# A Note on the Averaging Analysis for One-Dimensional Pulsating Detonations

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## 1 Introduction

It has been well established, from both experiments and numerical simulations, that gaseous detonation waves are inherently unstable [1]. To elucidate various dynamics of the detonation wave, its unstable structure needs to be fully described. Experimentally, it is challenging to quantitatively measure the detonation structure or even to unambiguously determine the wide spectrum of unstable detonation cell sizes. For practical purposes, there is a need to define at least a length scale to characterize the overall thickness of the unstable cellular front [2, 3]. Despite the fact that gaseous detonations are highly unstable and transient, it is hoped that one can at least define a steady, one-dimensional, average "effective thickness" of the detonation in its direction of propagation. This effective thickness is generally referred to as the "hydrodynamic thickness" of the detonation. Once such a length scale is obtained, it can be used to develop empirical correlations or models for other detonation dynamic parameters (i.e., initiation energy, critical tube diameter, propagation limit, etc.).

The definition of the hydrodynamic thickness is not unique. Experimentally, attempts have been made to measure the location of the sonic plane from the detachment of the bow shock on a blunt body placed in the path of the detonation [4] and hence to define the hydrodynamic thickness. However, it is difficult to distinguish the detachment distance for the case of unstable cellular detonations. Numerically, recent attempts have been made to simulate a two-dimensional cellular detonation and perform averaging of the flow quantities in order to determine the mean flow field or an equivalent one-dimensional ZND wave [2, 3]. In this manner, the hydrodynamic thickness is determined from the mean profile at the plane when all fluctuations are equilibrated. Such an averaging approach is found useful and has been used subsequently in many recent numerical studies [5, 6]. Despite further work performed, there remain some issues such as the sampling size invoked and the validity of the different averaging methods.

In this study, we re-visit the averaging approach for analyzing the unstable detonation propagation. This work focuses upon the simplest model of one-dimensional pulsating detonations, of which the instabilities and non-equilibrium fluctuations are restricted to the longitudinal direction. The focus of this

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research is to explore in greater detail the mean structure of pulsating detonations with increasing instabilities towards chaotic behavior and, particularly, the discussion on the effect of applying different averaging methods.

## 2 Numerical Methodology and Averaging Analysis

The unsteady, nonlinear dynamics of the propagation of a one-dimensional pulsating detonation wave are modelled by solutions of the one-dimensional inviscid compressible, time-dependent reactive Euler equations with a single-step irreversible Arrhenius kinetic rate law. These governing equations are solved numerically using a second-order centered scheme, namely the SLIC (Slope Limiter Centered) scheme; its detailed description can be found in [7]. The computational setup follows previous studies by fixing the dimensionless parameters with the values $Q = 50$ and $\gamma = 1.2$ while varying the activation energy $E_a$ as a control parameter [8, 9]. For all the simulations, a numerical grid resolution of 100 points per half reaction zone length $L_{1/2}$ of the steady ZND detonation is used to ensure the detailed features of the pulsating front are properly resolved. The computations are initialized by the steady solution of the ZND detonation.

In order to obtain the mean structure of the one-dimensional pulsating detonation wave, the computational results are analyzed via a density-weighted (Favre), spatio-temporal averaging method. The averaging analysis was introduced to the field of detonation by Lee & Radulescu [2] and Radulescu et al. [3], and recently employed by Sow et al. [5] and Mi et al. [6]. Two techniques of averaging were considered: (1) using a coordinate moving at the average propagation velocity of the detonation wave and (2) an instantaneous, shock-fixed frame analysis. In a reference frame moving at the average velocity $V_{avg}$, the spatial coordinate and particle velocity are transformed as $x' = x - V_{avg}t$ and $u' = u - V_{avg}$, respectively; in a reference frame moving at the instantaneous propagation velocity $V_{ins}$, $x$ and $u$ are transformed as $x' = x - \int_0^t V_{ins}(\tau)\mathrm{d}\tau$ and $u' = u - V_{ins}(t)$, respectively. A simple time averaging, or Reynolds averaging procedure, is then applied to density $\rho$ and pressure $p$ as follows:

