

# The mean pressure evolution in detonation cells

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## 1 Introduction

Detonation waves in gases take on a cellular structure. The reaction zone is not laminar nor one-dimensional, as modelled by the steady Zel'dovich - Von Neumann - Doering (ZND) model [1]. The front is marked by very large velocity excursions around the mean, typically  $\pm 20 - 30\%$  [2], with ensuing induction kinetics varying by orders of magnitude in the gases shocked by the different fronts. Transverse shocks further heat the shocked gases, sometimes becoming internal detonations, non-steady effects slow the reactions and deflagrative fronts consume large portions of gases with long ignition delays. Due to these complex physical phenomena, detonations require high-fidelity numerical simulations for their prediction. This is still not possible for irregular structure detonations, which currently fall in the "no model" category.

Nevertheless, at a macro-scale, a long-held modeling approach of detonations is akin to Reynolds averaging in turbulence modeling, whereby one can define statistically stationary field variables meant to represent the mean variables inside the detonation structure, phased averaged over a few cells [3–5]. Closure of the modeling requires the formulation of a local reaction rate conditioned on the mean variables, lead shock statistics, non-stationarity of the gasdynamic evolution in the reaction zone and diffusion-controlled burning of pockets. Modeling of the equivalent to Reynolds stresses involving the correlations among the various fluctuating components is also required - not in the context of isotropic turbulence, but in the context of cell-averaged dynamics. While simple empirical closures for the reaction rate have been attempted with some success [6], a rational closure presents a formidable task, and very little progress has been made so far [2, 7]. Gamezo [8], Radulescu [5] and their colleagues have attempted to reduce the large numerical data obtained in numerical simulations of cellular detonations to extract the mean profiles. Of particular interest is the study of Reynaud et al. [9] who assessed whether this modeling approach is meaningful *in the presence of losses*. This led to somewhat promising results, whereby the effective thickening of the mean structure compared with the ZND model explained the higher propensity of these detonations to fail in the numerical experiments with increasing instability; see also the analysis of Lalchandani [7]. Nevertheless, this was found in contradiction with experimental trends [10], leading to questioning the fidelity of the physics included in the cellular detonation calculations in the first place, such as the absence of turbulent assisted burning and over-simplification of the kinetic models used: namely that one step Arrhenius chemical models give the incorrect time scales of induction and reactions. It is thus preferable to extract the mean profile evolutions from experiment directly in order to meaningfully test this hypothesis: *is a mean-field approach a meaningful modeling approach for detonations?*

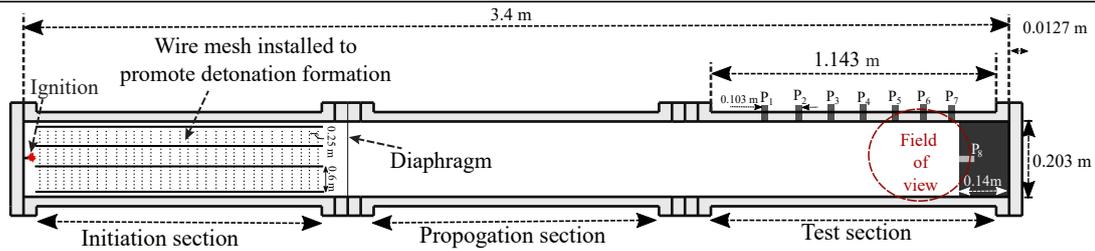


Figure 1: Schematic of the shock tube used in the experiment.

