One-dimensional stability analysis of vibrational nonequilibrium effect on detonation neutral stability

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1 Introduction

Detonation often exists in unstable form during propagation and is difficult to be observed experimentally. To investigate the instability of detonation wave, it is common to solve the steady one-dimensional conservation equations first and introduce small perturbations in the solution later to see if the amplitude of the perturbations grows or decay. In the mid of 20th century, Erpenbeck [1-3] has conducted an extensive study on this problem using an initial value Laplace transform approach. Thereafter Lee & Stewart [4] revisited the problem by using a normal mode approach in the linear stability analysis. With the increase of computational power in recent decades, parametric studies with dependence on activation energy, overdriven factors, heat release, etc. have been thoroughly demonstrated with simplified chemical models. Different scenarios of detonation problems such as chemistry involving two-step chain-branching reaction model, cylindrically and spherically expanding detonation and pathological detonation were discussed [5-7].

Nevertheless, recent researches have suggested that the vibrational relaxation mechanism is crucial in gas detonation to account for the difference of cell sizes between experiments and simulations and in the flame ignition and stabilization of supersonic scramjet combustion [8, 9]. Shi et al. [10] has simulated both onedimensional (1D) and two-dimensional (2D) argon-diluted hydrogen-oxygen detonation and reported that vibrational relaxation elongates the half reaction length and enlarges of detonation cell size. The computed cell size becomes comparable with the experimental one and the significant influence of vibrational relaxation effect is therefore concluded. To theoretically reveal the physical mechanism of vibrational relaxation effect on half reaction length and the cell size, Uy et al. [11] has proposed a modified ZND model with simplified chemical-vibrational coupling mechanism. A critical time ratio of the chemical time scale to the vibrational time scale, above which the vibrational relaxation effect becomes insignificant, has reported in the parametric studies.

In this report, single-step chemistry coupled with vibrational relaxation mechanism is considered in hydrogen-related detonation stability analysis. The present study aims to numerically investigate the shift of neutral stability range at the fixed activation energy under different time scale ratio of the chemical time scale to the vibrational time scale.

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2 Governing Equations and Numerical Method

To simulate the propagation of the detonation wave, 1D reactive Euler equations are considered and the energy equation is coupled with vibrational energy term. Equations are presented in normalized form as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0 \tag{1}$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} = 0$$
⁽²⁾

$$\frac{\partial(\rho e)}{\partial t} + \frac{\partial[u(\rho e + p)]}{\partial x} = 0$$
⁽³⁾

With the specific internal energy e, specific translational energy e_{tr} , and specific vibrational energy e_v described as

$$e = e_{tr} + \frac{u^2}{2} - \lambda Q + e_v \tag{4}$$

$$e_{tr} = \frac{f}{2} T_{tr}, f = \frac{2}{(\gamma - 1)}$$
(5)

$$e_{v} = \frac{\vartheta}{exp(\vartheta/T_{v}) - 1} \tag{6}$$

where ρ , u, p, Q, γ , f, ϑ and T_v are the density, velocity, pressure, local heat release, ratio of specific heats, degree of freedom of reactant (or product) molecules, characteristic vibrational temperature and vibrational temperature, respectively. Gas constant R is not shown in Eq. (5) and (6) because they are in non-dimensional form (presented in Eq. (9) later).

Chemical kinetic and vibrational relaxation models are introduced to couple with the energy equation. A simplified single-step Arrhenius model is applied to describe the chemical reaction process:

$$\frac{\partial(\rho\lambda)}{\partial t} + \frac{\partial(\rho u\lambda)}{\partial x} = -\rho k\lambda \exp\left(-E_a/T\right)$$
(7)

where λ , k, E_a and T denote the reaction progress variable, pre-exponential factor, activation energy and temperature respectively. λ is equal to unity at the upstream state and is equal to 0 at the downstream state, representing the completion of reaction.

Considering the vibrational relaxation mechanism, the Landau-Teller model is adopted to describe the energy mode exchange between translational-rotational mode and the vibrational mode. The equation is then formulated as:

$$\frac{\partial(\rho e_v)}{\partial t} + \frac{\partial(\rho u e_v)}{\partial x} = \rho \frac{e_v^{eq} - e_v}{\tau_v}$$
(8)

where e_v^{eq} and τ_v are the vibrational energy at the equilibrium state and the vibrational relaxation time, respectively. To describe e_v^{eq} , T_v in Eq. (6) is replaced by translational-rotational temperature T_{tr} , with the assumption that the translation mode and the rotational mode attain the equilibrium state right after the shock. Park's two-temperature model [12] with the geometrical average temperature $T_{avg} = \sqrt{T_{tr}T_v}$ is selected to manifest the chemical-vibrational coupling effect because of its simplicity, which has been applied in related studies [10]. Therefore, T in Eq. (7) will be replaced with T_{avg} .

Notably, normalized parameters are applied in the above equations with the unburned state values which are denoted with the subscript 0: (the superscript * represents the dimensional quantities)

$$\rho = \frac{\rho^*}{\rho_0}, p = \frac{p^*}{p_0}, T = \frac{T^*}{T_0} = \frac{\rho_0 R T^*}{p_0}, u = \frac{u^*}{\sqrt{RT_0}}, x = \frac{x^*}{\mathcal{L}_{1/2}}, \vartheta = \frac{\vartheta^*}{T_0}$$

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$$t = \frac{t^*}{\mathcal{L}_{1/2}/\sqrt{RT_0}}, Q = \frac{Q^*}{RT_0}, k = \frac{k^*}{\sqrt{RT_0}/\mathcal{L}_{1/2}}, E_a = \frac{E_a^*}{RT_0}$$
(9)

where $\mathcal{L}_{1/2}$ is the half reaction length and is defined as the distance from the shock to where one half of the reactant is consumed. In the present study, $\mathcal{L}_{1/2}$ is set as unity and only k is varied, with E_a , Q and γ fixed. The unsteady Euler equations presented above are then solved by the conservation element and solution element (CE/SE) method with second-order accuracy [13-18]. The computations are initially set up with the steady solution of the ZND detonation coupled with vibrational energy term. An effective numerical resolution of 128 points per half reaction zone length is suggested for the convergence in these analyses according to the previous researches [19]. The code is validated by reproducing the case of 1D piston-supported detonation case with $E_a=50$, Q=50 and $\gamma=1.2$ [20].

