On Chapman-Jouguet deflagrations

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Abstract

While the Chapman-Jouguet (CJ) criterion for predicting the detonation speed is well established, the same criterion also predicts CJ deflagrations. From purely thermodynamic and gasdynamic considerations, one can also define a CJ deflagration speed, with a corresponding limiting characteristic. The speed of deflagration waves observed in practice, however, is significantly lower than this value, and is dictated by the rate at which heat and species diffuse across the reaction front. In the presence of turbulence, however, the flame speed may be significantly enhanced. We isolate experimentally such CJ deflagrations following the interaction methane-oxygen detonation interaction with a column of cylinders. A self-similar multiple discontinuity model similar to previously proposed models by Chao and Chue et al. with an embedded CJ deflagration is formulated, and the results are found in excellent agreement with the experiments. Detailed flow visualization of the dynamics of these high speed deflagrations illustrate that they undergo a continuous amplification process. The front organizes into fewer modes and culminates with one of them being sufficiently strong to trigger a detonation.

1 Introduction

Detonation waves propagate at a speed dictated by thermodynamic and gasdynamic considerations. Within the reaction zone, pressure waves are continuously amplified and sustain the motion of the leading shock front [1, 2]. At the end of the reaction zone, a limiting characteristic propagates at a speed equal to $u + c$, which needs to coincide with the speed of the leading front D; here u is the particle velocity in the laboratory frame and c is the local sound speed. Along the path of this limiting characteristic, no net energy is released. This wave isolates gas-dynamically the reaction front from the trailing flow field. The simultaneous vanishing of the exothermicity with the sonic flow in the frame of the wave motion is the so-called generalized Chapman-Jouguet (CJ) criterion. This criterion has been very successful in predicting the detonation speed of detonations with area divergence, frictional losses, multiple competing reactions and turbulence [3].

From purely thermodynamic and gasdynamic considerations, one can also define a CJ deflagration speed [3], with a corresponding limiting characteristic (sonic outflow in the wave fixed frame). The speed of deflagration waves observed in practice, however, is significantly lower than this value, and is dictated by the rate at which heat and species diffuse across the reaction front. In the presence of turbulence, however, the flame speed may be significantly enhanced. For sufficiently high burning rates, exceeding the CJ deflagration speed, there is a strong experimental evidence that gasdynamic choking controls the deflagration propagation, as anticipated from purely gasdynamic considerations [4]. Such gasdynamic choking has also been observed in numerical simulations of deflagration to detonation transition [5] for flame speeds exceeding the CJ deflagration wave speed in a turbulent flow field. In experiments of flame propagation in obstacle laden tubes, where the obstacles generate their own large scale disturbances and turbulence, the reaction front also propagates at a speed close to the sound speed in the combustion products - known as the choking regime [3, 6, 7]. This regime corresponds to a turbulent reaction zone driving a shock ahead of it. Since the local post-reaction gas speed u observed is close to zero, the speed of these waves is thus well predicted by the speed of a limiting characteristic compatible with the CJ deflagration hypothesis [8].

Most observations of fast reaction waves compatible with a CJ deflagration have been made for obstacle laden tubes, leading to auto-ignition spots by wave reflections [9] or other forms of externally induced turbulence, such as shock-flame interactions [10] or transverse pressure wave generation in rough walled tubes [11]. There is however evidence that *flame-generated* turbulence may also permit to sustain such high speed deflagrations in smooth tubes. Simulation of flame acceleration in smooth narrow channels predict that precursor CJ deflagration waves can form as intermediate quasi-steady-states prior to the detonation formation [12]. Chao also showed that when a detonation wave interacts with a perforated plate, a meta-stable supersonic wave is formed downstream of the plate, which propagates at constant supersonic speed [13] before transiting to a detonation. Chao also speculated that these waves may be CJ deflagrations. Grondin and Lee [14] and Maley et al. [15] also observed such high speed meta-stable waves in a similar set-up.

In the present work, we extend the experiments reported by [13–15] for detonation interaction with a perforated plate and determine whether the transmitted meta-stable waves are CJ deflagrations. This set-up provides the least ambiguous setting for modeling the flow field, since the transmitted wave propagates unimpeded by obstacles. The assessment of whether these waves are CJ deflagrations is made on the basis of an analysis of the wave interactions using multiple discontinuities. The closed-form gasdynamic model formulated is similar to the one formulated by Chao [13], although Chao's model had one adjustable parameter for the dissipation in the choked under-expanded jets, which we treat in closed form by gasdynamic considerations following [16–18]. The paper is organized as follows. First, we report the results of the experiments, followed by the model formulation and validation with experiments and numerical simulations.

