Nonlinear dynamics and chaos regularization of one-dimensional pulsating detonations with small sinusoidal density perturbations

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Abstract

In this work, we explore the effect of initial density variation in the combustible mixture on the nonlinear dynamics of one-dimensional gaseous detonation propagation. Studies of nonlinear dynamical behavior of one-dimensional pulsating detonation are frequently based upon the reactive Euler simulations with one-step Arrhenius chemistry. In regions of the control parameters space, i.e., activation energy E_a, the 1-D detonation dynamics are shown to exhibit chaotic behavior at values of 28.5 and 30.0. Using small sinusoidal initial density perturbations, this investigation shows the emergence of various nonlinear temporal patterns as a function of the perturbation wavelength. It demonstrates that the cooperative behavior between the intrinsic instability and imposed small perturbation can lead to regularization of chaotic oscillations in one-dimensional gaseous pulsating detonation. Hence, by means of a small perturbation, an otherwise chaotic motion is rendered more stable and predictable. This result thus has implications for how intrinsically unstable detonation dynamics can be controlled.

***Keywords**:* Pulsating detonation, density perturbation, chaos, nonlinear dynamics

1. Introduction

Under realistic conditions with unsupported boundary, gaseous detonation waves are inherently unstable [1]. Evidence from both experimental and numerical simulations shows that the unsteady dynamics of detonation propagation is described by an ensemble of interacting transverse waves and small-scale instabilities embedded within the frontal wave structure. The mutual interactions between different waves create a cellular detonation structure, the so-called detonation cells, along its propagation direction. The cellular instability has also been probed by hydrodynamic stability analysis, particularly the normal mode analysis, on the one-dimensional steady Zel'dovich – von Neumann – Döring (ZND) structure, which reveals the growth and frequency of various inherent unstable modes giving rise to the cellular structure [2, 3]. Evolution equations are also derived under some asymptotic limits to describe the cellular detonation propagation, see [4-6], also [7] and reference therein.

As a first step to elucidate the unstable structure of detonations, a wealth of studies, starting from the pioneering work of Fickett & Wood [8] can be found on the simplest problem of one-dimensional (1D), time-dependent dynamics of planar detonations with simplified chemistry, e.g., [9-18] or more recently with detailed chemistry [19-21]. It is also becoming a canonical problem for testing and developing more accurate numerical schemes for detonation simulations [22-26]. In the one-dimensional treatment, the dynamic structure manifests itself through longitudinal pulsation. A number of high-resolution numerical simulations focus on examining the long-time evolution of the longitudinal instability and explore the role of chemical kinetics on the nonlinear instability spectrum far from the stability limit [14, 23]. One of the salient observations in many of these simulations is that varying a chemical parameter, such as the activation energy E_a in a one-step Arrhenius kinetic model, can cause the temporal pattern of the pulsation to pass from regularly periodic to highly irregular (or so-called chaotic structures) through a successive temporal symmetry breaking. In fact, studies have shown that the degree of nonlinear longitudinal instability and chaos can be correlated qualitatively with the regularity of cellular pattern observed in multidimensional settings, i.e. that closer or below the 1D stability limit the cellular structure is more regular or vice-versa [18, 27, 28].

It was found recently that additional finite, small flow disturbances in the quiescent mixture can provide a mechanism to excite hidden unstable modes in detonation systems [29]. Similar effect has also been observed for unsteady flame propagation in systems perturbed with spatially discrete sources [30]. Contrarily, in the field of nonlinear dynamics and chaos, an approach to stabilize a chaotic system can also be done by means of small system perturbations on the initial conditions, without significantly modifying the overall dynamics of the system, e.g., the Ott, Grebogi, Yorke (OGY) method [31]. The use of a small disturbance is to encourage the dynamical system to remain near one or a few limited unstable, periodic orbits embedded in its original chaotic attractor. The result is to render an otherwise chaotic motion more stable, regular, and predictable. This idea that the critical response of a chaotic system to small changes in its initial conditions may be, in fact, very desirable in application practices of gaseous detonations. It is thus the objective of this work to explore such method in controlling the chaotic dynamics of detonation phenomenon.

