An Approach to Modulate the Frontal Detonation Structures in Numerical Simulations

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1 Introduction

Detonation in gases has long been known to exhibit an unstable cellular frontal structure [1], which plays an important role in their propagation and dynamics at critical phenomena [2]. In recent years, various fundamental investigations have been made with the goal to modify this dynamic structure to isolate and demonstrate its significant effects, notably, by damping out the transverse waves using porous media [3, 4], by perturbing it locally using small obstacles [5-7], or modifying globally the inherent unstable structure using rough-walls resulting in a quasi-detonation [8] or in a spatially inhomogeneous reactive medium [9, 10], etc. In all these situations, a simultaneous change in the frontal strength, e.g., a velocity deficit, would unavoidably occur, preventing the role of the hydrodynamic frontal instability to be investigated in an isolated manner. With the increasing focus to develop practical detonation-based engines, other practical techniques to modify the dynamic detonation structure have also been revisited by changing the chemical kinetics process with the use of sensitizer species added in trace amounts to the combustible mixtures, such as ozone O_3. The presence of additives in trace amounts does not significantly modify the overall thermodynamic properties of the system, hence the wave strength, and has a similar effect of reducing the overall activation energy of the system and thus causing a change in the detonation sensitivity of the mixture and thus, the cellular instabilities [11-14].

In this study, we propose a simple numerical study to modify the frontal characteristics of a self-sustainably propagating detonation front by using a series of micro-plates embedded in the quiescent combustible mixture. These obstacles are sufficiently large ($\omega >$ the induction zone length Δ_I) to induce transverse flow perturbations but thin enough ($\eta << H$) to not cause any velocity deficit in the wave propagation direction. With the obstacle scale, the resulting perturbations are thus affecting solely the flow within the hydrodynamic thickness. A study is performed on the spacing of these micro-plates in order to modulate the cellular dynamics and instabilities to different degrees.

This modification of the detonation structure is further motivated. Within the detonation structure there are in general two modes of combustion, shock compression and slower diffusive burning [2, 15]. To understand this complicated structure is an ongoing challenge as reaction rates can differ by more than two orders of magnitude [2]. By modulating the detonation in this way, i.e., by controlling the

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cellular front dynamics without changing the detonation velocity, the slower diffusive burning can be reduced or eliminated, producing a wave where combustion is governed solely by shock compression. This modulated detonation wave may be easier to understand, and therefore also to control and predict.

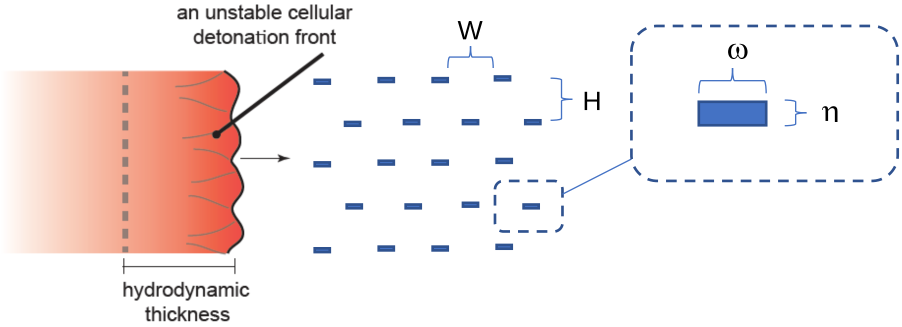

Figure 1: Numerical problem setup.

2 Simulation setup and numerical details

Focusing on the gasdynamic effects and the unstable frontal structure, the present numerical experiment considers the two-dimensional, reactive Euler equations governed by the two-step induction-reaction kinetic model [16]. The state and flow variables are non-dimensionalized with respect to the unburnt state and the non-dimensional parameters are Q = 50, γ = 1.2, while the chemical kinetics parameters are $\varepsilon_I = 9\,T_s$, $\varepsilon_R = T_s$, and $k_R = 0.8$. The induction pre-exponential constant k_I is scaled such that the induction zone length Δ_I of the corresponding steady Zeldovich-von Neumann-Döring (ZND) solution is unity.

The problem setup is illustrated in Fig. 1. An incident Chapman-Jouguet (CJ) detonation is initiated and propagates into the matrix of small, stationary obstacle plates with width ω = 15 and height η = 0.5. These are separated with spacings W = 25, 30, or 50, and H = 7.5, 10, 12.5, or 15.

The simulation code is based upon a uniform Cartesian grid with a resolution of 10 grid points per ZND induction zone length Δ_I. The MUSCL-Hancock scheme with the van Leer non-smooth slope limiter and a Harten-Lax-van Leer-contact (HLLC) approximate solver for the Riemann problem are used as described by Toro [17]. To accelerate the simulation run-time, the entire flow solver was implemented using NVIDIA CUDA programming language (NVIDIA Corp.) and run on an NVIDIA graphics processing unit (GPGPU) [18]. A periodic boundary condition is applied to the top and bottom boundaries of the domain, while a reflecting boundary condition is used for the obstacles.

