# Controlling Parameters for Detonation Re-initiation After Interaction with Cylinders in Hydrogen and Hydrocarbon Mixtures

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## 1 Introduction

Understanding the behavior of detonation transmission across a bank of cylinders is critical for both detonation physics and applications related to the design of detonation arrestors. Upon passing through the obstacles, the detonation waves generally go through a sequence of local diffraction and reflection processes at each pore between the obstacles [1–3]. This behavior is similar to the propagation of a detonation through porous media or perforated plates. However, the configuration of a bank of cylinders provides more detailed observation of the local wave dynamics during the passage of the detonation. The diffraction process cools down the gas in the reaction zone and leads to a decouple of the shock and the flame interface, while the local shock reflection immediately beyond the obstacles further enhance the shock strength. Depending on the mixture sensitivity, the detonation wave can exhibit different behaviors: it may successfully transmit, decouple during diffraction yet re-initiate from Mach reflections, quench during diffraction but experience hot-spot ignition behind the Mach shock, or undergo complete quenching following the interaction with obstacles. Understanding the mechanism of the re-initiation of the failed detonation is not only important in the applications in detonation arresting configurations. The acceleration of the shock-flame complex obtained through the interaction of a detonation wave with obstacles also resembles the last stage of the deflagration to detonation transition (DDT). At this stage, the mechanism for the fast flame propagation is presently not well understood, sometimes even referred to as a “strange wave” [4].

Over the past decade, extensive experiments have been conducted by Radulescu and his students using the detonation-obstacles interaction to isolate the high-speed waves without relying on a prior low speed flame acceleration. The original interest was motivated by understanding the mechanisms of fast flames acceleration into detonation waves, as the configuration can reproducibly form the shock-flame complex prior to the onset of a detonation. They found that for most hydrocarbon mixtures, the quenched detonation can re-amplify after traversing a substantial distance past obstacles, with the turbulent reaction zone structure closely coupled with the leading shock [3,5–7]. This re-amplification has been demonstrated to correlate well with the mixture sensitivity parameter $\chi$. However, later observations suggested that such fast deflagration waves are not possible in hydrogen mixtures [5,7], despite having a very large $\chi$ which

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Table 1: Experiments Conducted. $d$ and $n_{obs}$ represent the obstacle diameter and number. $L_{DDT}$ is the detonation re-initiation length, and $n_M$ is the number of Mach reflections before re-initiation.

| Mixtures | BR | $d$ (mm) | $n_{obs}$ | Ref. | $L_{DDT}$ (m) | $n_M$ | $P$ (kPa) |
|---|---|---|---|---|---|---|---|
| $CH_4$+$2O_2$ | 75% | 152.25 | 1 | [5,9] | 0.84 | >3 | 6.9 |
| $CH_4$+$2O_2$ | 75% | 30.45 | 5 | [5,9] | 0.91 | >3 | 6.9 |
| $CH_4$+$2O_2$ | 75% | 15.23 | 10 | [6,10] | 0.45 | >3 | 7.6 |
| $CH_4$+$2O_2$ | 90% | 2.03 | 10 | [6,10] | 0.87 | >3 | 13.1 |
| $C_2H_6$+$3.5O_2$ | 75% | 15.23 | 10 | [6,10] | 0.54 | >3 | 4.1 |
| $C_2H_6$+$3.5O_2$ | 90% | 2.03 | 10 | [6,10] | 0.51 | >3 | 9.6 |
| $C_2H_4$+$3O_2$ | 75% | 15.23 | 10 | [6,10] | 0.6 | >3 | 4.1 |
| $C_2H_4$+$3O_2$ | 90% | 2.03 | 10 | [6,10] | 0.62 | >3 | 7.0 |
| $C_3H_8$+$5O_2$ | 75% | 15.23 | 10 | [6,10] | 0.38 | >3 | 3.8 |
| $C_3H_8$+$5O_2$ | 90% | 2.03 | 10 | [6,10] | 0.58 | >3 | 6.3 |
| $C_2H_2$+$2.5O_2$ | 75% | 15.23 | 10 | [8] | 0.33 | >3 | 1.5 |
| $C_2H_2$+$2.5O_2$+10.5Ar | 75% | 15.23 | 10 | [6,10] | 0.27 | 1 | 10.1 |
| $C_2H_2$+$2.5O_2$+10.5Ar | 90% | 2.03 | 10 | [6,10] | n/a | n/a | No re-intiation up to 17.9 kPa |
| $2H_2$+$O_2$ | 75% | 152.25 | 1 | [5,9] | 0.36 | 1 | 12.4 |
| $2H_2$+$O_2$ | 75% | 30.45 | 5 | [5,9] | n/a | n/a | No re-intiation up to 18.6 kPa |
| $H_2$+$O_2$ | 60% | 30.45 | 4 | [8] | 0.14 | 1 | 8.9 |
| $1.5H_2$+$N_2O$+$O_2$ | 75% | 30.45 | 5 | New | 0.28 | <=3 | 11.7 |
| $H_2$+$N_2O$ | 75% | 30.45 | 5 | New | 0.76 | >3 | 13.4 |
| $H_2$+$N_2O$ | 67.5% | 30.45 | 4.5 | New | 0.074 | <=3 | 7.6 |