In this work, high-resolution numerical simulations of the long-term dynamics of an idealized pulsating detonation are performed using the reactive Euler equations with a single-step Arrhenius chemical kinetics subject to an initial sinusoidal density perturbation in the reactive mixture. A spectrum of nonlinear dynamics and instabilities resulting from the change in perturbation wavelength is presented and examined. It is worth noting that, despite its simple formulation, this study has significant implications on how to control unstable gaseous detonations and affect their critical phenomena, and further understand its propagation dynamics into a spatially non-uniform medium with density heterogeneity, as often experienced in practical propulsion systems such as pulsed and rotating detonation engines (PDEs or RDEs) due to jet injection and incomplete mixing [32, 33].

2. Simulation details

Following the canonical numerical setting [34], the reactive Euler equations with single-step Arrhenius kinetics are solved using a second-order Weighted Average Flux (WAF) scheme with the van Leer limiter [35] to simulate the inviscid, unsteady, one-dimensional propagation of a detonation wave. The computational domain is given by a Cartesian grid arrangement of the size 200 $l_{1/2.}$ The boundary conditions for the left and right side of this domain are both transmissive. A "patching" technique is used to improve the simulation efficiency, i.e., when the detonation reaches a position 10 numerical grid points before the right boundary, a computational window of 190 $l_{1/2}$ enclosing the detonation structure is extracted and patched back at the left boundary, allowing the detonation to propagate again to the right and continue the evolution [36-38]. Only a small shift is introduced and the long downstream domain's back boundary does not influence the front dynamics. Accordingly, the corresponding density variation is thus continuously imposed and adjusted on the 10 $l_{1/2}$ in front of the leading detonation shock. The computations are initialized with the steady solution of the ZND detonation. A rightward-propagating detonation was initialized by imposing the steady ZND-wave solution on the grid in a region 10 characteristic reaction-zone lengths away from the left end of the domain. The detonation is allowed to propagate over a sufficient distance before it encounters the perturbation in order to reach the "converged" propagation and to eliminate influences from the rear boundary of the system. The non-uniform density perturbation with different wavelengths are imposed in front of the incident detonation given by:

$$\rho_0 = 1.0 + A \cdot \sin\left(\frac{2\pi}{\lambda} x\right) \tag{1}$$

where A is the amplitude fixed at 0.10 and λ is the wavelength of the sinusoidal disturbance, see Fig. 1. It is important to note that a sufficiently moderate value of A is required to excite and show clearly different behaviors of the nonlinear system. However, too large of perturbation amplitudes may overdrive the detonation [39] or cause pre-ignition in the reactants. It is thus found A = 0.10 most representative of the system dynamics. Furthermore, the one-dimensional unsteady detonation is allowed to propagate for a sufficiently long time into mixtures with different perturbation wavelengths λ, and the final nonlinear dynamics of the unstable detonation behavior are then analyzed.

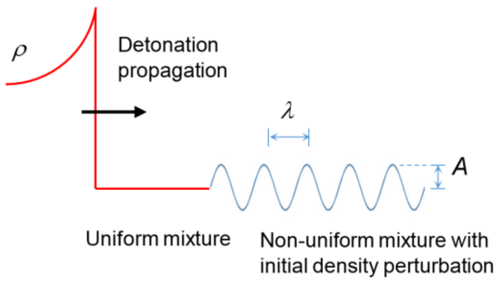

Fig. 1. A schematic representation of the problem.