3 Statistical methodology

3.1 One-dimensional average profile

The two-dimensional flowfield was first spatially averaged to obtain a one-dimensional flowfield by averaging across the vertical y-axis. The spatially averaged data was then also temporally averaged. To perform temporal averaging, the flowfield data were transformed to a wave-attached reference frame, which in this case is a frame moving at the CJ speed. The average profiles were calculated over a wave propagation distance of around 1000Δ_I, which contains ~2000 flowfield snapshots. Where the bar accent represents these spatially and temporally averaged values, the average reaction rate is given by,

$$\bar{\Omega} = \bar{\rho} k_R (1 - \overline{\lambda_0}) e^{(E_R/\bar{T})}.$$

3.2 Maximum pressure statistical analysis

A novel method of characterizing the strength of the detonation cellular front is proposed. The maximum pressure, p_{max}, obtained at each computational grid point is recorded in the numerical soot foils. These data are used to calculate a probability density function (PDF) over this variable p_{max}. Therefore, the PDF shows the distribution of shock pressures at the detonation front. For the PDF, the range of p_{max} considered, i.e., the minimum and maximum values are 20 and 80, respectively. This ranges from approximately half to twice the von Neumann shock pressure ($p_{\mathrm{vn}} \cong 42$) in order to capture the majority of shock pressure values. Again, the statistics are gathered over a wave propagation distance of at least 1000Δ_{I}, which contains $\sim 3\mathrm{x}10^7$ data points.

