Stability of One-dimensional Detonation Driven by Lokta-Volterra Oscillating Chemical Schemes

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1 Introduction

In unsteady one-dimensional (1D) simulation, the multi-dimensional cellular structure translates into a more or less regular longitudinal oscillating/pulsating behavior if the mixture properties enable the development of instability. Such an approach enables to access the complete range of non-linear dynamics of 1D detonations and can provide detailed information on the flow field. Using 1D numerical simulation driven by an irreversible one-step reaction model, Eckett et al. [1] showed that the neutral stability curves collapse to a single curve in the θ_{CJ}-M_{CJ} plane where θ is the reduced activation energy, M is the Mach number, and the subscript CJ designates a detonation propagating at the Chapman-Jouguet velocity. A similar result was obtained by Ng et al. [2] but when plotting the χ parameter as a function of the detonation Mach number, where $\chi = \theta(\Delta_i/\Delta_r)$ corresponds to the ratio of induction (Δ_i) to the reaction zone (Δ_r) length, multiplied by θ. These two parameters are widely employed to categorize detonation as weakly, moderately, or highly unstable, depending on the distance to the neutral stability curve. The non-linear stability of 1D propagating detonation has been investigated in a number of studies which considered a variety of reaction models from irreversible one-step to fully detailed ones [2, 3]. Typically, as the global activation energy of the chemical process is progressively increased, period-doubling bifurcation events are occurring and eventually lead to a chaotic behavior of the pulsating detonation which is characterized by sharp and large pressure jumps and low-amplitude oscillations, see [4]. Despite the large number of studies on the non-linear stability of detonation, to the best of our knowledge, the effect of complex, multi-step heat release profile has never been investigated.

A limited number of chemical systems exhibit multi-step heat release behavior. These include nitromethane containing mixtures, [5], rich fuel-NO_2/N_2O_4 mixtures where the fuel can be H_2, CH_4, or C_2H_6, [6–9], very lean H_2-N_2O mixtures [9], rich dimethyl ether-oxygen (DME-O_2) mixtures [10, 11], rich silane-nitrous oxide mixtures [12], and C-O mixtures relevant to detonation in type Ia supernovae, [13]. Recently, we have proposed the utilization of modified Lokta-Volterra (LV) auto-oscillating chemical schemes as a simple approach to generate multi-step heat release profiles [14]. The characteristics of the steady detonation solutions, the direct detonation initiation (DDI) process, as well as the two-dimensional cellular structure were investigated for various LV schemes. Concerning steady detonation, up to 8 peaks of heat release could be obtained depending on the specific kinetic parameters employed. It was also found that strong velocity oscillations could be generated at large over-drive during the DDI process. Finally, multi-scale cellular structures were observed for some of the LV schemes. Although different aspects of detonation driven by LV schemes were studied, their non-linear stability remains unknown. In the present study, we have performed high-resolution numerical simulations for such unsteady detonations, driven by LV schemes which demonstrate single- or multi-step heat release profiles. A number of analyses were performed to characterize the dynamics of the system. These results contribute to a better understanding of the effect of multi-stage heat release on detonation dynamics.

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2 Simulations and analysis

2.1 Numerical simulation

To simulate the 1D pulsating detonation, the in-house code ASURF has been employed and the planar geometry was considered. All the simulations were performed using the Euler equations

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = S_R \tag{1}$$

where t and x are the temporal and spatial coordinates. U, F(U), F_v(U), and S_R are defined as:

$$U = \begin{pmatrix} \rho Y_1 \\ \vdots \\ \rho Y_n \\ \rho u \\ E \end{pmatrix} ; \; F(U) = \begin{pmatrix} \rho U Y_1 \\ \vdots \\ \rho U Y_n \\ \rho u^2 + P \\ (E+P)u \end{pmatrix} ; S_R = \begin{pmatrix} \omega_1 \\ \vdots \\ \omega_n \\ \\ 0 \\ 0 \end{pmatrix} \tag{2}$$

In the equations 2, ρ, u, E, Y_k, ω_k, P, are the density, flow velocity, total energy per unit mass, mass fraction of species k, the production rate of species k, and the pressure.