2 Experiments

The experiments were conducted in a 3.5-m-long thin rectangular channel, 203-mm-tall and 19-mm-wide, as described by Maley et al. [15]. The last meter of the channel was equipped with glass windows allowing to visualize the flow evolution by via high-speed large scale shadowgraphy. A row of cylindrical obstacles of 16-mm-diameter were placed at the entrance of the visual section of the shock tube to allow for visualization of the fast flames established downstream. The mixture studied was stoichiometric methane-oxygen. The gases were mixed in a separate vessel and left to mix for a minimum of 24 hours before an experiment. Varying the initial pressure, p_0, of the test mixture permitted us to control the reactivity of the mixture.

Figure 1 shows the interaction of a multi-headed detonation wave with the row of cylinders at an initial pressure of $p_0 = 3.4$ kPa. Frames *a* to *e* show the multi-headed detonation prior to its interaction with the row of cylinders. Following the detonation interaction with the cylinders, multi-headed wave interactions occur as each wavelet exits from each hole and reflects with shocks from neighboring holes - see Maley et al. and Bhattacharjee et al. for a detailed study of these wave interactions [15, 19]. Frames k through r show the organization of the front into fewer stronger modes. Auto-ignitions are observed behind the strongest portion of the front, such as the bottom of frame o. These amplification events give rise to a structure that is very similar to the detonation structure, albeit on much larger scales [20]. The volumetric expansion of the gases undergoing rapid ignition drive strong perturbations on the resulting burning fronts, which become significantly wrinkled. For reference, the speed of the front, recorded along the center-line of the channel is shown in Fig. 2. The transmitted wave has a speed of approximately 1500 m/s.

A further increase in pressure yielded more prompt amplification of this meta-stable fast deflagration. Figure 3, for example, shows the structure of the transmitted wave at an initial pressure of $p_0 = 9.1$ kPa. Following the interaction of the incident detonation on the row of cylinders, a thick wave structure is established with the characteristic triple shock interactions driven by the cylinders. As the wave travels further downstream, fewer stronger modes are established. The amplification is more rapid, owing to the fact that the kinetics are faster at this higher pressure (and hence higher density and faster molecular collision rates). Near the end of the channel, one of the modes becomes sufficiently strong to cause the onset of detonation near the top wall. This onset of detonation is also marked by a transverse detonation wave propagating through the shocked un-reacted gas. By the end of the channel, the entire front propagates as a detonation wave. The speed of the front, recorded along the center-line of the channel is shown in Fig. 2. While the incident wave has a velocity close to the CJ detonation speed, the transmitted wave has an average speed of approximately 1750 m/s, and displays much stronger fluctuations, before the final establishment of a detonation. Further increase of the initial pressure lead to more rapid amplification.

3 Self-similar gasdynamic model

The transmission of a detonation wave is modeled following previous work performed for inert shock transmission across a perforated plate [16–18]. A sketch of the quasi-one-dimensional model is shown in Figure 4. The incident wave *I* is assumed to give rise to a reflected shock *R*, and a transmitted shock *T*. The over-expanded sonic jet flow exiting through the pores, which is characterized by a series of shock diamonds, is modeled by an auxiliary shock *A*. The jet head, separating the gases which were originally on the left of the obstacle row, from the gases on the right, are modeled by a contact surface. The flow from state 2 to state 3 is assumed to be isentropic nozzle flow, while the shock transitions obey the usual shock jump relations. In the inert case, the deflagration wave *F* is not present and states 5 and 6 are identical. In the reactive case, the jump conditions across the flame obey the usual Hugoniot jump conditions [3, 8]. In the past, this model has been shown to be quite successfull in capturing the attenuation of inert shocks passing over wire screens and other obstacles [16–18]. We have further validated the model using numerical simulations for a perfect gas in the inert case, for which we found excellent agreement.

