# Comparison of models predicting the mode of ignition behind reflected shock waves in the context of DDT

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#### 1 Introduction

The phenomenon of deflagration-to-detonation transition (DDT) has been widely studied experimentally, numerically and analytically. Flame acceleration processes, leading up to the critical conditions for onset of detonation, depend largely on the specific geometry considered. Effects such as flame and flow instabilities, turbulence-flame and shock-flame interactions need to be captured to model flame acceleration accurately. These effects contribute to a different extent in different mixtures and geometries so that a generalized description of flame acceleration is not expedient. However, there may exist a common mechanism accomplishing the actual onset of detonation: The notion that the onset relies on a gradient mechanism independent of the geometric situation has been stated [1, 2].

A central interest is to predict the critical conditions for onset of detonation. Historically, the observation has been made that flames in closed tubes need to accelerate to flame speeds near the speed of sound in the burned mixture for onset of detonation to occur [3]. Note that the accuracy of flame speed measurements largely depends on the type of diagnostics applied, which can vary from coarse point-measurements of flame arrival (photo-diodes, ionization probes, thermocouples, etc.) to high-speed optical measurements. Although this empirical criterion is not directly tied to the physics of the onset process, it is widely referred to. However, at large scale without significant confinement [4], in medium-scale semi-confined situations [5], and in highly reactive mixtures [6], onset of detonation has been reported at lower instantaneous flame speeds, as low as speed of sound in the unburned mixture.

In obstructed tubes, the most common mechanism leading to the onset of detonation is the reflection of precursor shock waves at obstacles and channel walls, causing local strong ignition [7, 8]. This mechanism can be isolated and studied scientifically in shock tubes. A critical incident shock Mach number can be obtained leading to onset of detonation upon shock reflection. For simplicity, we consider normal reflection of shock waves from flat walls. It is well known that reflection from concave surfaces such as parabolic reflectors [9, 10] leads to higher local pressures and temperatures, promoting the initiation of detonation. This needs to be considered in practical analyses. However, normal shock wave reflection represents a scientifically simple and historically well-documented configuration and thus an appropriate vehicle to study ignition modes from shock reflection. This work analyzes models from literature for the prediction of ignition mode behind reflected shock waves in the context of DDT.

# 2 Ignition by reflected shock waves

Two modes of ignition behind reflected shock waves are distinguished: Strong (sharp) and weak (mild) ignition. These modes have first been named by Voevodsky and Soloukhin [11]. To establish a clear terminology, we shall call ignition "strong" if detonation is initiated directly at the reflecting wall upon shock reflection, whereas "weak" ignition will refer to the initiation of deflagration. Alternatively, the term strong ignition is often used to identify reaction occurring homogeneously at the reflecting wall, whereas weak ignition shows reaction taking place in distributed ignition kernels away from the reflecting wall. It is known that also weak ignition can lead to delayed detonation originating from individual ignition kernels. This regime is understood as a transition between weak and strong ignition.

Several groups have suggested models and parameters to predict the mode of ignition behind reflected shock waves. These models assume different physical mechanisms being responsible for controlling the ignition mode.

Voevodsky and Soloukhin [11] argued that in hydrogen-oxygen mixtures, the ignition mode may depend upon the dominating chemical pathway during the induction period: At high temperature, branchedchain reaction dominates, whereas at lower temperature a straight chain involving HO<sub>2</sub> and H<sub>2</sub>O<sub>2</sub> dominates. The extended second explosion limit [12] delineates branched and straight-chain reaction. Voevodsky and Soloukhin suggested that strong ignition requires branched reaction. This notion has also been supported by Belles [13] in his study on mixture detonability and adopted, for example, by Ng et al. [14].

Meyer and Oppenheim [15, 16] introduced a coherence theory which predicts strong ignition if chemical reaction rates exhibit a sufficiently low sensitivity on temperature. For stoichiometric hydrogen-oxygen mixture, strong ignition was observed experimentally if  $(d\tau_{ign}/dT)_p \gtrsim -2 \,\mu s/K$ .

Grogan and Ihme [17] proposed that shock wave bifurcation due to the interaction of the shock wave reflected at the closed end of a tube and the wall boundary layer generates non-uniformity leading to weak ignition. They postulated a Damköhler number for shock wave bifurcation,  $Da_{bif} = \tau_{bif}/\tau_{ign}$ , which compares the shock bifurcation time scale,  $\tau_{bif}$ , to the ignition delay time,  $\tau_{ign}$ , where  $\tau_{bif} = D/(4u_2h'_{bif})$ , D denoting the tube diameter,  $u_2$  the flow velocity behind the incident shock wave, and  $h'_{bif}$  the bifurcation foot height growth rate, which is assumed constant and given by a modified empirical correlation based on Petersen and Hanson [18]. The authors found in simulations and comparisons with experiments from other groups that bifurcation leads to weak ignition for  $Da_{bif} \leq 1$ ; Strong ignition occurs for  $Da_{bif} \gtrsim 1$ .

For the specific case of normal shock reflection at a flat-plate obstacle mounted at a channel wall, which is a typical case studied in DDT experiments, Thomas et al. [19] argued that onset of detonation occurs if the ignition delay time behind the reflected shock wave is sufficiently short, compared to the velocity of the expansion wave (equal to the speed of sound in the post-reflected shock gas) originating at the obstacle corner traveling along the obstacle face. The authors proposed the parameter  $\eta = h/(a_r \tau_{ign})$ , where h is the obstacle height and  $a_r$  is the speed of sound in the gas behind the reflected shock wave. This parameter can be interpreted as a Damköhler number for expansion. In experiments, the parameter  $\eta$  needed to exceed a value of 3 for onset of detonation to occur upon shock reflection at a flat-plate obstacle.