To date, the mean profiles have seldom been extracted from experiments, with only a few exceptions: Soloukhin [11], pursuing the averaged description explained above, measured mean pressure, density and temperature and found that these decay in approximately  $4 \mu\text{s}$  to the expected Chapman-Jouguet values in the acetylene-oxygen system studied; this corresponds to approximately one detonation cell width  $\lambda$ . Subsequent effort has been made to locate the mean sonic surface of detonations in order to establish the global thickness of detonations as a characteristic length scale. Edwards et al. monitored the decay of transverse wave strength and onset of a Taylor expansion wave to infer the location of the sonic surface; it was estimated to lie 4 to 6 cell widths downstream of the front [12]. Vasil'ev [13] and Weber & Olivier [14] attempted to locate the instantaneous sonic surface at various locations in the cell. They took the sonic point in the lab reference frame as a lower bound estimate to the sonic surface in the detonation reference frame. The location where the flow transits from supersonic to sub-sonic in the lab frame was deduced by observing when the bow shock attached on a needle placed in the path of a the detonation detaches and moves upstream. Their estimates differed from each other and placed the sonic surface between  $\lambda/3$  and several cells behind the front. The uncertainty in the hydrodynamic thickness precluded models to be developed for its prediction.

In the present study, we reconstruct the average pressure evolution in cellular detonations by phase and ensemble averaging with sufficient resolution to establish meaningful results. Two types of detonations are probed: detonations in  $\text{H}_2\text{-O}_2\text{-Ar}$ , which display a very regular structure, and detonations in  $\text{CH}_4\text{-O}_2$ , which display a very irregular one. These two mixtures lie at the extreme of cellular regularity, physical processes controlling the global reaction rate and stability characteristics of the underlying ZND structure. The experimental results are compared with structure predictions made on the basis of the ZND model and account for losses, in order to draw conclusions on the meaningfulness of the mean description of the structure.

## 2 Experimental method

The experiments were performed in a 3.4-m-long shock tube, with 0.019-m-thickness and 0.203-m-height. The schematic illustrating the experimental set-up is shown in Fig. 1. Mesh wires were placed in the initial section of the shock tube to ensure the formation of detonation within this segment. Subsequently, the detonation propagated through the second section to reach a steady propagation speed before entering the third test section. The two mixtures studied were  $\text{CH}_4 + 2\text{O}_2$  at an initial pressure of  $p_0 = 6\text{kPa}$  and temperature of  $T_0 = 293\text{K}$  and  $2\text{H}_2 + \text{O}_2 + 7\text{Ar}$  at  $p_0 = 4\text{kPa}$  and  $T_0 = 293\text{K}$ . The selection of these two mixtures was based on their significant differences in cellular regularity. The initial pressure of the mixture was selected to ensure a single cell was present inside the channel. The hydrogen experiments were repeated twelve times under identical conditions, while the methane ones were repeated thirteen times.

Each mixture was prepared in a separate mixing tank by the method of partial pressures and was then left to mix for more than 24 hours. Monitoring of the mixing process was done using an Omega PX409-

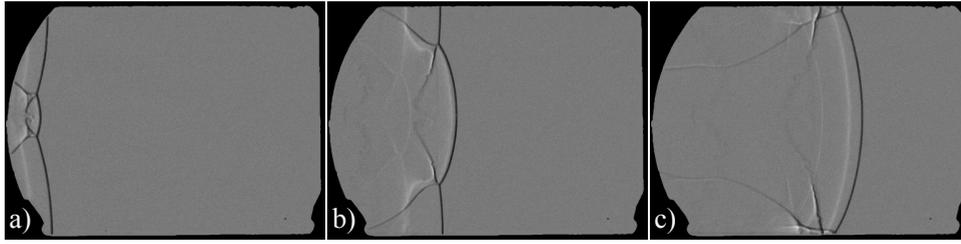


Figure 2: Detonation structure evolution in  $2\text{H}_2/\text{O}_2/7\text{Ar}$  at  $p_0 = 4$  kPa.