A high numerical resolution of 100 points per half-reaction zone length of the steady ZND detonation $l_{1/2}$ is used to ensure the characteristic features of the pulsating front are properly resolved [12, 40]. A CFL number of 0.80 is considered. All variables are non-dimensionalized by the initial uniform conditions. The dimensionless heat release parameter and specific heat ratio are $\tilde{Q}/\tilde{\mathrm{R}}\tilde{T}_0 = 50^*$ and γ = 1.2, giving the corresponding Chapman-Jouguet (CJ) detonation velocity and von Neumann shock pressure D_{CJ} = 6.81 and p_s = 42.06, respectively. In previous investigations, the activation energy E_a is often used as a control parameter. In certain regions of this control parameter

* Tilde "~" denotes dimensional quantities.

space, the 1-D detonation dynamics are shown to exhibit chaotic behavior. Two values where the detonation pulsation is chaotic, i.e., $E_\mathrm{a} = \tilde{E}_\mathrm{a}/\tilde{\mathrm{R}}\tilde{T}_0$ = 28.5 and 30.0 are chosen in this work. The shock pressure evolution for these two cases are given in Fig. 2. With the use of a shock-capturing scheme, a subroutine is needed to detect the location and pressure of the leading shock front [14, 27, 28, 34]. The highest pressure value closest to the maximum pressure gradient defines the leading shock front's location. In detail, at each computation time step, the leading shock detection algorithm first finds the maximum pressure gradient $(\mathrm{d}p/\mathrm{d}x)_{\max}$ near the detonation front to locate the leading shock and search the few neighboring numerical grids for correctly recording the maximum shock pressure value p_s due to the smearing effect inherent to the shock capturing scheme. Also shown in Fig. 2, the red dashed line indicates the average value of the oscillations. Chaotic features such as random peak oscillation and a wide range in the frequency spectrum are seen for these cases.

3. Results and discussion

Results obtained for the case of E_a = 28.5 with various sinusoidal density perturbation wavelength λ are first presented in Figs. 3-6, showing again the leading shock pressure evolution of the unsteady detonation as it propagates into the initial density disturbance. The corresponding fast Fourier transform (FFT) spectrum for each case is also provided. Starting from Fig. 3, it is observed that for relatively small wavelength $\lambda < 190$, the presence of the initial density perturbation appears to cause the oscillatory behavior to tend toward low-frequency modes, and the occurrence of additional high frequency unstable modes. It can be seen from the FFT spectra that the dominant frequencies shift to lower values as λ increases, resembling to the chaotic behavior of the higher activation energy case (Fig. 2 b). In addition, with increasing λ, the oscillations of the leading shock pressure become more regular, as also seen in the FFT plots showing more discrete peaks.

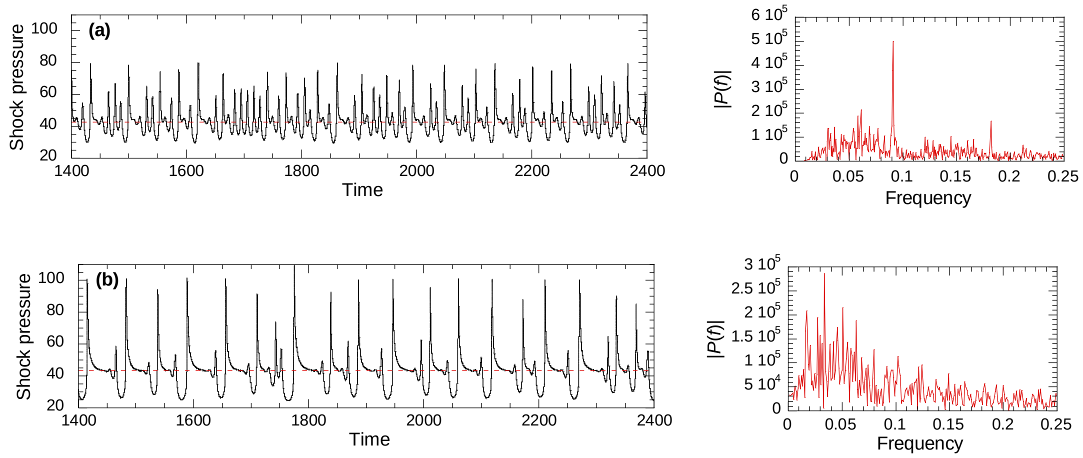

Fig. 2. Leading shock pressure history and its FFT frequency spectra showing the detonation chaotic propagation behavior for activation energies a) E_a = 28.5; and b) 30.0.