Concerning the numerical methods: (i) second-order Strang splitting fractional-step procedure was utilized to separate the time evolution of the reaction term S_r from that of the convection term; (ii) the Euler explicit scheme was used for temporal integration; and (iii) the HLLC scheme was used to calculate the convective flux. The simulations were initiated by mapping the ZND solution onto the 1D domain. The instability grows from the numerical error of unsteady code initialization. At the right boundary, through which the fresh mixture is fed into the domain, the transmissive boundary condition is employed. At the left boundary, a moving wall condition is imposed. Multi-level adaptive mesh refinement has been employed. Following a grid convergence study based on the approach of Hwang et al. [15], we employed a grid resolution of at least 200 points/Δ_i.

To generate chain-branching driven single- and multi-step of heat release in the ZND temperature or thermicity profile, we employed modified Lokta-Voltera (LV) reaction models [14], described as

- R_0: $A \rightarrow X$ $\quad k_0 = A_0 T^{B_0} \exp^{\frac{-E_{a,0}}{RT}}$
- R_1: $A + X \rightarrow 2X$ $\quad k_1 = A_1 T^{B_1} \exp^{\frac{-E_{a,1}}{RT}}$
- R_2: $X + Y \rightarrow 2Y$ $\quad k_2 = A_2 T^{B_2} \exp^{\frac{-E_{a,2}}{RT}}$
- R_3: $Y \rightarrow B$ $\quad k_3 = A_3 T^{B_3} \exp^{\frac{-E_{a,3}}{RT}}$

where A is the reactant, B is the product, and X and Y are radicals, k is the rate constant, E_a is the activation energy, R is the perfect gas constant, T is the temperature, and i is the i^{th} reaction.

2.2 Wavelet transform analysis

To characterize the stability and dynamics of the pulsating detonation, we have employed wavelet transform (WT), which enables to unfold a signal into both time and frequency. The WT analysis consists in using analyzing functions, i.e., the daughter wavelets, which essentially act as pass-band filters. For a discrete data series, the wavelet transform (W) of a function $f(t)$ takes the form

$$W_n(s) = \sum_{n'=1}^{N} \left(\frac{\delta\tau}{s}\right)^{1/2} f(t) \Psi^*_{s,\tau}\left(\frac{(n'-n)\,\delta\tau}{s}\right), \tag{3}$$

where n is the time index; s is the scale dilation parameter; N is the number of data points, $\delta\tau$ is the time between two consecutive data points; and $\Psi^*_{s,\tau}$ is the complex conjugate of the daughter wavelet. The wavelet power spectrum (P_Ψ), corresponding to the energy at scale s, is obtained from

$$P_\Psi(s) = |W_n\left(s\right)|^2. \tag{4}$$

Because it provides a good compromise between time and frequency localizations, We have chosen to employ as the mother wavelet the complex Morlet wavelet function given as

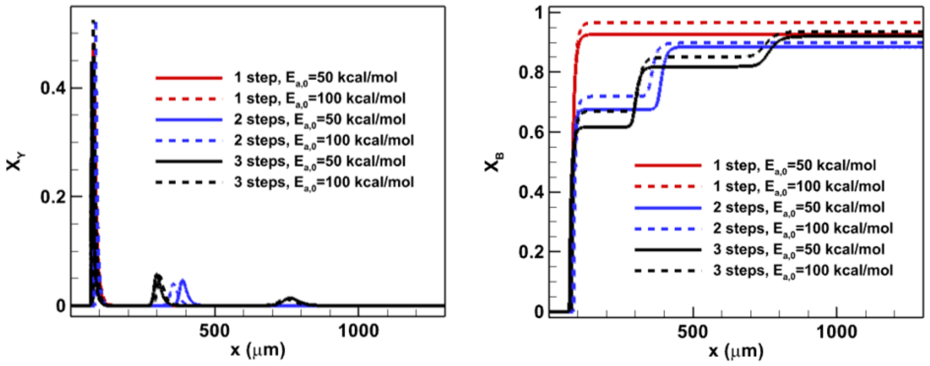
$$\Psi_0\left(\eta\right) = \pi^{-1/4} e^{i\omega_0\eta} e^{-\eta^2/2}, \tag{5}$$

where η is a non-dimensional time parameter; and i is the imaginary unit; and $\omega_0 = 6$.