$$\overline{\rho}(x') = \frac{1}{t_2 - t_1}\int_{t_1}^{t_2} \rho(x',t)dt \;\; ; \;\; \overline{p}(x') = \frac{1}{t_2 - t_1}\int_{t_1}^{t_2} p(x',t)dt$$

with $t_1$ and $t_2$ denoting the start and end of the averaging period. The bar "–" indicates time-averaged variables. Favre averaging (i.e., density-weighted averaging) is applied to particle velocity and specific energy as follows:

$$u'^* = \frac{\overline{\rho u'}}{\overline{\rho}} \text{ and } u' = u'^* + u'' \;\; ; \;\; e^* = \frac{\overline{\rho e}}{\overline{\rho}} \text{ and } e = e^* + e''$$

where superscript "*" and ″ indicate Favre-averaged variables and fluctuating quantities, respectively. The mean structure of the wave is therefore governed by the solutions of the one-dimensional, stationary Favre-averaged Euler equations expressed below:

$$\frac{\partial}{\partial x'}\left(\overline{\rho}u'^*\right) = 0$$

$$\frac{\partial}{\partial x'}\left(\overline{\rho}u'^{*2} + \overline{p} + \overline{\rho u''^2}\right) = -\overline{\rho\dot{V}}$$

$$\frac{\partial}{\partial x'}\left(\overline{\rho}e^*u'^* + \overline{\rho}(e''u'')^* + \overline{pu'}\right) = -\overline{\rho u\dot{V}}$$

In the equations above, terms $\overline{\rho \dot{V}}$ and $\overline{\rho u \dot{V}}$ represent the inertial (pseudo-) force and the work done by it due to the transformation to a reference frame moving at $V$. Note that these two terms are zero for a steady wave propagation or in a reference frame moving at $V_{avg.}$

## 3 Results and Discussion

The parameter that controls the 1-D detonation stability is the activation energy. Above the neutral stability boundary of $E_a$ ~ 25.2 for the given mixture conditions, the steady ZND detonation becomes unstable. The instability manifests itself as a pulsating behavior of the detonation front. Figure 1 shows the results for an activation energy of $E_a$ = 27 with the instability manifested as periodic oscillations after the initial transient. Pressure profiles at different instants over a pulsating cycle elucidates the unstable flow field within the detonation structure and fluctuations convected downstream in the wake.