015AV pressure transducer with the accuracy of  $\pm 0.08\%$ . The shock tube was evacuated to a pressure below 80 Pa before filling it with the gas. The initial ignition of the premixed combustible mixture was achieved using a capacitor bank discharge [15], charged to 25 kV. For the hydrogen experiments, a driver section filled with  $\text{C}_2\text{H}_4/3\text{O}_2$  was used to help in the detonation formation with an initial pressure 2.4 times larger than the test gas. A linear arrangement of two 113B24 piezoelectric PCB pressure sensors, followed by five 113B27 sensors, was evenly distributed along the top wall of the shock tube. The sensors have a natural frequency of 500kHz, while the pressure signals during the experiments were recorded at a rate of 1.5 MHz. All pressure gauges used in the experiments have a diameter of 5.5-mm and a maximum error of 1.3%, as determined from the calibration data. The signal conditioners used for these pressure sensors are the PCB Piezotronics model 482C05 and 482C16. To improve the quality of the pressure signals and minimize noise, a filtering process was applied to the raw data using a cut-off frequency of 250 kHz. This frequency selection aimed to preserve crucial information regarding the smallest spatial scales observed in the detonation structure during the experiments. Furthermore, the propagation process was visualized by utilizing the classical Z-type schlieren technique with the Phantom v1210 camera with  $12.9 \mu\text{s}$  inter-frame time.

### 3 Experimental results

The detonation structure obtained in the hydrogen mixture is shown in Fig. 2. A single cell was obtained propagating at an average speed of  $1285 \pm 40$  m/s. It takes on the characteristic structure with the induction zone terminating behind the transverse waves. A detailed discussion of the structure at these conditions is discussed elsewhere [16, 17].

Figure 3a shows the superposition of 72 pressure signals recorded by pressure sensors on the top wall following the passage of the detonation wave, with the average pressure indicated by the solid line. The time origin for every curve is the time at which the shock reached the sensor. The wide variability among each trace is due to the sampling of different points inside the cellular structure. We are interested in the mean pressure evolution, which represents the phase averaged and ensemble averaged pressure. This average pressure is shown in Fig. 3b.

In order to estimate the location of the sonic surface, we computed the location of the expected pressure at the sonic surface. If one seeks the solution of the detonation structure where transient and curvature effects are perturbations [17], the expected pressure at the sonic surface is uniquely dependent on the mean propagation speed. If one assumes a strong detonation, the pressure at the sonic point is given by

$$p_{sonic} = p_{CJ} \frac{D^2}{D_{CJ}^2} \quad (1)$$

The average pressure crosses this expected sonic point pressure after approximately  $160 \mu\text{s}$ . This also corresponds approximately with a sudden change in mean pressure evolution, which we associate with

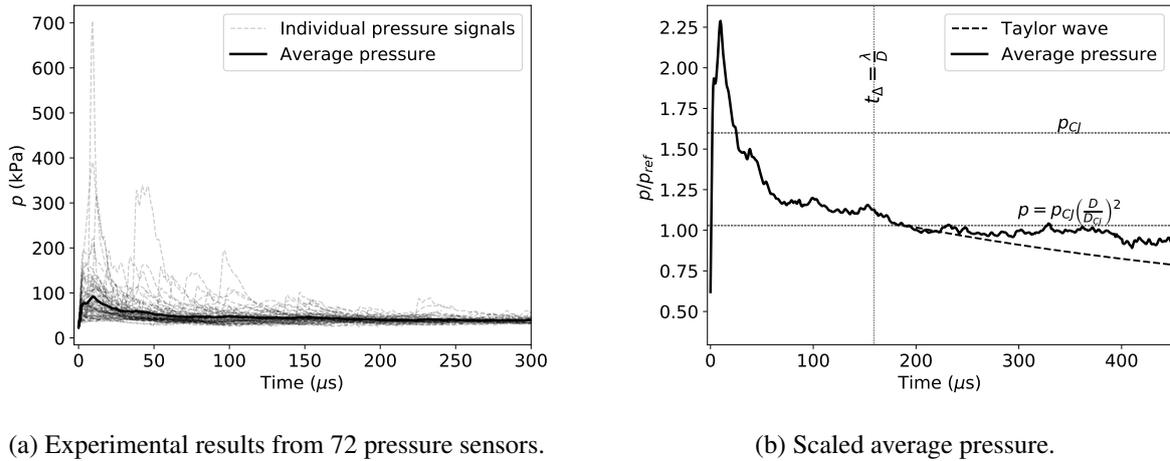


Figure 3: Temporal evolution of the incoming detonation wave pressure measured on the top wall in the mixture of  $2\text{H}_2/\text{O}_2/7\text{Ar}$  at  $p_0 = 4$  kPa.