3 Results and discussion

3.1 Chemical schemes and steady structure

Lokta-Volterra schemes with 1-, 2-, and 3-steps of heat-release with the activation energy of initiation reaction, $E_{a,0}$ equal to either 50 or 100 kcal/mol, have been employed. For all the schemes, the heat capacity ratio is fixed at 1.5. To facilitate the control of the heat release profile, reactions 0 to 2 are thermally neutral and only reaction 3 is exothermic. Therefore, the temperature and mole fraction of B have exactly the same temporal evolution. For all the reactions, B_i are set to zero to avoid the explicit temperature-dependence of rate constants. The activation energy for all the reactions are equal to zero, except the one for the initiation reaction. The pre-exponential factors for each scheme was chosen so that the induction length with respect to the first stage of heat release, Δ_1, for all the cases when $D = D_{CJ}$, was 80 μm $\pm$ 12.5% and the maximum thermicity of the first stage, σ_1, was 2.75×10^7 1/s $\pm$ 20%. Different cases with $D = 1.0D_{CJ}$, $1.2D_{CJ}$, $1.4D_{CJ}$, and $1.6D_{CJ}$ were used to study the effect of detonation velocity on stability.



a) Mole of fraction of Y b) Mole of fraction of B

Figure 1: Mole fraction profiles obtained by ZND calculation for a LV chemical scheme with one, two and three stages of heat-release with different $E_{a,0}$ and $D = D_{CJ}$.

The ZND profiles of Y and B mole fractions obtained for the schemes with 1- to 3- steps of heat-release, and $E_{a,0}$=50 and 100 kcal/mol are shown in Fig. 1. The profiles of X_Y clearly demonstrate either a single peak or multiple peaks. The first peak is the highest and narrowest, whereas the subsequent ones are much smaller and tend to spread over larger widths. The profiles of X_B are characterized by a single increase or by several successive phases of increase. Before each rapid increase, the mole fraction of B remains essentially constant. Table 1 presents the characteristics of ZND solution for various LV chemical schemes. From the reported θ and χ values, the ZND calculations indicate that the stability of unsteady detonation should decrease when the activation energy of the initiation step is increased from 50 to 100 kcal/mol. The change of stability parameters are not consistent for the same $E_{a,0}$, when the number of heat-release stages changes: when $E_{a,0}$=50 kcal/mol, χ decreases from 11.7 for mixture with 1-step to 1.9 for the one with 3-steps heat-release; however, for the same $E_{a,0}$, θ increases from 2.1 for mixture with 1-step to 7.6 for mixture with 3-step of heat-release. Such an inconsistency is also observed when $E_{a,0}$=100 kcal/mol. This contradiction between θ and χ, means that it is unclear whether a stabilizing or a destabilizing effect of the multi-step heat release should be expected. Unsteady simulation is necessary to determine which criterion is correct. To conclude this section on the steady structure, we note that the multi-step heat release is suppressed for over-driven detonations.

Table 1: Characteristics of the ZND solutions for various Lotka-Volterra chemical schemes. In all cases: D/D_{CJ}=1. The θ and χ are based on the first peak of heat release regardless of the total number of peaks. $E_{a,0}$ in kcal/mol, Δ_i in μm, σ_i is the maximum thermicity in 1/s.

peaks	$E_{a,0}$	Δ_1	Δ_2	Δ_3	σ_1	σ_2	σ_3	θ	χ
1	50	80.0			2.74E7			2.1	11.7
1	100	80.1			2.74E7			4.1	22.3
2	50	79.9	389		2.74E7	2.25E6		10.9	2.0
2	100	86.9	357		3.17E7	1.88E6		17.6	2.6
3	50	72.5	300	763	2.23E7	2.29E6	5.35E5	7.6	1.9
3	100	79.2	310	749	2.57E7	2.08E6	4.41E5	12.3	2.4

