entire fresh gas cone until no further auto-ignition waves remain.

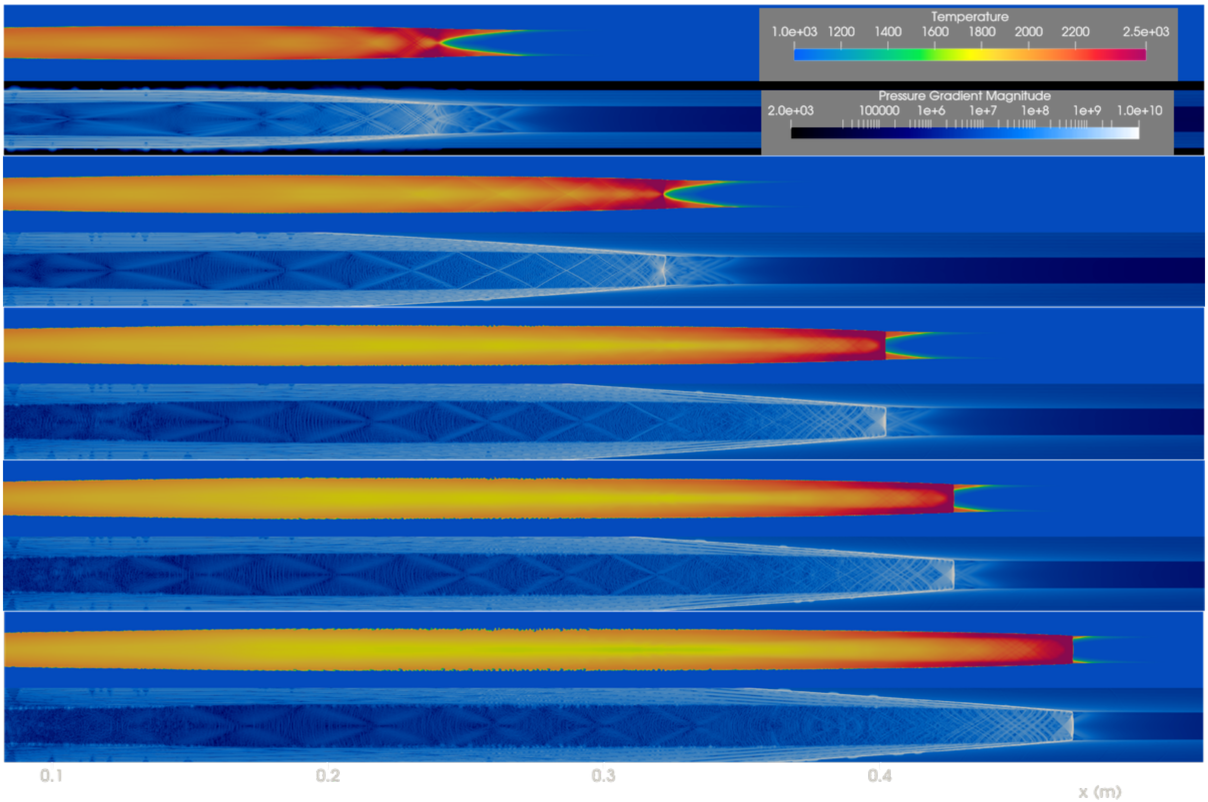

Figure 5: Hot spot precursor of DDT at the burned gas side of the collision point. Temperature field in K and pressure gradient field in Pa/m

3.4 Multiple Precursor Shocks and Conclusions

This canonical configuration, defined by three parameters (S_n, α, d), allows for the exploration of a wide range of transition scenarios, providing insights into phenomena observed in more realistic numerical simulations [13] and even in experiments. For instance, Figure 6 presents a particularly intriguing case ($\alpha = 3\pi/90$, $S_n = 50\,\mathrm{m\,s^{-1}}$, $d \approx 6.5$) where multiple hot spots appear almost simultaneously in the fresh gases. As a result, the reactive layer is pinched at several locations, ultimately leading to the formation of fresh gas pockets.

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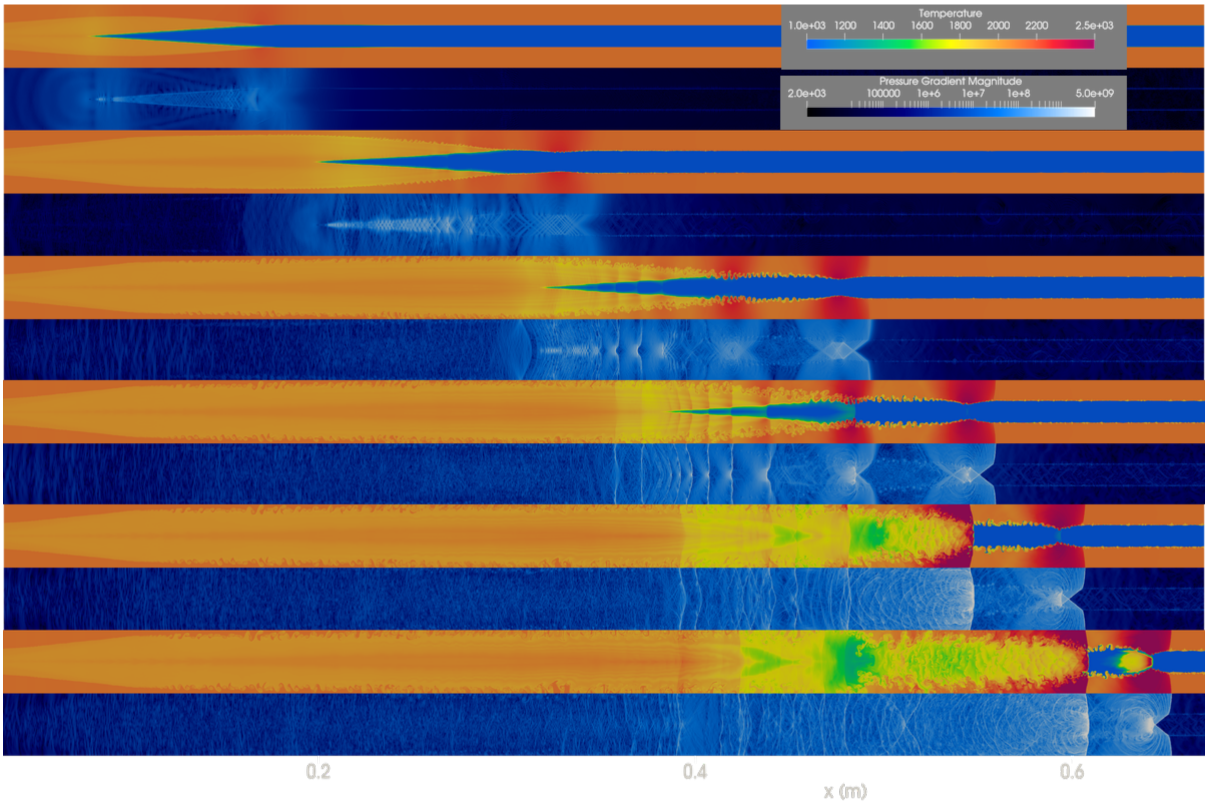

Figure 6: Multiple Precursor Shocks and fresh gas pockets formation. Temperature field in K and pressure gradient field in Pa/m

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