Numerical Study of Detonation Instability for a Two-Step Kinetics Model

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Introduction

Most of the works on the stability analysis of detonations have used one-step, irreversible reaction with an Arrhenius form of the reaction rate (e.g. [1]&[2]). The first formal linear stability studies were conducted by Erpenbeck, who used a Laplace transform approach to study the behavior of small-amplitude disturbances for a plane steady detonation wave [1]. Normal mode approach to the linear stability problem were developed by Lee & Stewart and also sharp ([2]&[3]). In parallel with linear stability analyses, there have been numerous studies concerned with the numerical simulation of the pulsating detonation instability with Arrhenius one-step reaction kinetics. In one-dimensional calculations, the detonation instability appears as oscillatory behavior of detonation front. Using advanced numerical techniques, a significant improvement in the quality and accuracy of such simulations was attained (e.g. [4]&[8]). Those simulations were able to obtain numerical results in close agreement with the theoretical predictions. Short and Quirk carried out a linear stability analysis by making use of a three-step chain-branching reaction [5]. In their work the chain-branching cross-over temperature was used as a bifurcation. A two-step reaction model was used by Sharp to study the linear stability of pathological detonations [6]. In his model the first step is endothermic and the second one is exothermic. He concluded that decreasing the value of Ea1-Ea2 (activation energy of the first step –activation energy of the second step) tends to stabilize pathological detonations.

Previous works indicated the important role of induction and reaction length on the instability. However, no attempt has been made to investigate these roles systematically. In this paper a two-step reaction model is used. The first is a non-heat release induction step and the second one is an exothermic reaction.

The method of study

The detonation is initiated using a blast wave. The chemical reaction is modeled by a two-step kinetics. The first step indicates induction delay where reactant A is converted to A^*. In the second step the energy of the reaction is released. These two steps can be shown by two reactions:

$$A \rightarrow A^*, \quad \text{and} \quad A^* \rightarrow B.$$

The rate of reactions progress are given by:

$$w_1 = \frac{d\alpha}{dt} = -K_1 \alpha \exp\left| \frac{-Ea_1}{RT} \right| \quad , \quad w_2 = \frac{d\beta}{dt} = -K_2 \beta \exp\left| \frac{-Ea_2}{RT} \right|$$

where $w1$ and $w2$ are reaction rates, $K1$ and $K2$ are constant of reactions, T is the absolute temperature, R is the specific gas constant, and $Ea1$ and $Ea2$ are activation energies. α and β are progress variables of two reactions. For induction step, $0 < \alpha < 1$ and $\beta = 1$, while in exothermic step, $\alpha = 0$ and $0 < \beta < 1$. The governing equations used are the one-dimensional reactive Euler equations:

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$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}=S \quad , \; U=\begin{vmatrix}\rho\\ \rho u\\ \rho e\\ \rho\alpha\\ \rho\beta\end{vmatrix} , F=\begin{bmatrix}\rho u\\ \rho u^2+p\\ u(e+p)\\ \rho u\alpha\\ \rho u\beta\end{bmatrix} \text{, and } \quad S=\begin{vmatrix}0\\ 0\\ 0\\ -\rho w_1\\ -\rho w_2\end{vmatrix}$$

Where variables ρ , u, p and e are density, particle velocity, pressure and specific internal energy, respectively. A polytropic equation of state and an ideal thermal equation of state are assumed,

$$e=\frac{p}{\rho(\gamma-1)}+\frac{u^2}{2}+Q\beta \quad , \qquad P=\rho RT$$

In this relation Q is the heat release per unit mass of reactant and γ is the ratio of specific heats. The dependent variables are non-dimensionalized with respect to the unburned mixture properties. Density is non-dimensionalized with ρ_0, and pressure with γp_0. For the velocity, the sound speed of the unburned mixture, Co, is used as the reference. The characteristic length scale, Lc, is half reaction length of steady ZND detonation. The characteristic time scale is $t_c = L_c / C_0$. In all calculations here, Q/RTo=50 and γ=1.2 are used.

In the present work, PPM (Piecewise Parabolic Method) is chosen as the main gasdynamics solver [9]. In analyzing the propagation of pulsating detonation, the tracking of the shock front has an essential role. For this purpose, conservative front tracking of Chern and Colella has been utilized [10]. Since all reactions are completed in a narrow region close to the shock, it is more economical to use fine meshes only in this region and coarse grids elsewhere. To fulfill this requirement, a simple version of the "Adaptive Mesh Refinement" of Berger and Colella has been utilized [11]. The developed code is validated via several test problems [8].

Results

Previous researches have shown that for one-step Arrhenius kinetic model the activation energy is the main parameter which determine the instability of CJ detonation (e.g., [1] and [2]). In one-step model, for a mixture with Q/RTo=50 and γ=1.2 the ZND structure is unstable for Ea/RTo higher than 25 ([1],[2]). Increasing the activation energy beyond this limit, the detonation front exhibits oscillatory behavior (Fig.1).

