

CORRELATION BETWEEN DYNAMICS AND CHEMICAL KINETICS PARAMETERS IN DETONATION WAVES

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Introduction

Several authors have tried to relate the velocity and the shock structure of detonation waves to provide a better understanding of the coupling between the front shock and the heat release resulting eventually in its sustenance.

The work focuses on the correlation between experimental properties, namely the ratio (t_{char}) of the length of the cellular structure (L) and the mean wave velocity (D), and the calculated mean induction time (t_{ind}). The ratio L/D has been reported by Libouton et al. [1] as the characteristic time of the detonation (t_{char}) and represent basically the period of the detonation wave. Previous workers [2] have noticed a linear correlation between the induction and characteristic times, i.e.

$$t_{\text{char}} = K \cdot t_{\text{ind}} \quad (1)$$

However, the factor K seems not to be a universal constant and depends sometimes on the chemical composition of the reactive mixture. Moreover, close to the detonation limits, the simple relation Eq. (1) does not stand anymore. Figure 1 shows a schematic of Eq. (1) and the potential evolutions of the correlation between both parameters as the detonation wave approaches extinction. Defining the factor K' as

$$K' = \frac{d t_{\text{char}}}{d t_{\text{ind}}} \quad (2)$$

where $K' = K$ when the linear relation Eq (1) is valid, we may observe two types of detonation failure:

- (1) K' increases close to the detonation limit (curve A in Fig. 1). In this case, the reactive system is affected mainly by the increasing wave period (L/D), resulting eventually in the failure of the detonation. We may qualify this type of failure as an acoustic or dynamic one.
- (2) K' decreases close to the detonation limit (curve B in Fig. 1). In this case, the chemical kinetics, and consequently the increasing induction time, mainly affects the reactive system. We qualify this type of failure as a chemical kinetics failure.

The above distinction between both types of failure does not exclude the fundamental coupling between the kinetic of the chemical reactions sustaining the detonation wave and the gas dynamics controlling the shape and the size of the detonation structure.

This work investigates these correlations for detonation waves at various initial conditions, namely:

- variable equivalence ratio (?) of the mixture with different initial pressures,
- variable inhibitor content (?) with different fuel compositions (?), and
- various initial pressures in three different tube cross-sections, including rectangular and diagonal types of detonation waves [3].

The table 1 describes the different ranges of conditions.

The experimental set-up used for this study is the typical detonation tube equipped with either ionization or pressure gauges and soot plates to record the detonation velocity and detonation structure, respectively. Detailed description of the apparatus is given in [1, 4].

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The mean induction time is calculated according to the following scheme:

- the temperature and pressure conditions are evaluated using the classical steady shock equations. The Mach number used in these equations comes from the experimental average detonation velocity,
- at these temperature and pressure, the Arrhenius rate constants k_b (chain branching reaction) and k_t (chain termination reaction) are calculated using the simple kinetic mechanism and data from Libouton et al. [2],
- the species concentrations are evaluated at these temperature and pressure as well,
- the induction time is then given by

$$t_{ind} = \frac{1}{k_b \cdot O_2 - k_t \cdot M} \quad (3)$$

A detailed description of these calculations is discussed in [2].

Experimental Results and Discussion

Series 1: Equivalence Ratio

Figure 2 shows the detonation velocity and the cell for mixture with 70% argon dilution and at three different initial pressures (see table 1 series 1). Similar results with mixtures diluted with 50% of argon are observed. The vertical hatched lines refer to the composition at which no detonation propagates in the given experimental conditions. Calculating the characteristic and induction times as described above, we plot the values of K (Eq. (1)) in Fig. 3. The K -values are rather constant for equivalence ratios ranging from 0.5 to 1.3. At low equivalence ratios ($\phi < 0.5$), the K -value increases sharply exhibiting the typical behavior of curve A in Fig. 1. A similar trend but less obvious is noticed also for rich mixtures ($\phi > 1.3$).

Series 2: Chemical Composition

For different fuel compositions, i.e. $\phi = H_2 / (H_2 + CO)$ (see table 1), we add up to 5 % of inhibitor (CF_3Br). The whole set of experimental results is given in [5]. The evolution of the characteristic times as a function of the induction times is represented in Fig. 4a. One observes that, irrespective of the fuel composition, the curves exhibit the behavior of curve B in Fig. 1. Mathematical fitting of these evolutions enables us to determine the K' parameter according to Eq. (2). The K' -values are collected in Fig. 4b and decay when the inhibitor content increases, i.e. when the detonation limit approaches. The decay is much more pronounced when the CO content is dominant, accounting for a large influence of the chemical kinetics on the sustaining mechanism of the detonation.