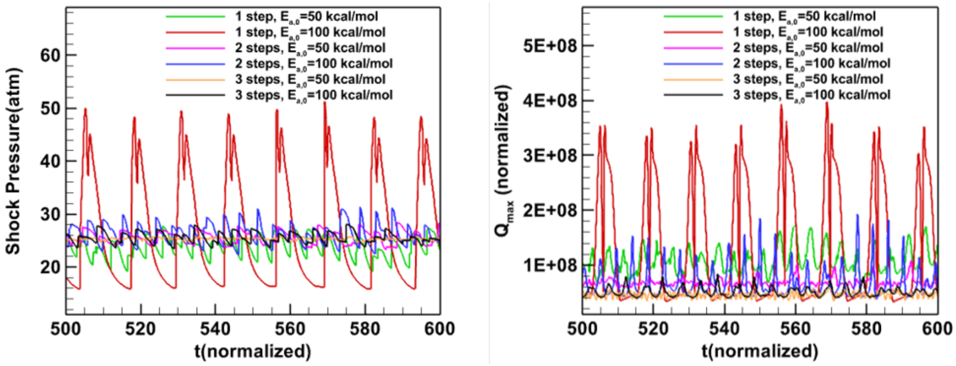
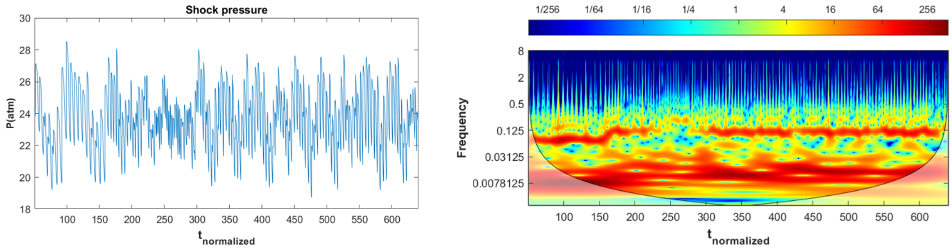


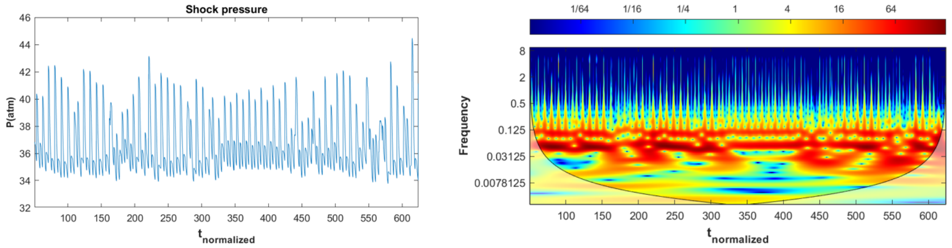
Figure 2: Shock pressure and heat release rate as a function of normalized time for unsteady detonation driven by LV chemical schemes. In all cases, the inflow velocity was $D = D_{CJ}$.

3.2 Unsteady detonation

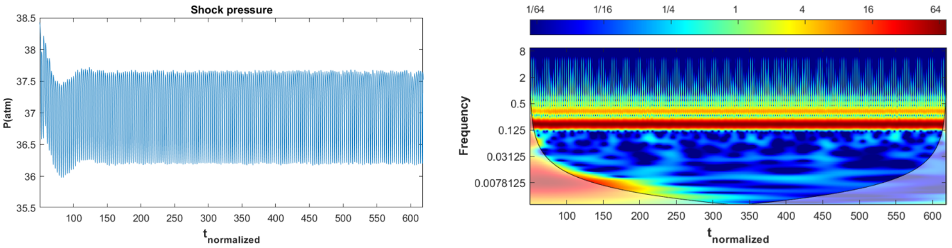
Unsteady simulations were performed under the same conditions as the ones illustrated in Figure 1 and Table 1. Figure 2 shows the shock pressure and maximum heat release rate profiles over the range 500$< t_{normalized} <$600, for which the detonations have already reached their long-term behaviors. The strength of the oscillations are very different for the different LV schemes, with the largest oscillations induced when $E_{a,0}$=100 kcal/mol and for only one step of heat release. The analysis of the power spectral densities (PSD) of the shock pressure history (not shown) indicates that the maximum power of the oscillations tends to decrease as the number of thermicity peaks increases, whereas no clear trends can be observed for the number of oscillation modes. The evolution of χ/θ with the number of heat release peaks is consistent/inconsistent with the decrease of the oscillation amplitude. Although increasing the overdrive does not lead to clear trends, we observed that at all velocities, stronger oscillations are generated when $E_{a,0}$=100 kcal/mol than when $E_{a,0}$=50 kcal/mol. In general, the amplitude of the oscillations decreases as the number of thermicity peak at D/D_{CJ}=1 increases.