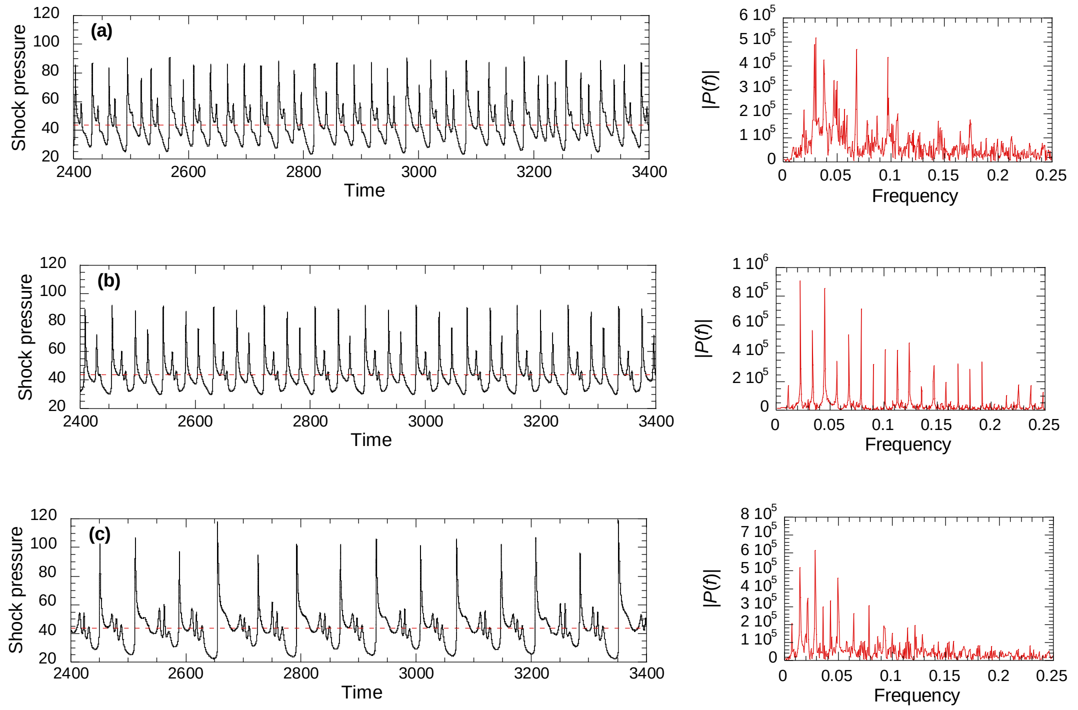

Fig. 3. Leading shock pressure history and its FFT frequency spectra of 1-D pulsating detonation with E_a = 28.5 subject to the initial density perturbation with wavelength λ equal to: a) 100; b) 150; and c) 190.

By further increasing the perturbation wavelength λ to the range of 220 – 265, the simulation results given in Fig. 4 show rather surprisingly regular oscillatory behaviors of the detonation propagation with different limit-cycle bifurcation modes, and with clear frequency modes and their harmonics in the FFT spectra. The oscillation amplitudes of these stable modes also decrease. Hence, the small initial sinusoidal density perturbation exerts a regularizing influence on the chaotic dynamics of the pulsating detonation. In other words, the introduction of a small, finite perturbation forces the originally chaotic attractor with many orbits to self-organize to limit cycles. Another band of chaos control is also observed approximately in the range around λ ~ 350 as shown in Fig. 5.