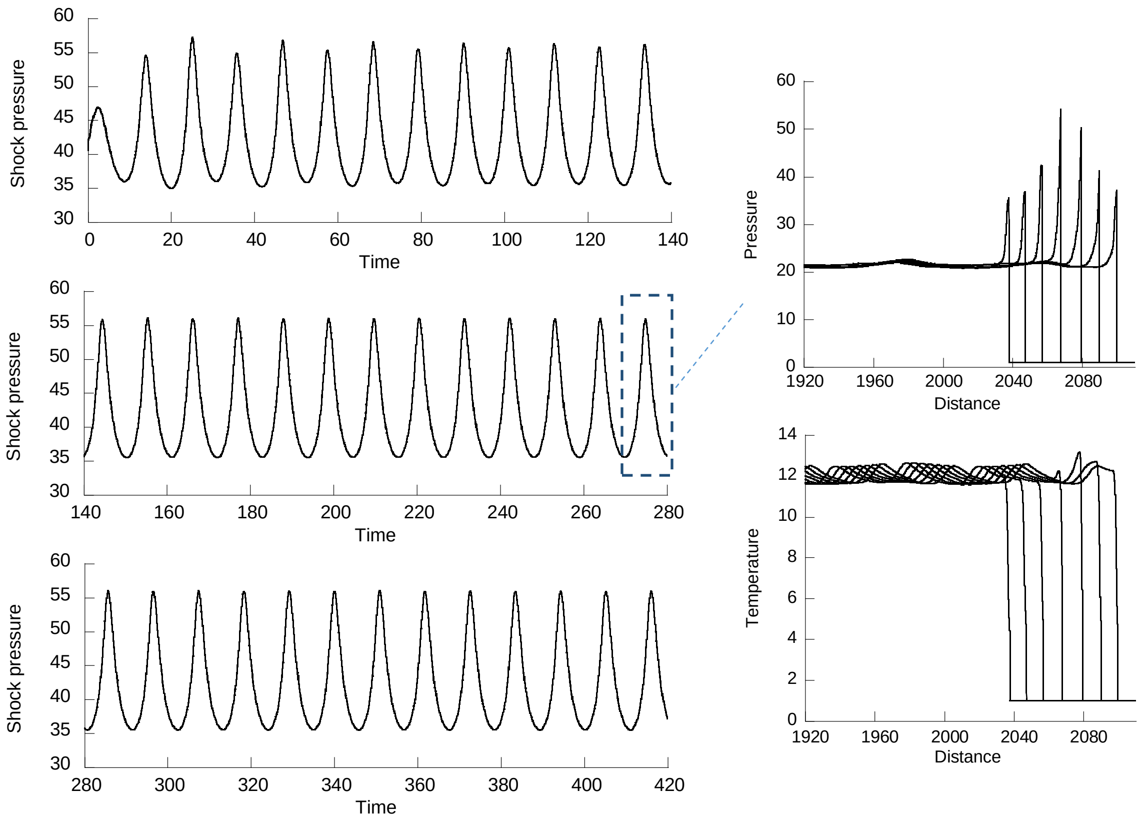


Figure 1. Leading shock pressure history for $E_a$ =27 and pressure and temperature profiles over a pulsating cycle

Figure 2a) shows the spatially averaged pressure profile computed using coordinates attached to the mean shock velocity and coordinates attached to the instantaneous shock location. The dashed line gives the ideal, steady ZND structure for the given mixture and initial conditions. Because of the periodic, oscillatory nature of the results, the average profile converges quickly with relatively limited sampling of the simulation. Globally, the averaged profile from the CFD results follows well the ZND solution. For the weakly unstable detonation, one can notice for the average structure a slight extension near the tail of the profile. Using the coordinates attached to the mean shock velocity, the averaging of the shock oscillation smears out the front shock and the resulting smoothing cannot capture the von-Neumann peak.

Figures 2 b) and c) give the $x'$-$t$ diagrams for the reactive progress variable $Z$ and the leading shock front position. From these plots, both the results obtained using average-velocity and instantaneous shock-attached frames yield similar hydrodynamic thicknesses. In Fig. 3b), the amplitude of the shock front oscillation is also close to the reaction length.

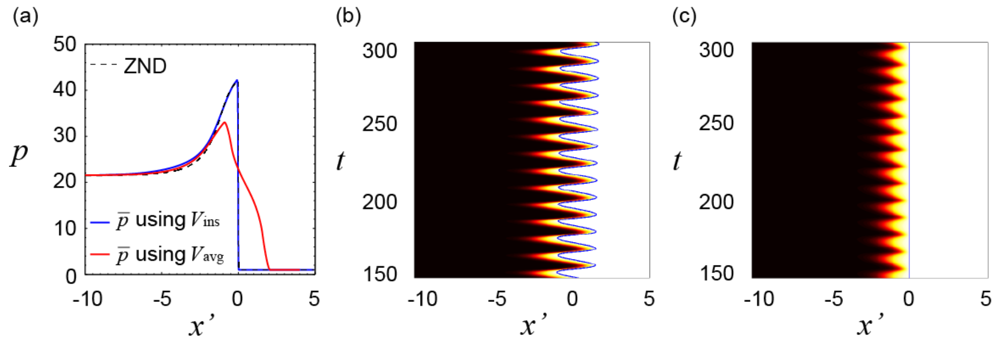


Figure 2 a) Spatial profiles of averaged pressure; b) contours of reactive progress variable $Z$ plotted in $x'$-$t$ diagrams using the coordinate attached to the mean shock velocity and c) the instantaneous shock-attached frame for the pulsating detonation with $E_a$ = 27.0. The trajectory of the leading shock is plotted as the blue line in (b) and (c).