3 Results on comparison with respect to different time ratio

In this report, $E_a=25.30$ is selected for the analysis, while Q=50 and $\gamma=1.2$ are fixed. According to the analysis by Ng et al. [21] on the similar settings under thermal equilibrium assumption, the neutral stability condition is at $E_a=25.26-25.27$. To account for the vibrational relaxation mechanism in H₂ detonation problem, characteristic vibrational temperature $\vartheta^*_{H_2}=5989$ K [22] is chosen for the analysis. The reason of choosing H₂ is due to the dominating role of it in this problem and has been discussed by Taylor et al. [8]. τ^* is introduced and is denoted as the time ratio of the characteristic chemical time scale τ_{chem} to the vibrational relaxation time τ_v , i.e. $\tau^* \equiv \tau_{chem}/\tau_v$, as discussed in Uy et al. [11]. In other words, τ_v can be evaluated by fixing τ^* and τ_{chem} , which is the current practice in this analysis. τ_{chem} is defined as the time for which one half of the reactant is consumed. Figure 1 shows the shock pressure profile, p, as a function of time, t, with (a) the benchmark case under thermal equilibrium assumption with vibrational energy term considered, and the cases under thermal nonequilibrium assumption with time ratio fixed at (b) $\tau^*=2$, (c) $\tau^*=4$ and (d) $\tau^*=6$.





Figure 1: Shock pressure history for E_a =25.30, Q=50 and γ =1.2, under (a) thermal equilibrium assumption and (b-d) thermal nonequilibrium assumption with time ratio fixed at (b) τ^* =2, (c) τ^* =4, and (d) τ^* =6, respectively. eq: vibrational equilibrium; Neq: vibrational nonequilibrium

Conventionally it is expected that $E_a=25.30$ is in the range above the neutral stability boundary and therefore the propagation should become unstable when time goes on. With the decrease in τ^* , the peak of the first pulse becomes higher and there is a maximum of 17% increase compared with the equilibrium case. This pulse is defined as the "ignition pulse" by Watt & Sharpe [6] and it has no relation with the stability of detonation propagation. Moreover, the smaller amplitude and lower frequency of the pulse afterwards under smaller τ^* ($\equiv \tau_{chem}/\tau_v$) implies that the pulse become less unstable under vibrational nonequilibrium effect. At $\tau^*>6$, the simulated pressure profile becomes comparable with the equilibrium case (a). This can be explained by the concept of critical time ratio proposed by Uy et al. [11], beyond which the vibrational relaxation becomes insignificant.



Figure 2: The variations of peak pressure difference with time for the thermal equilibrium case (*eq*) and thermal nonequilibrium cases (*Neq*) at $\tau^*=2$, 4, and 6.

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Figure 2 shows the temporal variations of peak pressure difference for the corresponding four profiles in Figure 1. The peak pressure difference is obtained by subtracting each peak pressure from the 2nd peak value in the corresponding pressure profile. Notably, the 1st peak is excluded because ignition pulse is irrelevant in the stability analysis. The first point in every case is zero since it is subtracted from the 2nd peak value itself and is denoted as the reference point. The thermal equilibrium (*eq*) case (a), and the thermal nonequilibrium cases (*Neq*) at $\tau^*=4$ (c) and $\tau^*=6$ (d) show general increases in amplitude overall when time goes on, which fit with the expectation of the mildly unstable case at $E_a=25.30$. However, the thermal nonequilibrium case (b) at $\tau^*=2$ shows a different trend and the pulsation decays with time. In other words, the detonation propagation is stabilized. This result indicates that there is a shift of neutral stability boundary to a higher value of E_a if vibrational relaxation is significant. The possible τ^* range in which the shift of neutral stability boundary becomes significant is at $\tau^* < 4$. Further study will be conducted to explore more on the vibrational nonequilibrium effect in the detonation stability.

4 Conclusion

A mildly unstable detonation is simulated to elucidate the shift of neutral stability boundary for the hydrogen detonation under thermal nonequilibrium assumption. The ratio of the characteristic chemical time scale to the vibrational time scale, τ^* , is introduced to describe the different degree of the vibrational nonequilibrium, following the work by Uy et al. Cases at $\tau^*=2$, 4 and 6 are simulated and compared with the benchmark case at thermal equilibrium. With the decrease of τ^* , corresponding to the case when vibrational relaxation effect is significant, the ignition pulse can reach to a maximum of 17% increase compared with the baseline case. Moreover, the smaller amplitude and lower frequency of pulsation under smaller τ^* suggests that the detonation instability is suppressed under increasing vibrational nonequilibrium. Furthermore, the simulated temporal variation of peak pressure at $\tau^*=2$ shows decay in contrast with the other cases at the fixed E_a . This implies that a shift of neutral stability boundary to a higher E_a will take place when vibrational relaxation relaxation is substantial. The possible τ^* range for the shift is at $\tau^*<4$ and requires further clarification.

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