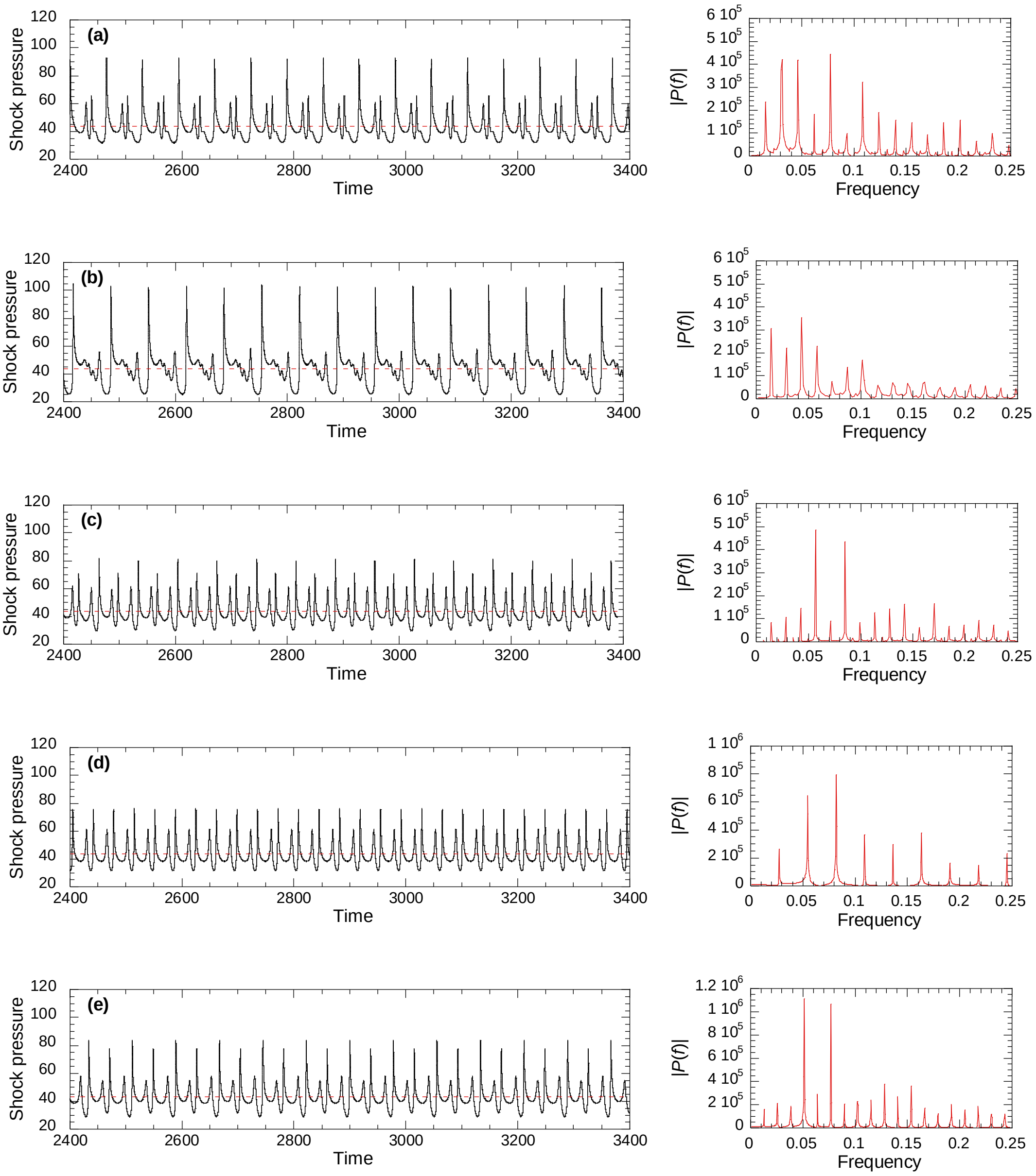

Fig. 4. Leading shock pressure history and its FFT frequency spectra of 1-D pulsating detonation with E_a = 28.5 subject to the initial density perturbation with wavelength λ equal to: a) 220; b) 230; c) 240; d) 250; and e) 265.