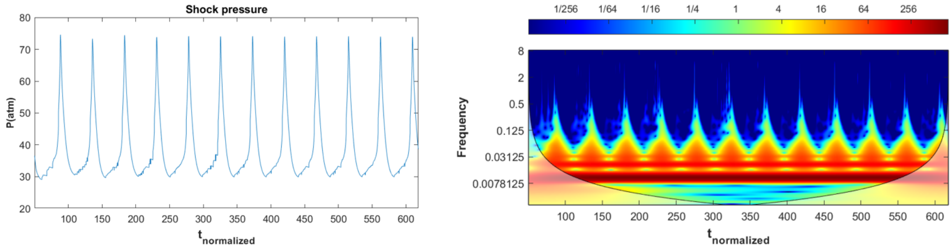
a) LV scheme with 1-steps heat-release and $E_{a,0}$ = 50 kcal/mol, $D = 1.0D_{CJ}$



b) LV scheme with 1-steps heat-release and $E_{a,0}$ = 50 kcal/mol. $D = 1.2D_{CJ}$



c) LV scheme with 2-steps heat-release and $E_{a,0}$ = 50 kcal/mol, $D = 1.2D_{CJ}$.



d) LV scheme with 2-steps heat-release and $E_{a,0}$ = 100 kcal/mol

Figure 3: Shock pressure and associated wavelet transform for several LV chemical schemes.

Figure 3 shows the shock pressure signals and associated wavelet transforms obtained with various LV schemes, illustrating the effects of over-drive (Fig. 3 a) to b)), of the number of heat release stages (Fig. 3 b) to c)), and of $E_{a,0}$ (Fig. 3 c) to d)). At D/D_{CJ}=1 for a LV scheme with 1-step heat release and $E_{a,0}$ = 50 kcal/mol, the pressure signal appears highly irregular with a dominant frequency in the wavelet power spectrum around 0.125, and a large band of high power in the range 0.0039-0.03125. At high frequency, the pressure peaks appear as elongated features. The maximum amplitude in the pressure profile is on the order of 8 atm. Increasing the velocity to D/D_{CJ}=1.2 does not fully stabilize the detonation. The pressure profile remains quite irregular and shows similarity with a typical multi-mode profile, with a maximum amplitude around 6 atm. The wavelet spectrum is characterized by two dominant, quasi-continuous bands at 0.125 and 0.0625, the latter being the fundamental frequency, while the former corresponds to an harmonic. The pressure spikes of the different oscillating modes appear as elongated features with more or less large base, possibly of triangular shape. Performing a same simulation but with a LV scheme that exhibits two steps of heat release leads to a dramatically different pressure profile. Once the long-term behavior has been established, the amplitude of the pressure oscillations is about 1.5 atm only, whereas the period of oscillation has largely decreased compared to the cases presented in Fig. 3 a) to b). In addition, the profile appears as highly regular. The wavelet transform spectrum demonstrates a very high-power, continuous band at a frequency slightly above 0.125. A band of significantly lower intensity is also present at a frequency approximately twice that of the high-intensity band. Thin elongated features are present in the high-frequency range. Increasing the activation energy of the initiation step from 50 to 100 kcal/mol, both the amplitude and the period of the pressure oscillations dramatically increases. The pressure amplitude reaches 35 atm, whereas the period increases by more than one order of magnitude. On the other hand, the pulsating detonation remains regular. The wavelet power spectrum exhibits a band of high power just above 0.0078125, as well as large triangular features, which are a result of the wide pressure spikes.

4 Conclusion

The non-linear stability of 1D detonations driven by various LV oscillating chemical schemes was studied using high-resolution numerical simulations. In general, the θ and χ parameters cannot provide reliable predictions of the stability characteristics of pulsating detonation driven by multi-step heat release. The LV schemes that exhibit several steps of heat release tend to lead to more stable detonation. The over-drive and $E_{a,0}$ have strong influence on the non-linear stability. In the future, the linear stability of LV-driven detonation should be investigated to help interpreting the results obtained in the present study.

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