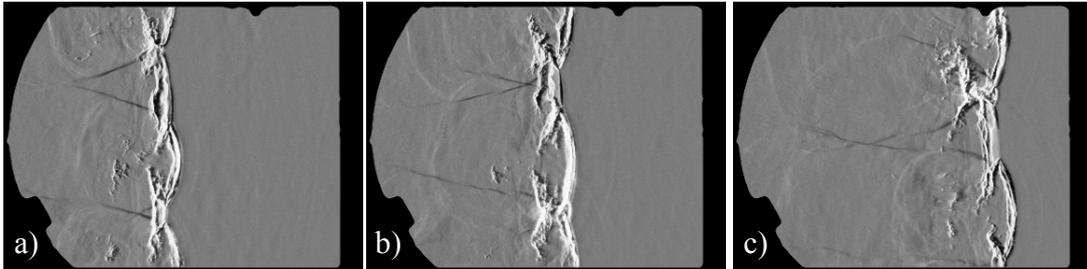


Figure 4: The detonation structure in  $\text{CH}_4 + 2\text{O}_2$  at  $p_0 = 6$  kPa.

the Taylor wave. Note that the subsequent pressure evolution is under-estimated by the Taylor wave solution. This is possibly due to the action that the driver has in the experiment on the post detonation gas dynamics.

The time to reach the sonic surface is seen to coincide approximately to a time given by  $t_{\text{sonic}} \simeq \lambda/D$ , the time it takes the front to advance approximately one cell width. It is difficult to accurately translate this into a length, since the flow speed is not known. Adopting the post-shock speed as characteristic speed, with  $u \simeq 0.3D$ , this gives a hydrodynamic thickness of  $\Delta_H \simeq ut_{\text{sonic}} \simeq 0.3\lambda$ . The estimate would be  $0.5\lambda$  if the particle velocity near the sonic surface was taken as characteristic speed. Our estimate is in excellent agreement with that of Weber and Olivier [14].

The experiments performed in the methane mixture captured a more complex detonation structure (fig. 4), similar to previous observations in this system [2, 5, 18]. The characteristic cell size  $\lambda$  in this mixture extracted from our experiments is 10 cm, or half the channel height. Non-reacted pockets are observed over a distance corresponding to approximately half of a detonation cell downstream of the lead shock. The transverse waves appear as non-reactive.

Figure 7 provides the pressure measurements in the methane mixture. The instantaneous pressure profiles again show a wide variability, reflecting the non-steady processes within the detonation structure. The mean pressure profile is shown in Fig. 5b. Scaling the pressure by the expected pressure at the sonic point as per (1), the pressure decay passes through the sonic point at a time of  $50 \mu\text{s}$ . This corresponds again to precisely the time scale  $\lambda/D$ . Note that this also corresponds to an abrupt change in the pressure decay rate, which we associate with the onset of the Taylor expansion wave. The measured pressure de-