The effect of activation energy on the detonation front behavior has been studied in this work. Calculations were arranged in two stages. In each stage, one activation energy was kept constant and the other one changed. The results of calculations are presented in Figures 2 to 8. In these figures the front shock pressure are plotted vs. the instantaneous shock location.

At first stage, the activation energy of the second step was kept constant (i.e., Ea2=20) and Ea1 was changed. The variation of shock pressure for Ea1=5 is demonstrated in Fig.2. It is seen that the front shows a regular oscillation, with small amplitude. Increasing Ea1 to 8, causes a larger amplitude (Fig.3). An irregular oscillation appears as the activation energy increased to 10 (Fig.4). In this case, it is observed that increasing the activation energy of induction step promotes the detonation instability. This result is similar to that of one-step model.

In the second stage of calculations, the effect of Ea2 on detonation instability has been studied while Ea1 was constant (i.e., Ea1=5). Fig.5 shows the variation of the front shock pressure for Ea1=5 and Ea2=15. A regular oscillation with large amplitude is observed. Increasing Ea2 to 20 causes a smaller amplitude of oscillation with respect to Ea2=15 (compare Fig. 5 with Fig. 6). As Fig. 7 shows, further increasing Ea2 to 25 stabilizes the front propagation. Finally, we increase Ea2 beyond the instability limit of one-step models, (i.e. Ea=25). Fig. 8 shows the detonation front behavior for Ea2=27. An oscillatory variation of the front pressure is observed for this case. Therefore, it may be concluded that increasing the activation energy of the exothermic step may stabilize a detonation.

Conclusion

The detonation instability with a two-step model of chemical kinetics has been studied in this work. It is shown that:

1. Increasing Ea1 (for a fixed Ea2), destabilizes a detonation, the same behavior as one-step model.
2. Increasing Ea2 (i.e. the activation energy of the heat release step), has a stabilizing effect for Ea2<25.
3. Increasing Ea2 to value higher than 25, has a destabilizing effect.
4. It seems that increasing the difference of two activation energies, (i.e., Ea1-Ea2), tends to destabilize the front propagation for Ea2<25. Sharp reported the same behavior for a pathological detonation regardless the value of Ea1 or Ea2 [6].

It should be noted that increasing Ea2, increases total induction delay (first step induction delay + second step induction delay), which has a destabilizing role [12]. However, the current study indicated that, the effect of exothermic length, which increases with increasing Ea2, may have a dominant effect[4].

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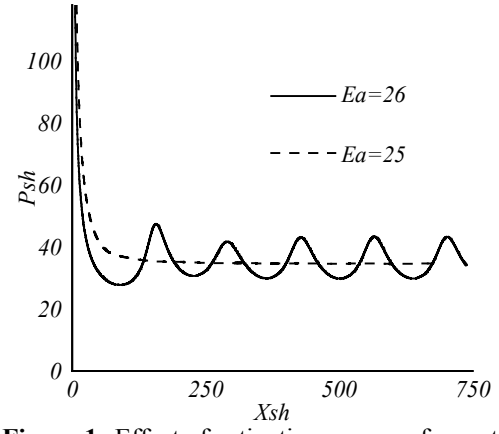

Figure 1: Effect of activation energy of one step model on detonation stability

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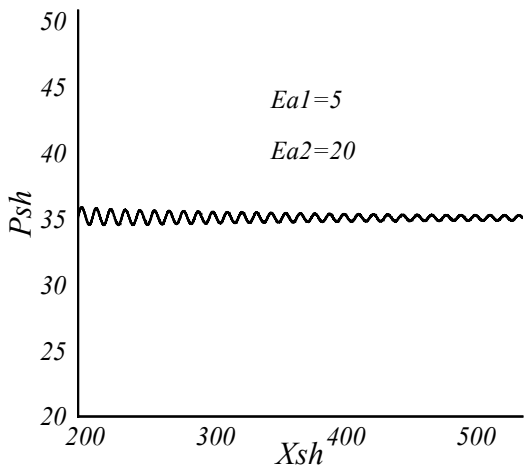

Figure2: Regular oscillation with small amplitude of

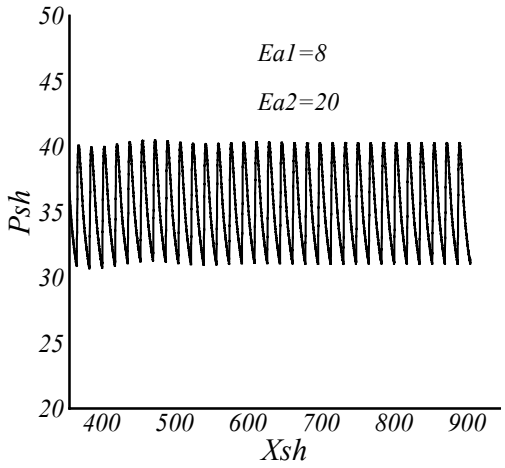

Figure 3: Regular oscillation with large amplitude of detonation shock pressure for Ea1=8