Series 3: Tube Cross-Section

The different tube cross sections used are: square tube ($9.2 \times 9.2 \text{ cm}^2$ cross section), rectangular tube ($9.2 \times 3.2 \text{ cm}^2$) and flat tube ($0.7 \times 3.2 \text{ cm}^2$). The initial pressure of the mixture ranges from 20 to 250 torr, 25 to 200 torr and from 125 to 200 torr for the experiments in the square, rectangular and flat tube, respectively. A post-process of the experimental data similar to the one described above (series 2) is applied and the results are presented in Figs 5a and 5b. Note that the data on Fig. 5b are plotted versus the inverse of the initial pressure to emphasize the evolution towards the detonation limit. We observe a change in the decaying behavior of the detonation wave as the confinement conditions varies: from tube heights going from 9.2 cm to 0.7 cm, the type of failure goes from the chemical kinetics one (curve A in Fig. 1) to the dynamics one (curve B in Fig. 1).

All these observations confirm that Eq. (1) is may be to simple to describe the behavior of the detonation close to the limit. A more appropriate description (Eq. (2)) leads to consider two types of failure and that consideration has already been made by Evariste et al. [4]. Extension to other initial parameters could be considered and will be dealt with.

References

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Table 1: Ranges of compositions and initial pressures covered by this study: ϕ is the dilution (% of diluant including the inhibitor content), ϕ_f is the ratio of fuels ($H_2 / H_2 + CO$), ϕ_e is the equivalence ratio, and ϕ_i is the percentage of inhibitor.

Series	Tube	Composition					Pressure (torr)
			ϕ	ϕ_f	ϕ_e	ϕ_i	
1	square	$H_2 - O_2 - Ar$	0.7	0.33 - 1.55	1.0	0.0	40, 125, 200
		$H_2 - O_2 - Ar$	0.5	0.5 - 1.4	1.0	0.0	20, 75
2	square	$H_2/CO - O_2 - Ar/CF_3Br$	0.7	1.0	1.0 - 0.1	0.0 - 0.05	200
3	square, rectangular and flat	$H_2 - O_2 - Ar$	0.7	1.0	1.0	0.0	20 - 250

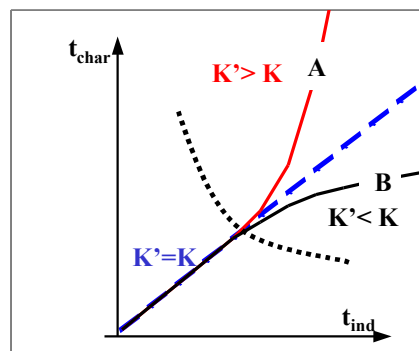


Fig. 1: Simplified evolution of the characteristic time of the detonation (t_{char}) vs. the chemical induction time (t_{ind}).

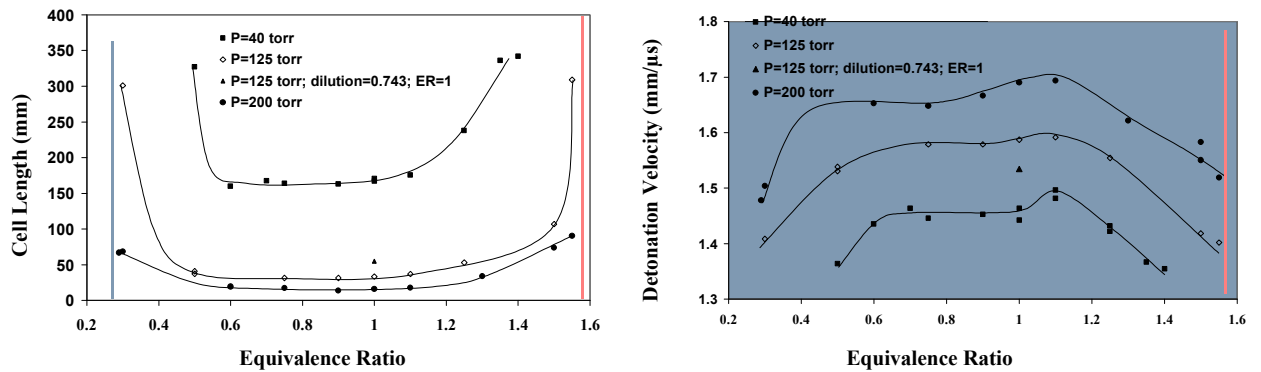


Fig. 2: Experimental cell length and detonation velocity vs. the equivalence ratio of the initial mixture (series 1 from table 1).