For the reactive case, following the work of Chue et al. [8], we use a two-gamma approximation, where the non-reacted and reacted gases are assumed to be polytropic gases with constant thermodynamic properties (i.e., constant isentropic exponents). The burned post detonation state (State 1) was assumed to be the CJ detonation state, and was computed using the NASA CEA code. The isentropic exponent γ for the burned gases, assumed constant for states 1 through 5 was evaluated from exact thermal equilibrium calculations at the computed state 1. The unburned isentropic exponent γ was evaluated at state 0. The heat release Q required for the calculation of the jump conditions across the deflagration F was estimated from the detonation jump conditions such that the correct Mach number is recovered.

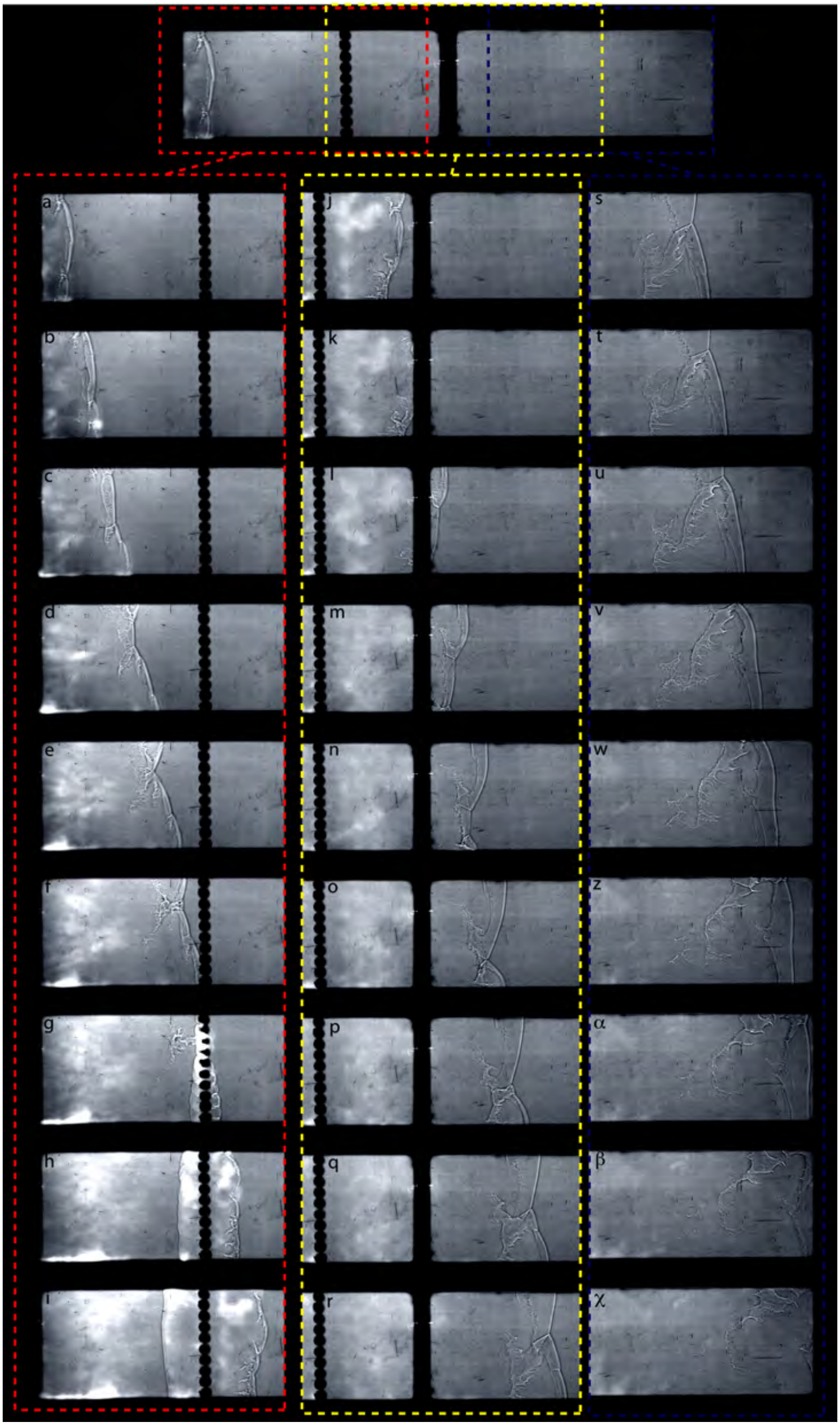

Figure 1: Detonation transmission through a row of cylinders as a fast speed deflagration in methane-oxygen at $p_0 = 3.4$ kPa; note the front organization into fewer stronger modes.