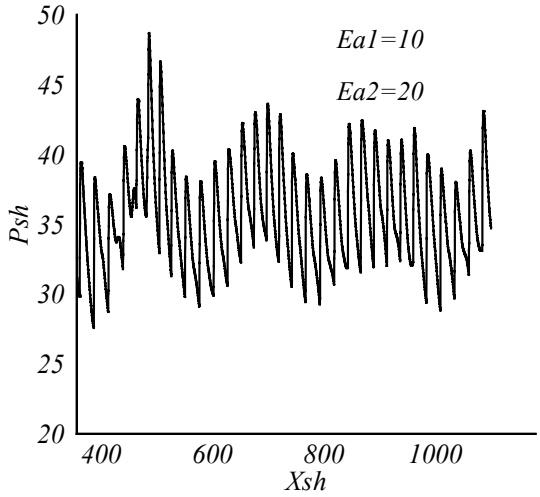

Figure4: Irregular oscillation with large amplitude of detonation shock pressure for Ea1=10

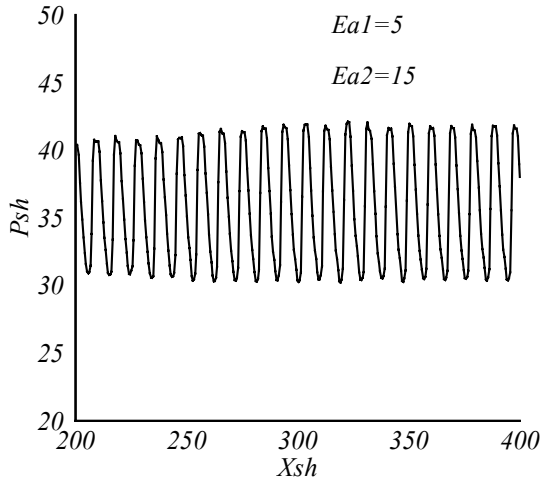

Figure 5: Regular oscillation with large amplitude of detonation shock pressure for Ea2=15

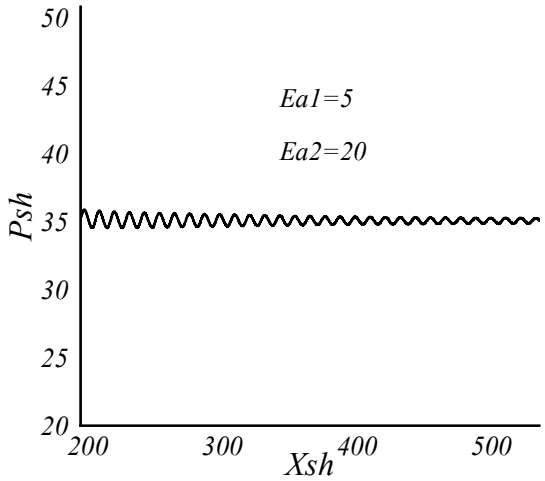

Figure 6: Regular oscillation with small amplitude of detonation shock pressure for Ea2=20

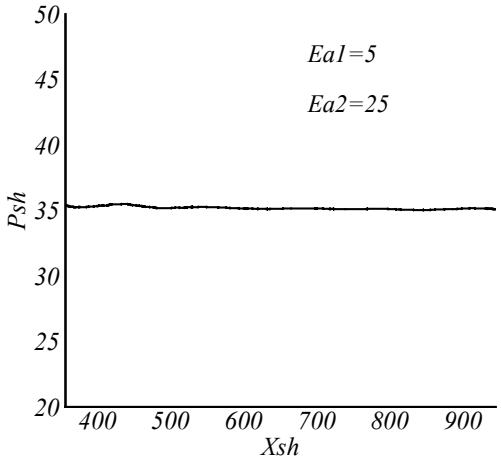

Figure 7: Stable behavior of detonation shock pressure for Ea2=25

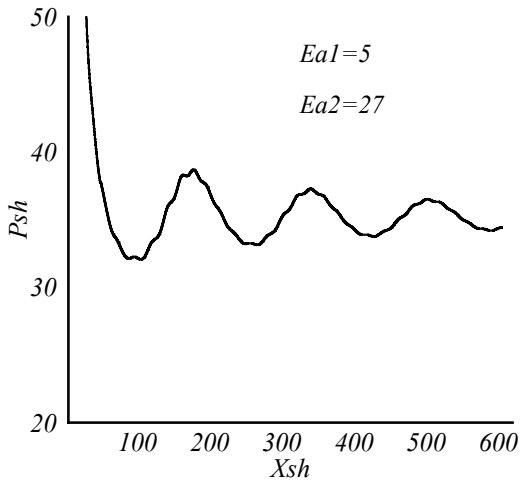

Figure 8: Oscillatory variation of detonation shock pressure for Ea2=27