4 Results and discussion

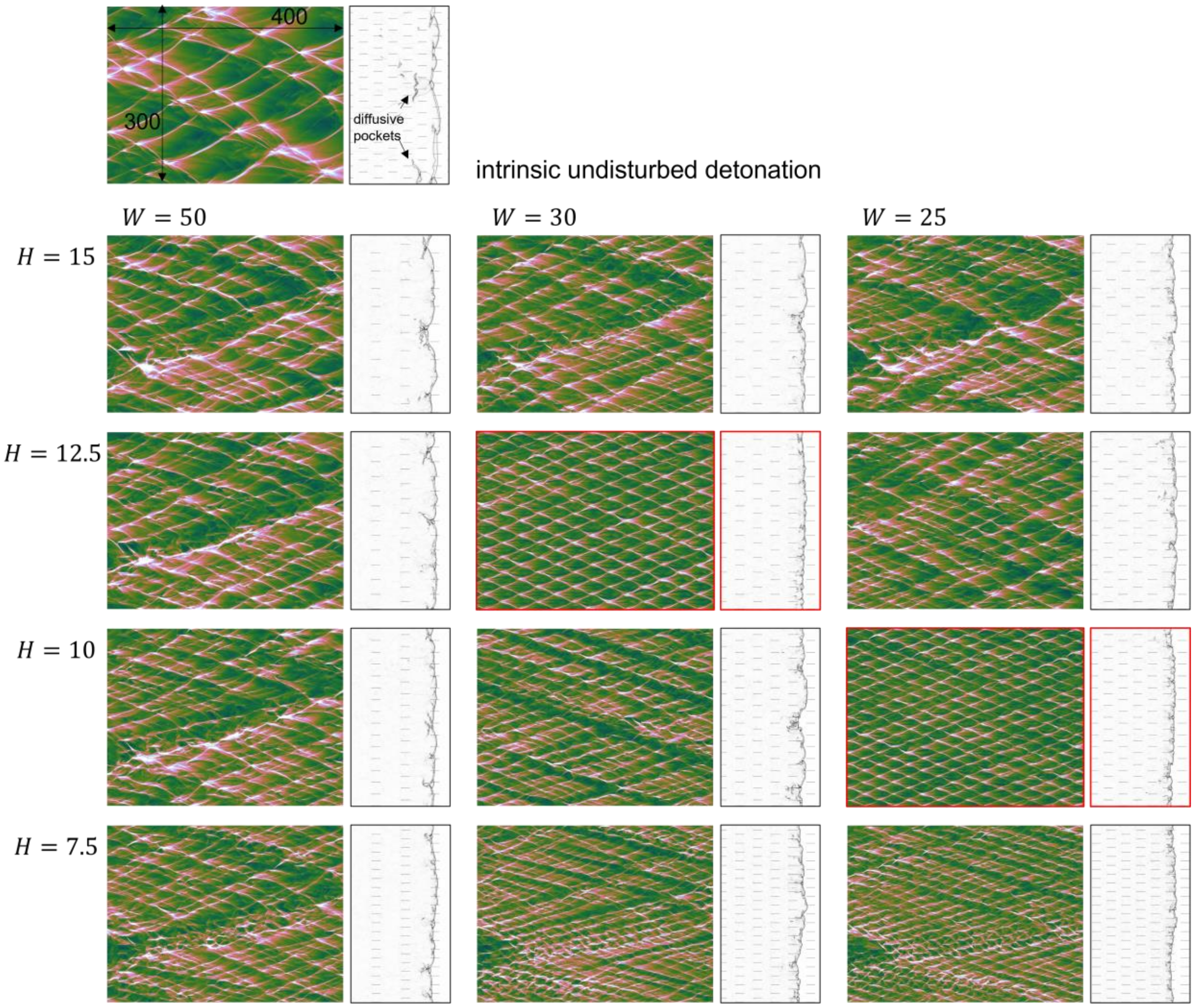

Figure 2: Numerical soot foils and typical schlieren images of the flowfield for the intrinsic undisturbed detonation and for the modulated detonations with different micro-plate spacings.

For a detonation in a given reactive mixture the simplest fundamental model is the ZND structure. In addition, the two-dimensional detonation wave has an inherent cellular structure. In this section, these two characteristic structures serve as benchmarks to which the modulated detonation produced by the embedded micro-plates is compared. They are henceforth referred to as the ZND detonation and intrinsic undisturbed detonation, respectively. It is important to emphasize that modulation by the micro-plates produces no velocity deficit in the direction of motion of the flow, hence, all waves propagate at velocities within 3% of the CJ value.

In Fig. 2, the intrinsic undisturbed detonation and the modulated detonations obtained with different micro-plate spacings are compared via numerical soot foils and schlieren images. Each column of images corresponds to a different micro-plate spacing in the x-direction, W, and each row to a different spacing in the y-direction, H. In its soot foil, the intrinsic detonation structure is irregular. For the modulated detonations, the cells are in general smaller, and for two specific cases, namely $W = 30\ \ H = 12.5$ and $W = 25\ \ H = 10$ (emphasized with red), the modulation produces highly regular cells. The accompanying schlieren images of the flowfield suggest a change in the combustion mechanism. In general, unstable mixtures with irregular cells do not burn by shock compression only, rather, some pockets of gas burn via slower diffusive processes downstream of the front [2, 15]. These pockets are visible in the intrinsic detonation structure. For the modulated detonations, these pockets are notably absent, implying that the gas burns more rapidly and mainly via shock compression, as is characteristic of stable mixtures with regular cells [15]. Moreover, for the specific cases of $W = 30\ \ H = 12.5$ and $W = 25\ \ H = 10$ with regular cells, the detonation front appears the most planar and uniform.

The detonation structures can be more directly compared via their average one-dimensional profiles. In Fig. 3(a), profiles of reaction rate are plotted for the intrinsic undisturbed detonation and the modulated detonations, along with the ZND structure. The two cases for which regular cells were obtained above are differentiated from the other modulated detonations (i.e., $W = 30\ \ H = 12.5$ and $W = 25\ \ H = 10$). The reaction zone is the shortest for the ZND wave since the gas is assumed to burn planarly by shock compression, and is the longest for the intrinsic detonation due to the slower diffusively burning pockets. Modulation by the micro-plates shifts the detonation structure closer to the ZND ideal, with the reaction zone becoming shorter. Moreover, the two differentiated cases with regular cells are the closest ZND approximation. This result is more quantifiable in Fig. 3(b), where the hydrodynamic thickness, defined by the location of the sonic point of the one-dimensional average structure, has been calculated and plotted. The x-axis is the ratio between the plate spacings in the x- and y-directions, i.e., W/H. The hydrodynamic thickness is seen to decrease slightly for all of the modulated detonations, with a more pronounced decrease for the special cases occurring at around $W/H = 2.5$. Also notice that in both Figs. 3(a) and (b), the case with $W = 25\ H = 10$ is more distinct.

Finally, in Fig. 4, the distribution in strength of the cellular shock fronts is compared via maximum pressure statistics. In Fig. 4(a) the x-axis is the maximum pressure, p_{max}, and the y-axis is the PDF, f. The vertical dashed line is the von Neumann shock pressure, p_{vn}. In general, for the modulated detonations, the PDFs suggest a higher concentration of shock pressure values near p_{vn}. More quantitatively, the median and standard deviation of p_{max} are plotted in Figs. 4(b) and (c). Compared to the intrinsic detonation, all of the modulated detonations are shown to have a reduced median which approaches p_{vn}, and a lower standard deviation. Therefore, for the modulated detonations the variation in shock pressure values at the cellular front is narrowed, and the front approaches that for the ZND structure with its non-fluctuating planar shock at p_{vn}.