favors the re-amplification process. Their experiments also showed that in mixtures with slightly lower sensitivities, i.e. lower initial pressures, ignition was altogether quenched. Yang et al. [8] suggested that due to the unique chain-branching characteristic of the hydrogen mixtures, the post-shock temperature falls into the chain branching cross-over ignition limit after past the obstacles. In this regime, the very long $t_i$ suppresses auto-ignition, while the high isentropic exponent $\gamma$ of hydrogen mixtures prevented further convective mixing required for re-initiation.

This paper aims to re-examine this problem by reviewing all the experiments in Radulescu group, supplemented with new experimental data. Table 1 listed the related mixtures reviewed in this study. In the new set of experiments, the oxygen in the hydrogen mixture was partly or fully replaced by nitrous oxide, which will support combustion to the same extent as oxygen yet has a lower isentropic exponent. The addition of the nitrous oxide serves to lower the isentropic exponents of the hydrogen mixtures to be similar to the oxi-hydrocarbon mixtures, while maintains the same orders of ignition delay times. The objective is to elucidate the parameters controlling the re-initiation of the failed detonation after interaction with obstacles in both hydrogen and hydrocarbon mixtures.

## 2 Experimental Details

All the experiments were conducted in a shock tube with dimensions of 3400 mm × 19.1 mm × 203.2 mm, as detailed in many of the references listed in Table 1. The last meter of the channel was equipped with glass windows allowing for schlieren and shadowgraph visualization. A bank of cylindrical and half-cylindrical obstacles was evenly placed at the beginning of the visualization section. As shown in

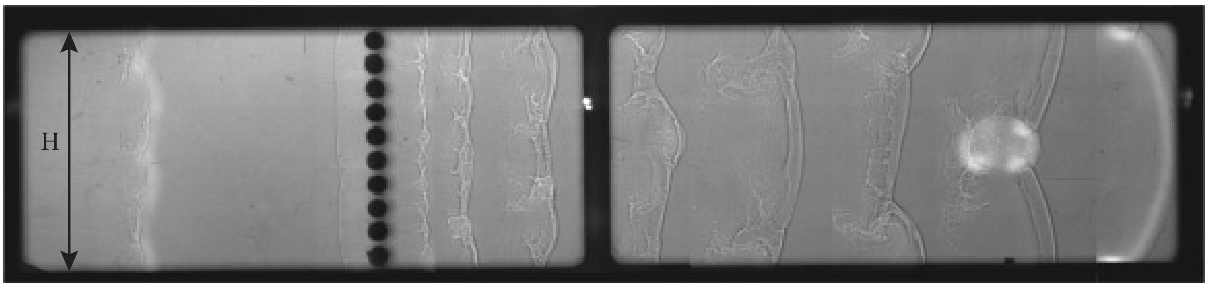
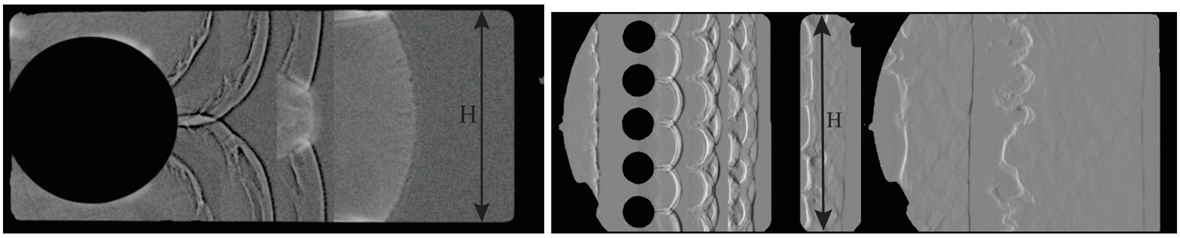


Figure 1: Composite shadowgraph images illustrating typical detonation re-amplification in a $C_2H_6$+3.5$O_2$ mixture at 3.4 kPa, see [6] for more details.