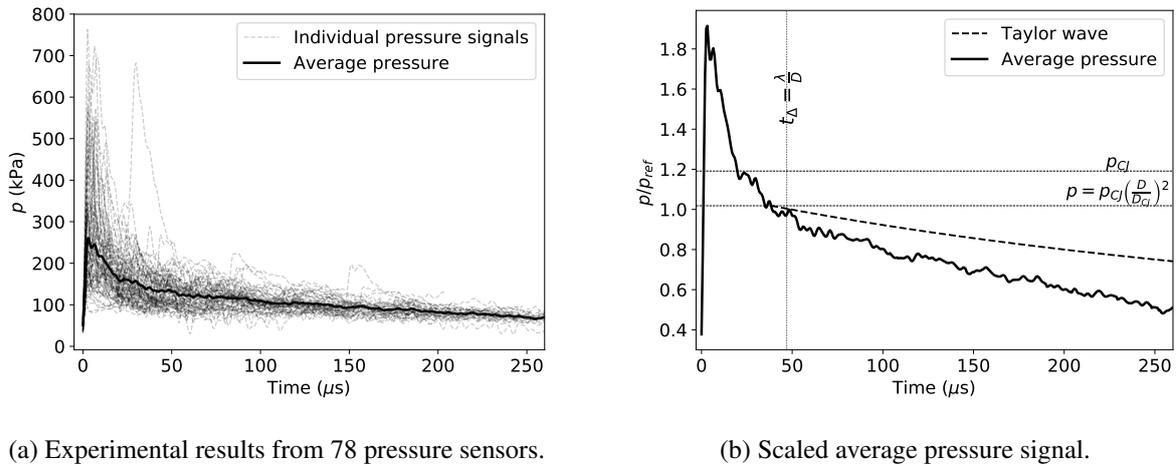


Figure 5: Temporal evolution of the incoming detonation wave pressure measured on the top wall in  $\text{CH}_4/\text{2O}_2$  mixture at  $p_0 = 6$  kPa.

cay is faster than the Taylor wave, as expected for this un-supported detonation in a thin channel. Large differences are expected due to boundary layer losses; substantial differences were noted in previous experiments [19]. The location of the sonic point correlates well with the distance at which the pockets disappear.

#### 4 Modelling

Simulations of the hydrogen detonations have recently been reported by us [17] using a calibrated two-step model for the kinetics and account for the wall losses. The details of the simulations are not reproduced here. Figure 6 illustrates the structure obtained numerically and its experimental counterpart at the same stage of the calculation. The excellent agreement permits to further use the simulation as a surrogate for the experiments. Simulations were also performed in 1D, for which the solution was a stable travelling wave with a speed deficit, owing to the losses.

The average velocity deficit of detonation propagation measured in one cell in the two-dimensional simulation ( $D/D_{CJ} = 0.82$ ) and the one-dimensional simulation (0.83) is in good agreement with the global velocity measured from the experiments (0.8). The pressure dynamics was extracted at 12 locations across one cell in the 2D numerical simulation. Figure 7a presents these pressure signals alongside the mean pressure profile. Remarkably, the average pressure measured from the simulation closely matches the experimental data, capturing both peak pressure and decay rate towards the plateau as shown in Fig. 7b. Of interest is that the 1D steady wave ZND solution captures remarkably well the mean profiles obtained by averaging the cellular dynamics. This is perhaps the first time where it is shown that the ZND structure provides a good model for the mean cellular dynamics in a regular structure detonation! This is perhaps not surprising, since it has been argued for a long time that the ZND structure provides an adequate model for modeling losses of detonations in systems with long reaction zones, such as hydrogen at low pressure [20]. Indeed, as first argued by Radulescu, when the exothermic reaction zone is much longer than the induction zone variations, one expects the coherent superposition of the power pulses into a wave form resembling the steady ZND structure [20, 21].

For the methane mixture, the ZND profile obtained with the model of Zangene using the San Diego 2016 kinetic mechanism [17] accounting for losses reproduces the mean velocity deficit (7% in the experiments and 6% model prediction), but not the global mean pressure profile (fig. 8). The experimental

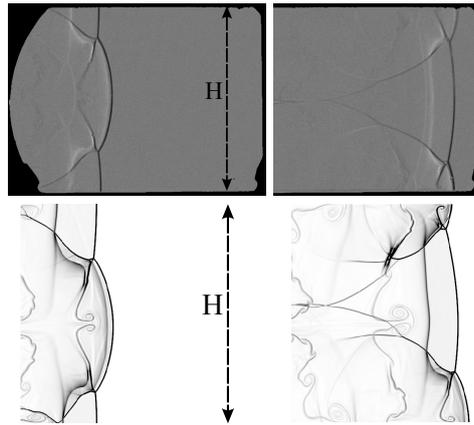


Figure 6: Comparisons of the gradient of the density of the incoming detonation and reflected wave from the quasi-2D simulation (bottom row) with the schlieren photos from experiment (top row) in  $2\text{H}_2/\text{O}_2/7\text{Ar}$  mixture at  $p_0 = 4$  kPa.  $H$  is the channel height of 0.203 m.