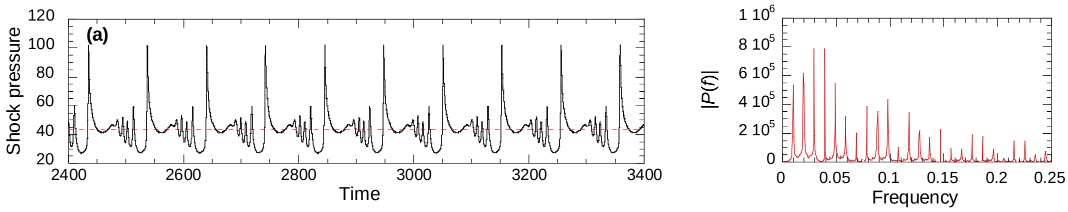

Fig. 5. Leading shock pressure history and its FFT frequency spectra of 1-D pulsating detonation with E_a = 28.5 subject to the initial density perturbation with wavelength λ = 350.

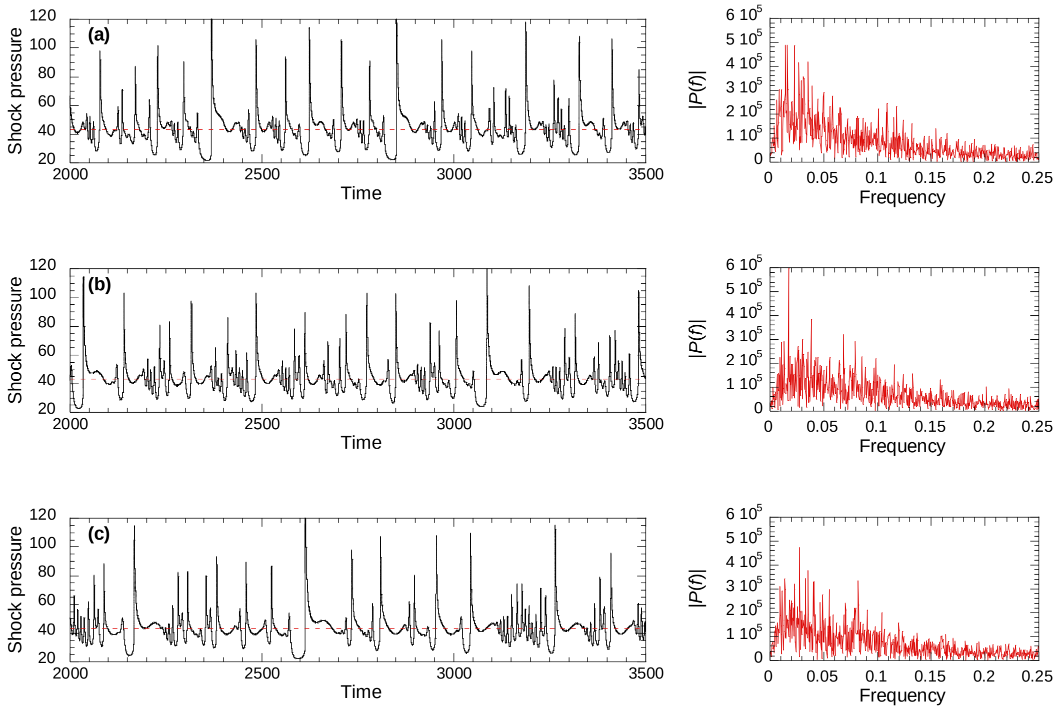

Fig. 6. Leading shock pressure history and its FFT frequency spectra of 1-D pulsating detonation with E_a = 28.5 subject to the initial density perturbation with wavelength λ equal to: a) 300; b) 400 and c) 500.