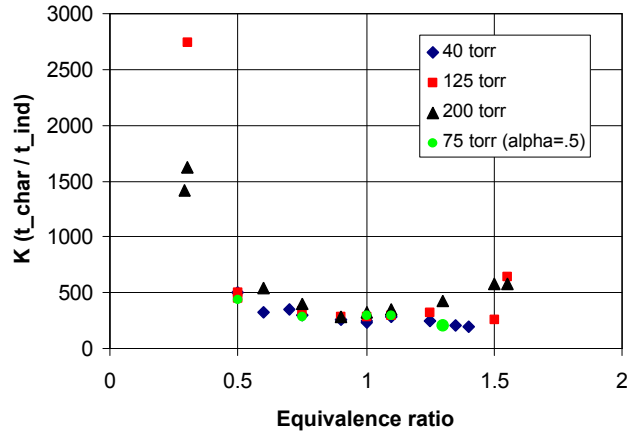


Fig. 3: Evolution of the ratio $K = t_{char}/t_{ind}$ vs. the equivalence ratio (?) of the reactive mixture, series 1 in table 1.

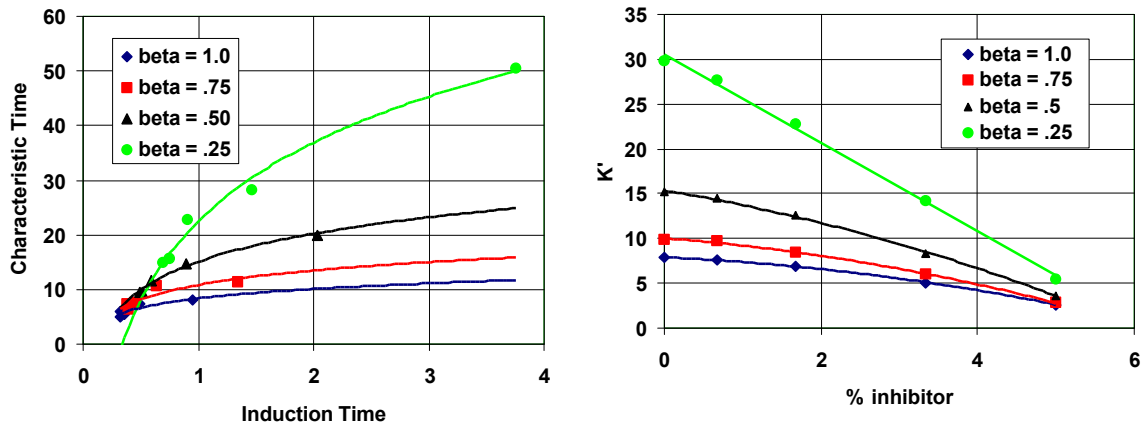


Fig. 4: Correlation between the characteristic and induction times and evolution of $K' = d t_{char}/d t_{ind}$ vs. the inhibitor content for different fuel composition (?), series 2 in table 1.

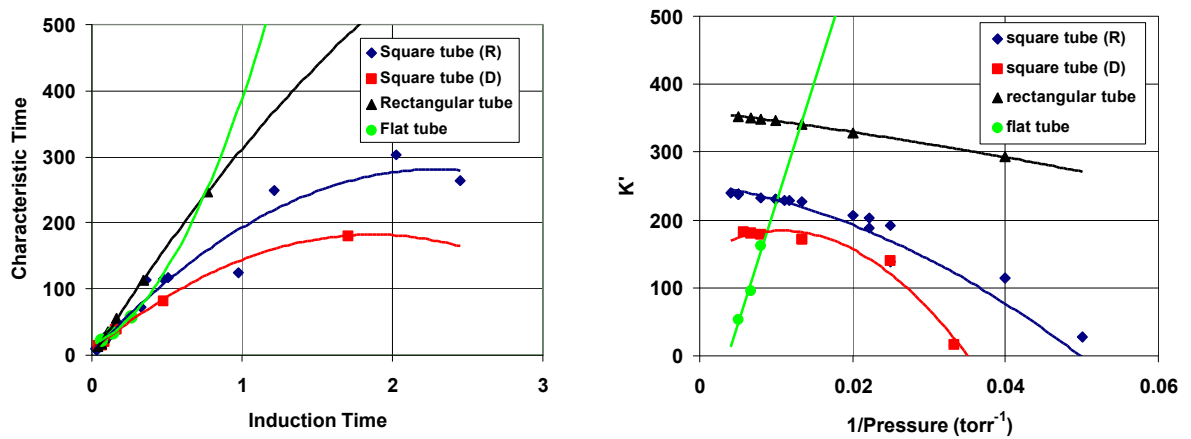


Fig. 5: Correlation between the characteristic and induction times and evolution of $K' = d t_{char}/d t_{ind}$ vs. the initial pressure in different tube cross sections, series 3 in table 1. The labels (R) and (D) refer to the rectangular and diagonal types of detonation propagations [3].