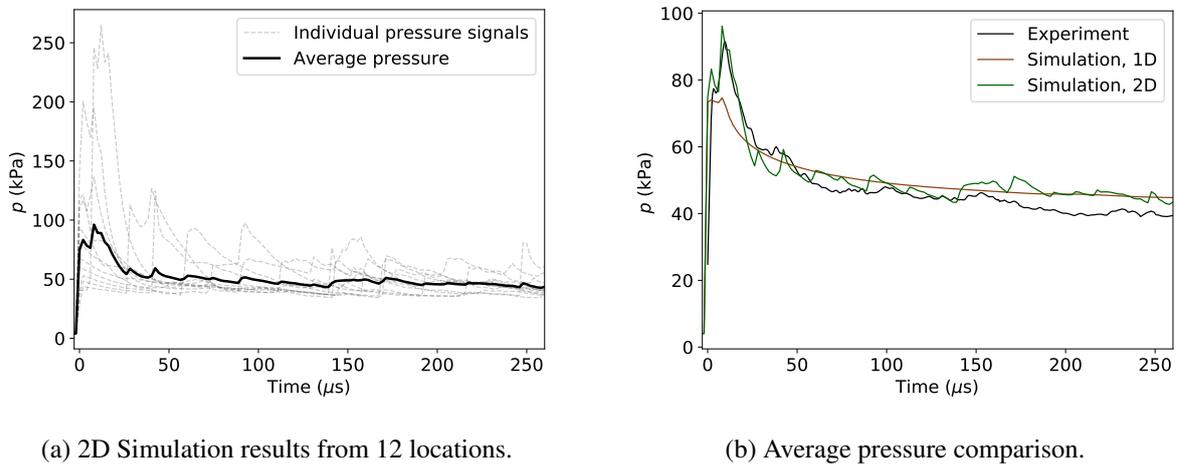


Figure 7: Temporal evolution of the incoming detonation wave pressure measured on the top wall in  $2\text{H}_2/\text{O}_2/7\text{Ar}$  mixture at  $p_0 = 4$  kPa.

pressure profile terminates at a sonic surface earlier than predicted by the ZND model with the same velocity deficit. This is again the opposite trend from the observations made by Reynaud et al. [9] from numerical simulations of inviscid detonations. We are planning numerical simulations of methane detonations with account of deflagrative burning of the pockets in order to further determine if the burnout of the non-reacted pockets controls the location of the sonic surface. The results will be presented at the Colloquium.

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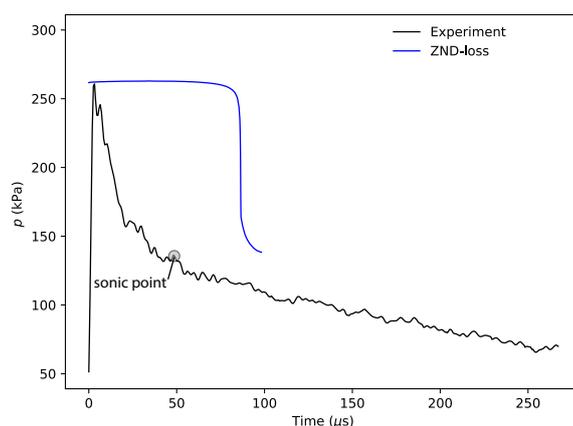


Figure 8: The mean detonation profile and the ZND prediction with losses for  $\text{CH}_4/2\text{O}_2$ .

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