### 3 Discussion

The models introduced in sec. 2 can be evaluated to obtain predictions for the critical Mach number of an incident shock wave causing strong ignition upon normal reflection. This evaluation is performed



Figure 1: Critical incident shock Mach number leading to strong ignition upon shock reflection, according to models introduced in sec. 2, for a stoichiometric hydrogen-air mixture at  $T_1 = 298.15$  K.

here for a stoichiometric hydrogen-air mixture at various initial pressures using the reaction mechanism by Ó Conaire et al. [20]. The effect of dilution as well as other fuels will be studied in the full-length paper.

Figure 1 shows that the extended second explosion limit criterion (circle symbols) predicts a monotonic increase of critical Mach number from 2.4 ( $p_1 = 5$  kPa) to 3.1 ( $p_1 = 101.3$  kPa). Meyer and Oppenheim's sensitivity parameter (evaluated for temperature sensitivities -1, -2 and -5  $\mu$ s/K, square symbols) predicts higher values than the explosion limit criterion at initial pressures  $p_1 \leq 20$  kPa, and lower values at higher initial pressure. A maximum in critical Mach number occurs at initial pressures around 60 kPa. At initial atmospheric pressure,  $p_1 = 101.3$  kPa, the critical Mach number ranges between 2.7 and 2.8. Interestingly, although based on a different physical understanding, Grogan and Ihme's bifurcation criterion (diamond symbols) shows very similar qualitative and quantitative results if evaluated for typical laboratory dimensions for tubes, 0.02 m < D < 0.1 m. Also Thomas' expansion criterion (star symbols), evaluated for obstacle heights 0.05 m < h < 0.2 m, results in similar critical Mach numbers in both models. For small geometric dimensions both criteria predict an increase in critical Mach number towards low pressure at high temperatures for hydrogen-air.

The understanding that the chemical pathway dominates the ignition mode has been questioned by Yamashita et al. [21]. The authors investigated shock-induced ignition of stoichiometric acetylene-oxygen mixture at laboratory scale and low pressure using high-speed optical diagnostics and numerical simulation. A gradual transition from weak to strong ignition was observed with increasing incident shock Mach number, which was characterized in terms of distance of ignition from the reflecting wall. No significant change in activation energy was observed between the ignition regimes. Qualitative

agreement of experimental data with Meyer and Oppenheim's sensitivity parameter was found with critical  $-1.0 \,\mu\text{s/K} \le (d\tau_{ign}/dT)_p \le -0.5 \,\mu\text{s/K}$ . However, their results were also reproduced at reasonable accuracy by Grogan and Ihme's bifurcation criterion [17].

It is evident from this comparison of models that the unambiguous validation of either model for strong ignition requires a variation of initial pressure and geometric scale. This has not been accomplished so far. Studies by Voevodsky and Soloukhin [11], Meyer and Oppenheim [15, 16], Grogan and Ihme [17] and Thomas et al. [19] were limited to low initial pressures around 10 kPa and laboratory scale. Experiments at higher pressures and larger scales are challenging, especially since optical visualization is desirable to clearly resolve ignition locations and the dynamics of detonation initiation.

In less confined situations at larger scale onset of detonation has been observed at low flame speeds well below the speed of sound in the burned products [4, 5]. At first sight this indicates that ignition by precursor shock wave reflection may not play a crucial role in these experiments since shock waves are expected to be weak. However, local flame acceleration effects may not be captured by large-scale instrumentation; It is not evident that no strong shock waves are formed locally and lead to the onset of detonation. Local instrumentation may help answer the question regarding the onset mechanisms dominating at larger scale. Similarly, experiments in highly reactive mixtures [6] showed onset at low instantaneous flame speeds. Due to the extreme local flame acceleration rates in such mixtures it cannot be inferred without doubt from these experiments whether localized shock reflection phenomena play a key role or not.

# 4 Conclusions

The present discussion concerned detonation initiation by shock reflection (strong ignition) as the final stage of deflagration-to-detonation transition as typically observed in obstructed tubes. Detonation initiation was treated in isolation from the flame acceleration process. Normal shock reflection at a flat wall was considered.

The discussion focused on the question of which fluid-mechanic, gas-dynamic and chemical-kinetic effects govern the mode of ignition upon shock reflection and eventually determine whether detonation is initiated directly. For this purpose, theoretical models from the literature were analyzed. These models by (i) Voevodsky and Soloukhin, (ii) Meyer and Oppenheim, (iii) Grogan and Ihme and (iv) Thomas et al. considered different mechanisms to determine the ignition mode: (i) the dominating chemical pathway, i.e., branched-chain vs. straight-chain reaction; (ii) sensitivity of ignition delay time on temperature; (iii) time-scale comparison between shock bifurcation and ignition delay; and (iv) time-scale comparison between expansion and ignition delay for shock reflection at flat-plate obstacles.

Critical incident shock Mach numbers leading to strong ignition based on these models were determined for a stoichiometric hydrogen-air mixture at initial pressures between 5 and 101.3 kPa and an initial temperature of 298.15 K. Initial pressure affects the results in all models, but only models (iii) and (iv) take into account the effect of geometric scale. A clear validation of any model requires the variation of initial pressure and geometric scale. A gradient mechanism acting during the onset of detonation was not considered by any of these models.

Future work may target a validation of models for strong ignition as part of an effort to better understand and predict deflagration-to-detonation transition. Eventually, a main question is which physical effect provides a lower bound for strong ignition by shock reflection, independent of geometric scale. Both experiments and numerical simulations may be interpreted regarding the critical conditions required to achieve transition to detonation. In addition, the intermediate regime between weak and strong ignition, where detonations occur due to a secondary DDT process, should be studied in the context of DDT due to its high practical (safety) relevance.

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