5 Concluding remarks

In the present study, a method of controlling the detonation structure by embedding a matrix of micro-plates in the reactive gas was proposed and demonstrated. Crucially, this modulation is able to alter the detonation structure without changing the detonation velocity. A reactive mixture which is inherently unstable with an irregular cellular structure was used. Modulation by the micro-plates was shown to reduce the variation in shock pressures at the cellular front, thereby enhancing gas burning via shock compression, and consequently reducing the size of the reaction zone and the thermodynamic thickness. Therefore, the modulated detonation was shown to be more akin to detonations in stable mixtures with regular cellular structures, and furthermore, more like the ideal ZND structure. Specifically, micro-plates with $W/H = 2.5$ (where W and H are the plate spacings in the x and y-directions, respectively) produced highly regular cells and the closest approximation. A resolution study is currently underway, as well as the inclusion of viscous effects in the governing equations.

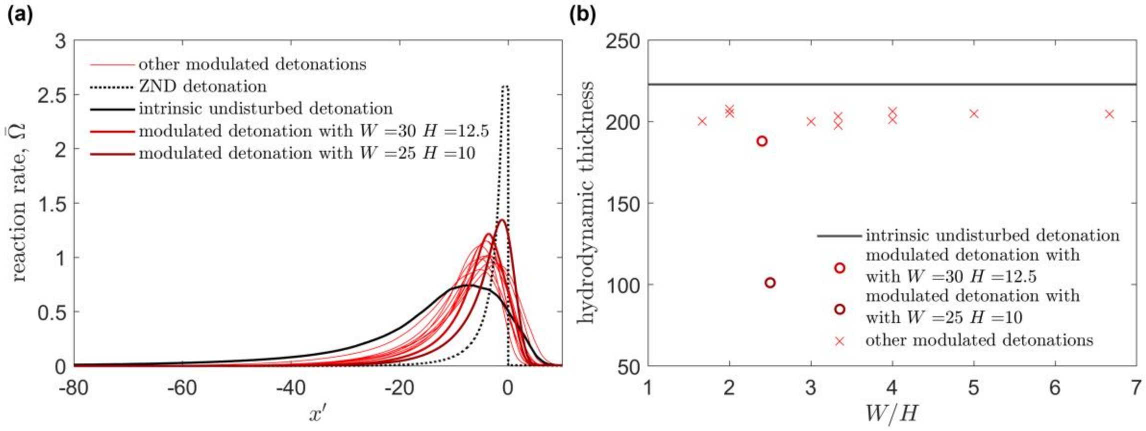

Figure 3: (a) The average one-dimensional reaction rate profile, and **(b)** the hydrodynamic thickness based on the location of the sonic point in the one-dimensional average structure, for the intrinsic undisturbed detonation and for modulated detonations with different micro-plate spacings compared to the ZND structure.

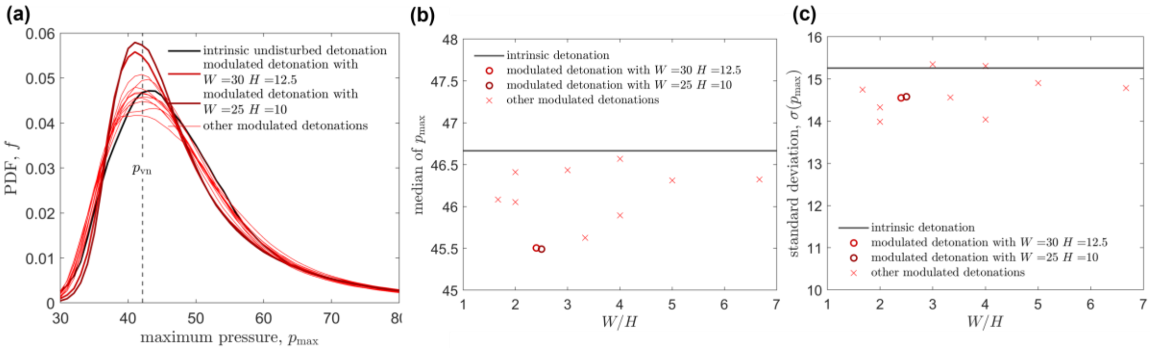

Figure 4: (a) The probability density functions (PDFs) of maximum pressure $\boldsymbol{p}_{\mathbf{max}}$, and **(b)** the median, **(c)** and the standard deviation of $\boldsymbol{p}_{\mathbf{max}}$, for the intrinsic undisturbed detonation and for modulated detonations with different micro-plate spacings. The vertical dashed line is the von Neumann shock pressure, $\boldsymbol{p}_{\mathbf{vn}}$.

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