Table 1, the blockage ratios (BR) occupied by the obstacles ranged from 60% to 90%, with the number of cylinders varying from 1 to 10. Table 1 listed the reactive mixtures studied in the current work and the mixture initial pressure for the case with detonation re-initiation. Note that the initial pressure $P$ in the table is not necessarily the initial pressure for the minimum re-initiation pressure. Instead it corresponds to the largest detonation re-initiation length. The experiments were all conducted at the initial temperature 294 K. The initiation of the detonation waves in the reviewed mixture was achieved by means of a capacitor discharge at the extreme left end of the channel, while a tungsten wire was used as a point source to initiate the mixtures in the new experiments. The detonations reached the CJ velocity before interacting with the obstacle for both initiation techniques. Aside from the hydrogen, methane, ethane, ethylene, acetylene, and propane mixtures in the references, three sets of new experiments were conducted to determine the influence of the isentropic exponent using $H_2$+$N_2O$ and 1.5$H_2$+$N_2O$+$O_2$ mixtures in an obstructed channel with 75% BR and $H_2$+$N_2O$ mixtures in an 67.5% BR obstructed channel. The new experiments were repeated at least five times for each set of mixtures to ensure reliability and consistency.

Figure 2 shows the typical successful detonation re-initiation scenarios for oxi-hydrocarbon mixtures. We observe an acceleration from the fast flame to detonation after a long distance, for which the Mach reflection occurs multiple times, in all 5 mixtures of stoichiometric methane, ethane, ethylene, acetylene, and propane with oxygen as oxidizer. As listed in Table 1, the shock can travel up to hundreds of obstacle size before it transits to a detonation wave. However, there is no evidence of re-amplification for both the stoichiometric and lean hydrogen mixtures. Similar evolution can also be found in the argon diluted acetylene mixtures. All the successful transmitted cases occur immediately past the obstacles due to the Mach reflection, as shown in Fig. 2a. Once the detonation fails to re-initiate within a few Mach reflections after the obstacles, although it might be able to ignite the gas behind the Mach reflection the shock-flame complex continuously decays without further re-amplification. As illustrated in Fig. 2b, a keystone-shaped hot spot emerges behind each Mach shock, the flame gradually falls further behind the leading shock.

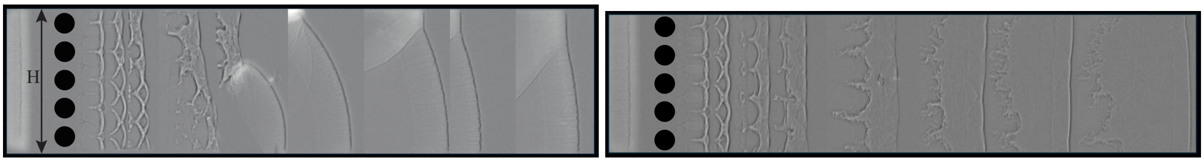
Replacing the oxygen with nitrous oxide in the hydrogen mixture reduces the isentropic exponent. A lower isentropic exponent enhances hydrodynamic instabilities, favoring turbulent mixing. Figure 3 compares the evolution undergone by the hydrogen detonation with different percentage of nitrous oxide in the channel with a BR of 75%. After passing through the obstacles, the leading shock of the 1.5$H_2$+$N_2O$+$O_2$ is curved due to the hot spots ignition behind the Mach shock. The overall evolution for both the successful detonation re-initiation and the completely quenching behavior is similar to that of the hydrogen oxygen mixtures. The detonation re-initiation is formed by the Mach reflection. In case of less strong Mach reflections, the distance between the flame and the leading shock becomes larger as it propagates further from the obstacles. Figure 4a depicts the leading shock velocity measured along



(a) Detonation re-initiation from the first Mach reflection in a $2H_2$+$O_2$ mixture at an initial pressure of 14.2 kPa, see [5] for more details.