In between the control bands of limit cycle-like oscillations, some chaotic behavior persists as seen in Fig. 6a for λ = 300 where the oscillatory pattern is dominated by low-frequency modes with randomly embedded high frequency oscillations during the decaying phase of the large amplitude oscillations. For the cases with a very large wavelength λ, i.e., 400 – 500 (Figs. 6b and 6c), chaos re-emerges. The leading shock pressure oscillations are characterized by irregular fluctuations and a wide FFT frequency spectrum is observed.

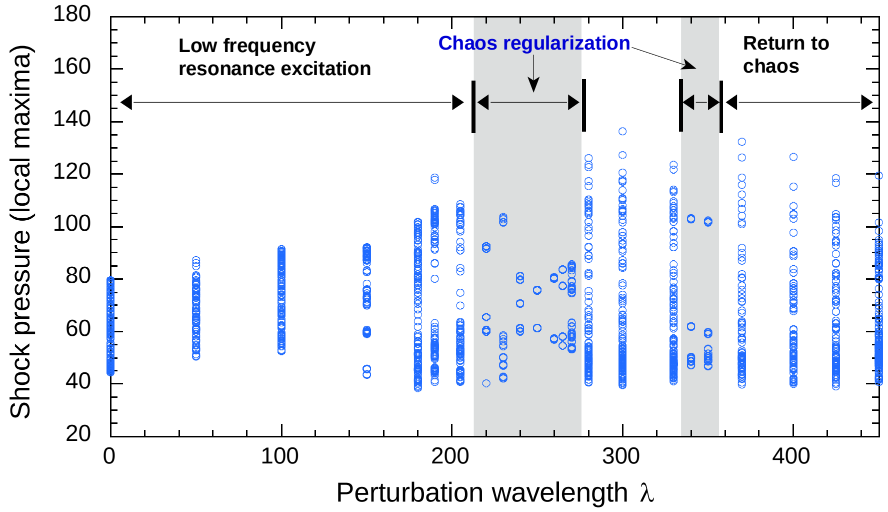

Fig. 7. Bifurcation diagram for 1-D pulsating detonation propagation with $E_a = 28.5$.

Using a MATLAB post-processing script to extract the local maxima of shock pressure oscillations from the numerical simulation's shock-pressure time-series, a bifurcation diagram is then constructed to demonstrate the modal evolution with varying wavelength λ, shown in Fig. 7. From this diagram, several regimes can be distinguished. Initially, for small λ, the perturbation effect is to excite higher amplitude, low-frequency modes, as shown in Fig. 3, and the 1-D detonation oscillatory behavior remains irregular with different modes given by a wide range of shock pressure values. As λ increases to a critical level, chaos regularization is observed via backward bifurcation where various unstable modes are restrained and the oscillations turn into limit-cycle types with fewer distinct peak values in leading shock pressure. Two bands of regularized chaos appear where the bifurcation plot shows only a limited number of oscillation peak pressures. For very large perturbation wavelengths λ, the oscillation patterns return to chaos.