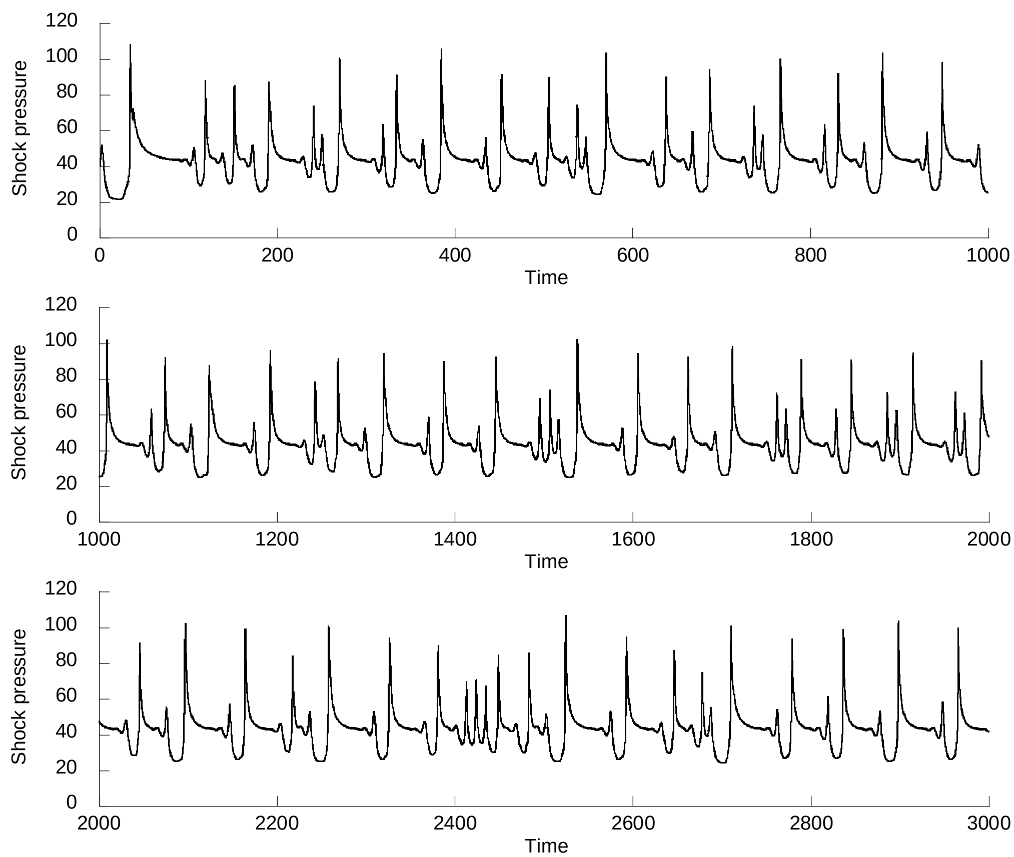


Figure 3. Long-time evolution of the leading shock pressure for $E_a$ =30 showing chaotic oscillations of the one-dimensional detonation propagation.

Increasing the value of the activation energy $E_a$ causes the pulsating detonation to undergo a series of period-doubling cascades and for $E_a$ = 30, the one-dimensional pulsating detonation exhibits chaotic behavior [8]. The time series of the shock pressure for $E_a$ = 30 showing the chaotic dynamics is given in Fig. 3.