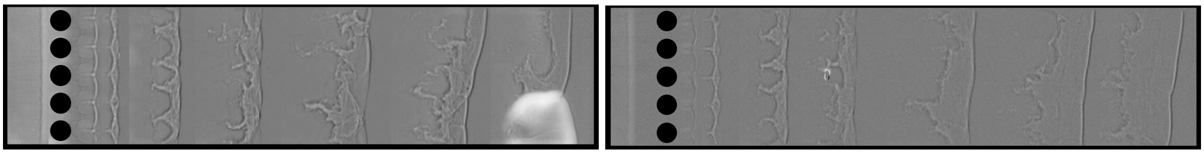
(b) Failed detonation with hot-spot ignition behind the first Mach reflection in a $H_2$+$O_2$ mixture at an initial pressure of 9 kPa, see [8] for more details.

Figure 2: Composite images illustrating typical hydrogen detonation transmission after passing through a column obstacles with a 75% blockage ratio.



(a) $1.5H_2$+$N_2O$+$O_2$, $P_0$ = 13.1 kPa

(b) $1.5H_2$+$N_2O$+$O_2$, $P_0$ = 11.0 kPa



(c) $H_2$+$N_2O$, $P_0$ = 13.4 kPa

(d) $H_2$+$N_2O$, $P_0$ = 13.1 kPa

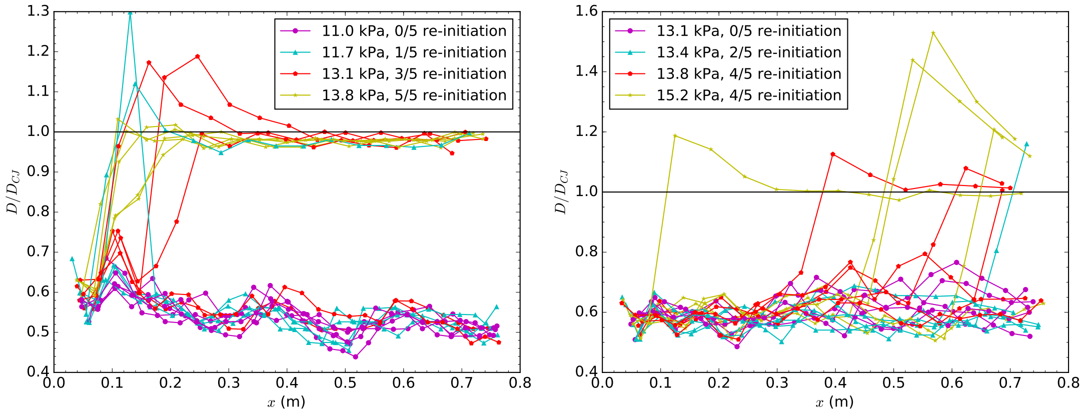
Figure 3: Composite shadowgraph images illustrating the evolution of the hydrogen detonation after passing a column obstacles with a 75% blockage ratio.

the bottom wall for a range of initial pressures corresponding to the critical re-initiation pressures. It can been seen that if the detonation fails to re-initiate within the first few Mach reflections, the leading shock speed will continue to decay. This is also consistent with the hydrogen-oxygen mixtures.

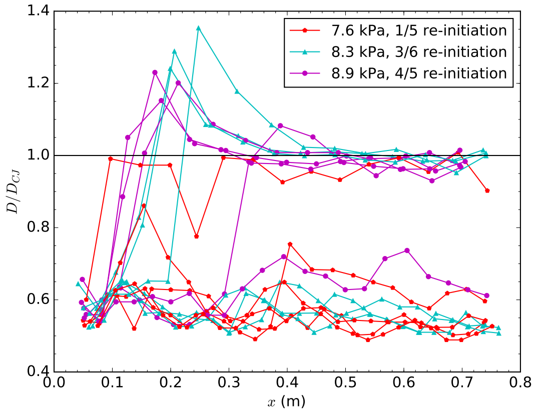
The $H_2$+$N_2O$ shows similar flame acceleration as the hydrocarbon mixtures in the channel with 75% BR. As shown in Fig. 3c, there is no obvious ignition behind the first formed Mach reflection. As compared to that of the $1.5H_2$+$N_2O$+$O_2$ mixtures, the shock is more flat and with the flame more closely couple with it for both successful and failed detonation re-amplification. As illustrated in the velocity plot in Fig. 4b, the closely coupled flames seem to be strong enough to support the shocks from decaying all the way to the end of the channel. With the decrease of the BR, the minimum initial pressure required for the $H_2$+$N_2O$ detonation re-initiation reduces (Fig. 3d). However, at these low pressure, the $L_{DDT}$ also decreases to be more close to the obstacles. For most cases, the initiation occurs immediately after the obstacles. The slowly increasing shock speeds in the no detonation re-initiation cases suggests a self-sustained fast flames propagation.