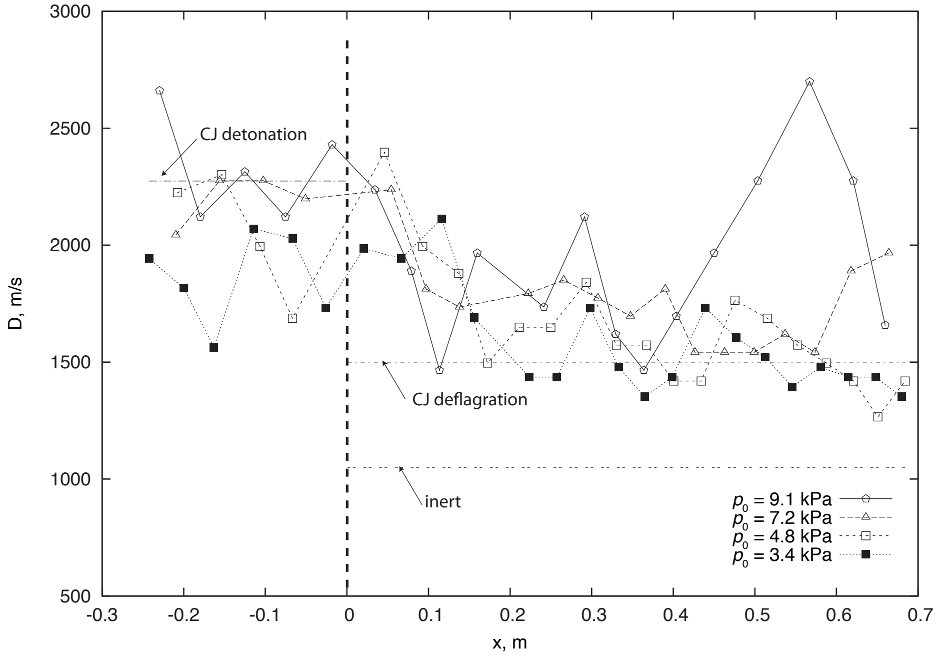

Figure 2: Speed of the front recorded along the channel center-line and comparison with the predicted transmitted wave speeds assuming an internal CJ deflagration or inert propagation.

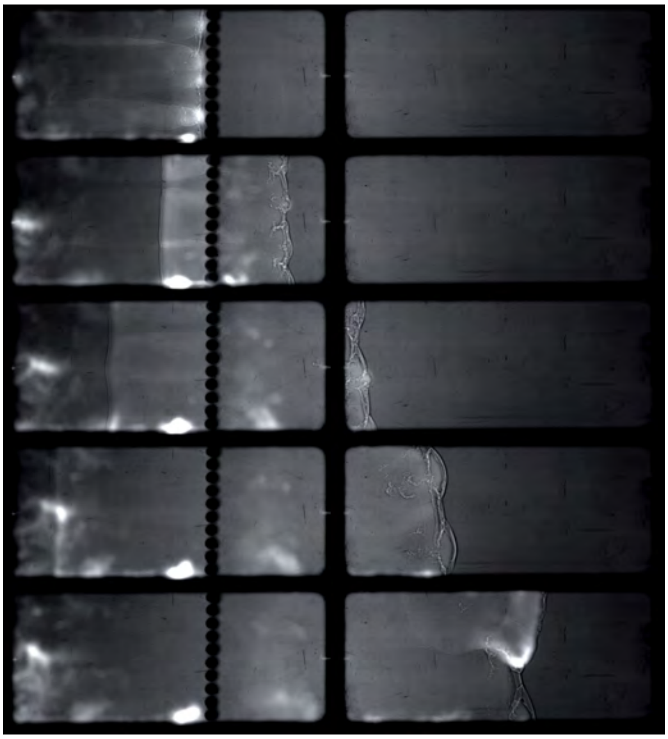

Figure 3: Detonation transmission through a row of cylinders as a fast speed deflagration in methane-oxygen at $p_0 = 9.1$ kPa.