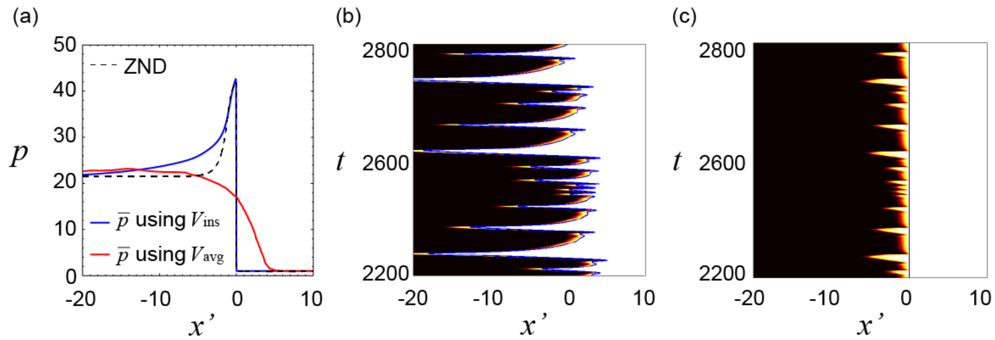


Figure 4 a) Spatial profiles of averaged pressure; b) contours of reactive progress variable $Z$ plotted in $x'$-$t$ diagrams using the coordinate attached to the mean shock velocity and c) the instantaneous shock-attached frame for the pulsating detonation with $E_a$ = 30.0. The trajectory of the leading shock is plotted as the blue line in (b) and (c).

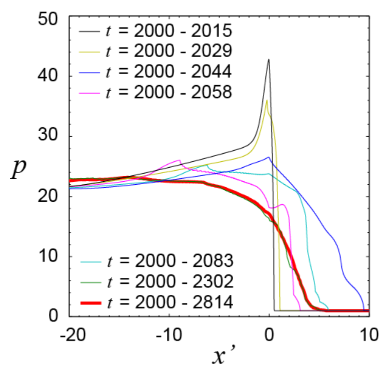


Figure 5. Spatial profiles of pressure averaged using the coordinate attached to the mean shock velocity with different sampling size (time interval).

For highly chaotic pulsations with $E_a$ = 30, the difference between the results becomes apparent. The average pressure obtained using both the coordinate moving at mean shock velocity and instantaneous shock-attached frame, shown in Fig. 4, deviates significantly from the ZND solution. The hydrodynamic thickness of the mean structure is larger than the ZND reaction zone length. Using the instantaneous shock-attached analysis, the von-Neumann peak is again well captured in the mean structure. It is interesting to note that the deviation from the ZND solution occurs around the ZND half reaction zone length with $Z$ = 0.50. For the averaging using coordinates attached to the mean shock velocity, the smearing becomes pronounced due to the high level of fluctuations in the shock velocity. The averaging appears to destroy or suppress all the main features of the detonation wave. In addition, it is also found that for the chaotic oscillation with large shock fluctuations, the average profile determined using the coordinate attached to the mean shock velocity is very sensitive to the sampling size (or time interval), as shown in Fig. 5. Also shown in Figs. 4 are the $x'$-$t$ diagrams for the reactive progress variable $Z$ where the highly fluctuating results in b) suggests a long sampling time is needed to have a converged average profile using the mean shock velocity analysis, while c) appears to reveal a clearer hydrodynamic thickness and the mean structure converges faster using the instantaneous wave-attached analysis.

## 4 Concluding Remarks

The use of averaging is a powerful technique to understand the detonation dynamics by obtaining a mean structure of the unstable detonation. However, the present results caution that care must be exercised when choosing the way to perform the averaging. Performing the averaging in a reference frame moving at the average velocity, the result is shown to be sensitive to the sampling length. Also, it does not really represent the mean structure of the reaction zone behind the leading shock wave. For all cases, the averaging based on the average velocity is related to the spatial extend of the shock fluctuation. Using the wave-attached analysis, the global structure resembles more closely the standard ZND profile. It does not consider the spatial fluctuations of the shock location and the leading front does not smear out. The setup is closer to averaging a sampling of particle paths undergoing different shock compression. The latter method seems to give a clear definition of the detonation thickness and the mean structure obtained converges with fewer samples of the simulation for both regular and chaotic pulsating detonation.

## Acknowledgment

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