## 3 Discussion

To determine whether a universal understanding can be established for all the hydrogen and hydrocarbon mixtures considered, the chemical effects — characterized by the ignition delay time ($t_i$) and mixture



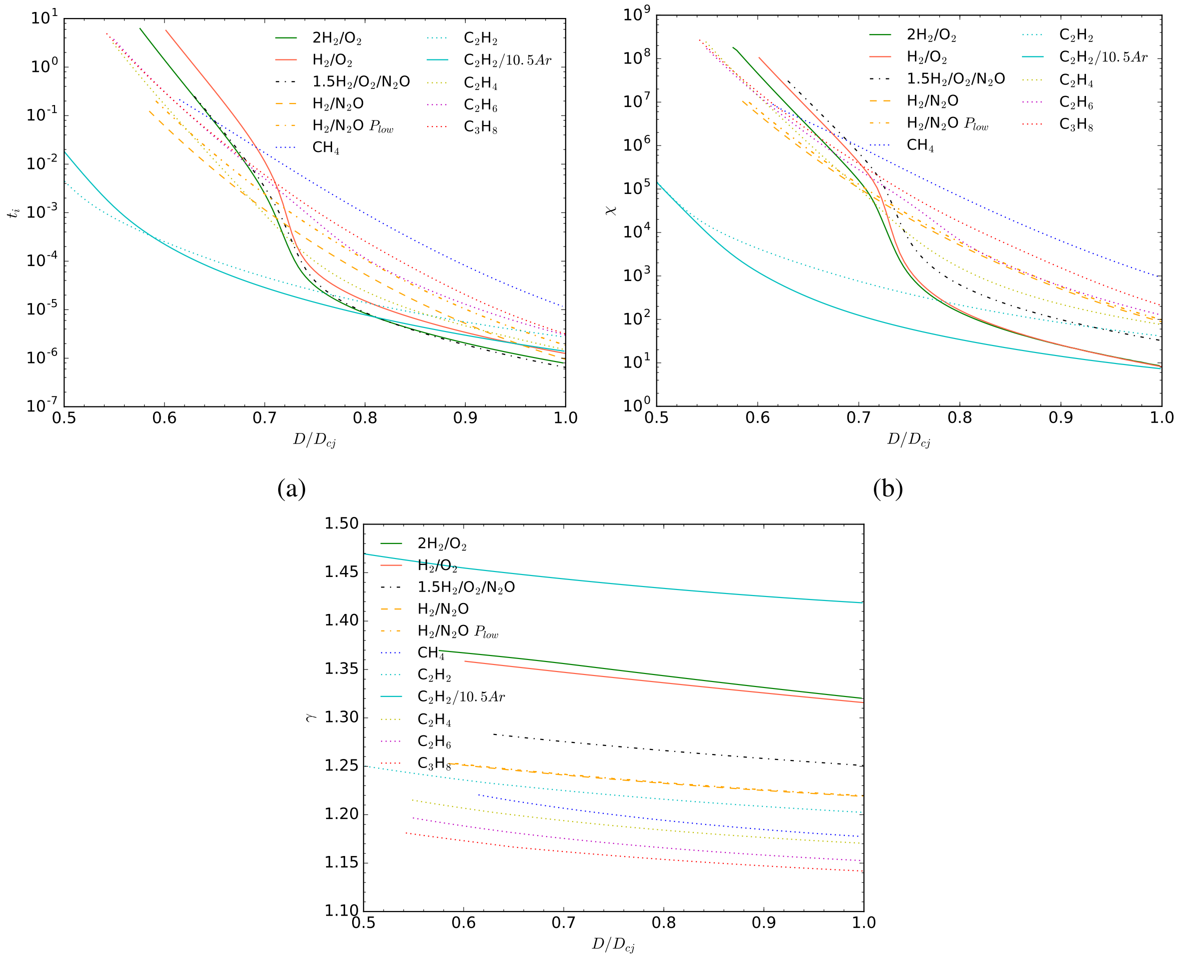
(a) 1.5$H_2$+$N_2O$+$O_2$, BR = 75% (b) $H_2$+$N_2O$, BR = 75%