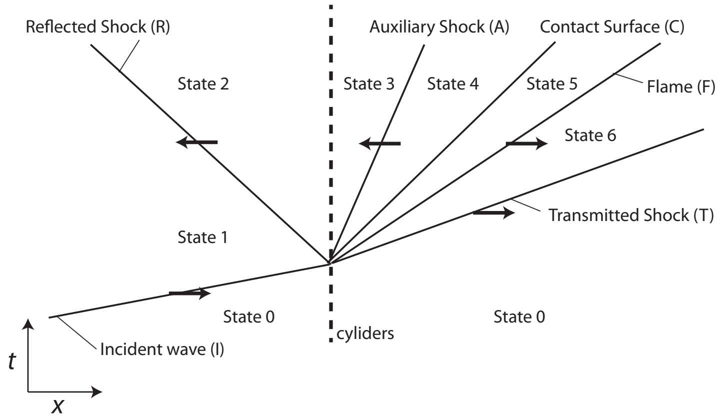

Figure 4: Space time diagram illustrating the self-similar gasdynamic model for a detonation interaction with a row of cylinders.

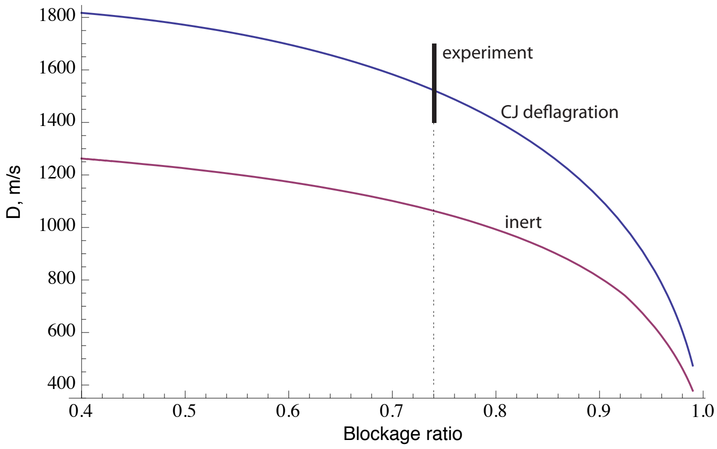

Figure 5: Predicted transmitted shock speed for the reactive case assuming an inner CJ deflagration or inert shock as a function of the obstacle blockage ratio for $p_0 = 7.2$ kPa.

Figure 5 shows the predicted speed of the transmitted shock in terms of the blockage ratio of the cylinder row. The two curves shown are for the flame F taken as a CJ deflagration and for an inert case, where no reactions occur downstream of the row of cylinders. The results corresponding to the two solutions are also shown in Fig. 2, for comparison with the experimental data for the blockage ratio of 0.75 used in the experiments. The comparison between the model and experimentally measured transmitted shock speed is very good. The speed of the transmitted shock in the presence of a CJ deflagration is 1500 m/s, in excellent agreement with the experimental measurements. This strongly suggests that the transmitted waves can indeed be modeled as CJ deflagrations.

4 CJ deflagration structure

The structure of the high speed deflagrations resembles that of unstable CJ detonations [20]. The front has a cellular structure, with its evolving triple shock reflections and complex flow at the surface of unburned pockets. The front is found to have a tendency to organize into stronger fewer modes - as first observed by Radulescu et al. [21] in similar experiments. This is not surprising, since compressible turbulence tends to display an inverse energy cascade, where compression waves of the same family tend to form fewer stronger ones [22]. In the context of high speed deflagrations, this organization into fewer stronger modes gives rise to local ignition spots, which then drive further instabilities [20].

That the transmitted deflagration waves propagate at a speed very close to that predicted by assuming a CJ inner deflagration suggests that a limiting characteristic exists, which isolates the deflagration dynamics from the following flow. Based on this observation, it can be speculated that these waves propagate similar to detonation waves [1]. The wave structure would correspond to the continuous amplification of pressure waves from the back the deflagration toward the front. The reactive field amplifies these waves, which in turn support the leading front. The last pressure wave at the end of the reaction zone is the limiting characteristic, which does not get any amplification. Its speed thus sets the speed of the deflagration structure.

The fact that the waves observed correspond to CJ deflagrations, and the front does not propagate at the CJ detonation speed, further clarifies the main ignition mechanism in these waves. In CJ detonations, the lead front triggers the ignition sequence by auto-ignition, and the limiting characteristic is thus in phase with the front. For CJ deflagrations, the lead shock is only a consequence of the rapid burning within the reaction zone, since the ignition delays behind the lead shock are a few orders of magnitude larger than required for a coherent propagation [15]. For this reason, the lead shock is only weakly coupled with the trailing flow, hence permitting to establish a quasi-steady state [8].

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