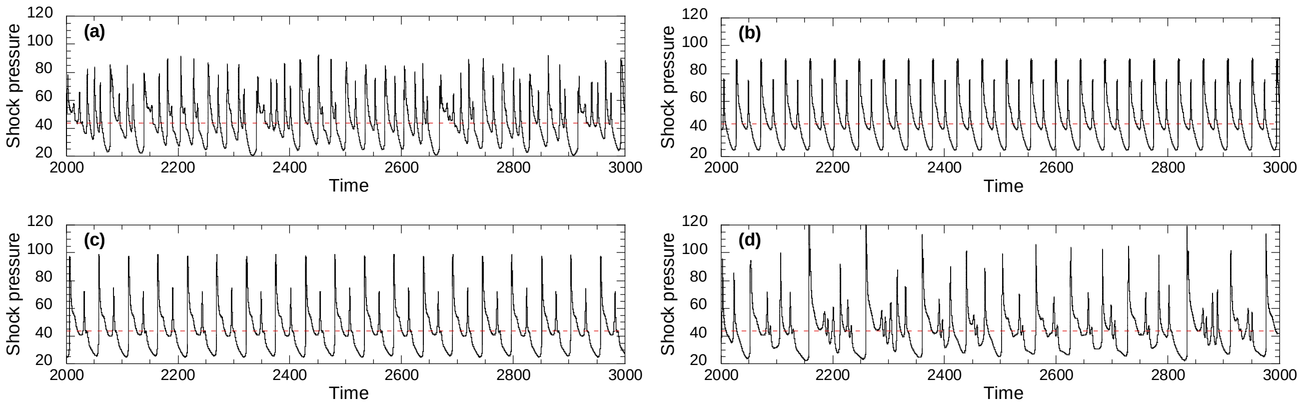

Fig. 8. Leading shock pressure history and its FFT frequency spectra of 1-D pulsating detonation with E_a = 30.0 subject to the initial density perturbation with wavelength λ equal to: a) 80; b) 100; c) 120; and d) 140.

Similar chaos control results were also obtained for E_a = 30.0, as shown in Fig. 8. For this activation energy value, Fig. 2b shows that even without the density disturbance, the oscillatory behavior of the 1D pulsating detonation is primarily dominated by low-frequency modes. It is found for E_a = 30.0, the chaos control is achieved at smaller perturbation wavelength λ (i.e., λ around 100 to 120) where limit cycle oscillations can be seen in Fig. 8.

The present results have demonstrated that the sinusoidal density perturbation can significantly affect the nonlinear dynamics of one-dimensional pulsating detonations and the perturbation wavelength λ is critical on both instability excitation and stabilization. It is worth recalling that high frequency unstable modes manifest at low activation energies with weak compression waves originating from the reaction zone, and reflected expansions originating from the shock front [15]. At higher activation energy, these disturbances are overshadowed by low-frequency, large fluctuations where the reaction's high temperature sensitivity causes disturbance characteristics originating at the end of the reaction zone and traversing the entire detonation length to be amplified by the heat release, i.e., through the shock wave amplification by coherent energy release (SWACER) mechanism [1]. Pulsating detonations are typically dominated by these low-frequency modes. In fact, the emerging chaotic behavior of pulsating detonations with high activation energies comes from the nonlinear interaction of the high frequency excitation of disturbances by the low frequency waves. Thus, additional high-frequency, weak density perturbation will only generate additional disturbances in the chemical reaction zone and likely excite further low-frequency modes without affecting the original intrinsic low frequency oscillation mode – similar to increasing the activation energy. Thus, for short wavelengths, one expects the density perturbation to have little effect on the chaos as shown in the work. To exhibit mode locking, the perturbation wavelength needs to be of the same order as the front's intrinsic low-frequency oscillation. From a nonlinear dynamics point-of-view, the perturbation's time-scale has to be sufficient to cause the initial chaotic attractor to remain in one or few dominant low frequency limit cycles for regularization. For future work, a characteristics analysis [15] should be considered to analyze the underling wave dynamics caused by the density perturbations of various λ.

4. Conclusion

In this study, we have examined numerically the possibility of using a small perturbation to vary the unstable dynamics of 1D pulsating detonation. A sinusoidal density perturbation was imposed in the fully manifested, chaotically propagating detonation and the effect of the perturbation wavelength λ on the nonlinear dynamics of the pulsating detonation was examined. It is found that small wavelength perturbations tend to excite low-frequency oscillation modes despite the propagation being still chaotic. Chaos regularization begins when the perturbation wavelength increases to a certain range and bands of chaos control are observed in which limit cycle type oscillations are achieved.

Despite only considering the simplest configuration of detonation dynamics, i.e., 1D longitudinal pulsation, the present results provide insights on how the perturbation technique can be considered to control the dynamic detonation parameters such as cell size or limits [1, 33, 41], which are related to the intrinsic instability of gaseous detonations.

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