(c) $H_2$+$N_2O$, BR = 60%

Figure 4: Leading shock speed profiles along the bottom wall.

sensitivity parameter ($\chi$) — and the hydrodynamic instability, represented by the isentropic exponent, were calculated for the gas in the post-Mach shock states. This was achieved using constant volume homogeneous reactor calculations implemented with Cantera thermal chemical tools and the Blanquart et al. mechanism (V2.3) [11] for the mixtures oxidized by pure oxygen and the Mevel mechanism [12] for the mixtures with nitrous oxide. The calculations were conducted at initial pressures corresponding to the critical re-initiation pressures. The available data from previous studies and the current experimental results show that the critical transmitted shock speed is in the range of $50 \sim 75\%$ of $D_{CJ}$ for all the mixtures considered, specifically 60% $D_{CJ}$ for the 2$C_2H_2$+5$O_2$/21Ar mixture. Figure 5 compares the calculated $t_i$, $\chi$ and $\gamma$ at such leading shock speeds, with the solid lines represent the cases without re-amplification. It can be observed that the re-initiation of the $C_2H_2$+2.5$O_2$ detonations is a result of auto-ignition because of the small $t_i$, whereas the $C_2H_2$+2.5$O_2$+10.5Ar fast flame falls into the chain-branching cross-over regime, similar to the oxi-hydrogen mixture, and fails to re-amplify. In other hydrocarbon mixtures, both the $t_i$ and $\chi$ are in approximately the same order as the oxi-hydrogen mixtures. Also, the gas behind the leading shock of the $H_2$+$N_2O$ mixtures has a lower $\chi$ as compared to that in the $H_2$+$N_2O$ mixtures, yet re-amplifications after a long distance from the obstacles were observed in experiments. This means that one cannot solely attribute the acceleration and re-initiation in these mixtures to auto-ignition and purely chemical kinetics. Instead, as shown in Fig. 5c, the $\gamma$ effect appears to have a better correlation for the re-initiation. All the mixtures failed to re-amplify seem to have a



(a)

(b)

(c)

Figure 5: Comparison of (a) ignition delay time $t_i$, (b) mixture sensitivity parameter $\chi$, and (c) isentropic exponent $\gamma$ as a function of leading shock speed for different hydrocarbon and hydrogen mixtures at initial pressures corresponding to the critical re-initiation pressures.

larger $\gamma$ as compared to the others. As is suggested by [13, 14], the decrease of $\gamma$ results in a stronger hydrodynamic jet behind the Mach shock. This $\gamma$ criteria seems to be compatible with all mixtures, suggesting that the hydrodynamic instability is important.

## 4 Conclusions

In summary, this study revisited the problem of fast flame re-amplification formed by detonation transmission through a bank of cylinders in hydrogen and hydrocarbon mixtures. When the detonation does not survive the diffraction process, the lead shock is found to decay to approximately 50% to 75% of $D_{CJ}$. All the oxygen-mixed methane, ethane, ethylene, acetylene, and propane mixtures show a similar trend of detonation re-amplification after a distance in the order of tens to hundreds of obstacle size. While once the oxygen-mixed hydrogen detonations fail to re-initiate in the first few Mach reflections, the shock-flame complex continuously decays. The fast flames of the $1.5H_2$+$N_2O$+$O_2$ and $C_2H_2$+$2.5O_2$+10.5Ar mixtures share a similar behavior as the oxi-hydrogen mixtures. One common feature shared by these mixtures is that the gas temperature behind the leading shock also falls into the chain-branching cross-over ignition limit, effectively quenching the ignition process. However, the $t_i$ and $\chi$ of these mixtures were found to be in the same order as other oxi-hydrocarbon mixtures which were able to re-amplify to detonations. Instead, the detonation re-initiation seems to be governed by the hydrodynamic instability, which is characterized by the isentropic exponent $\gamma$. All the mixtures that failed to re-amplify appear to have a larger $\gamma$ as compared to the others.

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