The Chemical-Gasdynamic Mechanisms of Pulsating Detonation Wave Instability.

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Abstract

The chemical-gasdynamic mechanisms behind the instability and failure of a one-dimensional pulsating detonation wave driven by a three-step chain-branching reaction are revealed by direct numerical simulation.

Introduction

Depending on the initial pressure, projectile velocity and mixture ratio of chemical reactant to diluent, two different regimes of pulsating detonation instability have been observed to occur when spherical objects are fired into a reactive atmosphere (Lehr 1972, McVey & Toong 1971, Alpert & Toong 1972, Kaneshige & Shepherd 1996). The first involves regular periodic oscillations of the flow field, while the second involves less regular but significantly larger amplitude oscillations. Alpert & Toong (1972) refer to the former as the regular regime and the latter as the large disturbance regime. In both cases, however, the characteristic hydrodynamic mechanisms of the pulsating detonation instability are still poorly understood, despite the number of semi-qualitative theories that have been put forward.

In the following, the mechanisms for the regular, irregular and failure modes of pulsating detonation wave instability are investigated by very high resolution direct numerical simulation. The chemistry is modelled by a three-step chain-branching reaction, having the distinct advantage over the standard one-step Arrhenius model of possessing a well-defined detonability limit (Short & Quirk 1997). The mechanisms driving both the instability and failure of the detonation wave are revealed by examining selected snap-shot profiles of the thermodynamic and chemical structure behind the detonation shock during the unsteady evolution. The use of adaptive mesh refinement allows an effective resolution equivalent to 320 points in the standard steady-wave half-reaction length. We find that the mechanisms for both the regular regime and large amplitude regime are found to differ from those proposed by McVey & Toong (1971) and Alpert & Toong (1972).

Model

The pulsating detonation instability is modelled by the one-dimensional, non-dimensional reactive Euler equations (Short & Quirk 1997)

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho\frac{\partial u}{\partial x^l} = 0, \quad \frac{\mathrm{D}u}{\mathrm{D}t} + \rho^{-1}\frac{\partial p}{\partial x^l} = 0, \quad \frac{\mathrm{D}e}{\mathrm{D}t} + p\frac{\mathrm{D}\rho^{-1}}{\mathrm{D}t} = 0, \tag{1}$$

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

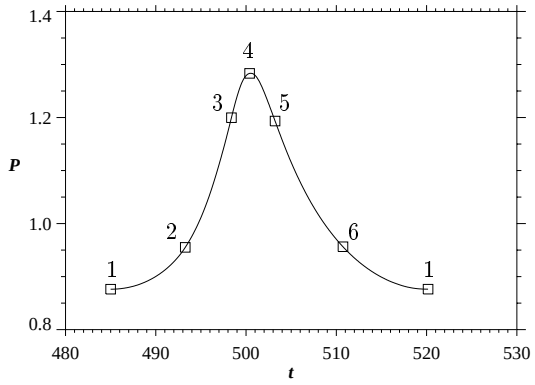
$$e = \frac{p}{(\gamma-1)\rho} - q, \quad T = p/\rho, \tag{2}$$

q represents the local chemical heat energy and T represents the temperature. The scales for the density, pressure, temperature and velocity are the steady-wave post-shock density, pressure, temperature and sound speed respectively.

The chemical reaction is modelled by the three-step chain-branching reaction

$$\begin{aligned} &\text{Initiation :} && F \to Y, \quad k_I = \exp\left(\tfrac{1}{\epsilon_I}\left(\tfrac{1}{T_I} - \tfrac{1}{T}\right)\right), \\ &\text{Chain-branching :} && F + Y \to 2Y, \quad k_B = \exp\left(\tfrac{1}{\epsilon_B}\left(\tfrac{1}{T_B} - \tfrac{1}{T}\right)\right), \\ &\text{Chain-termination :} && Y \to P, \quad k_C = 1, \end{aligned} \tag{3}$$

1(a)



1(b)

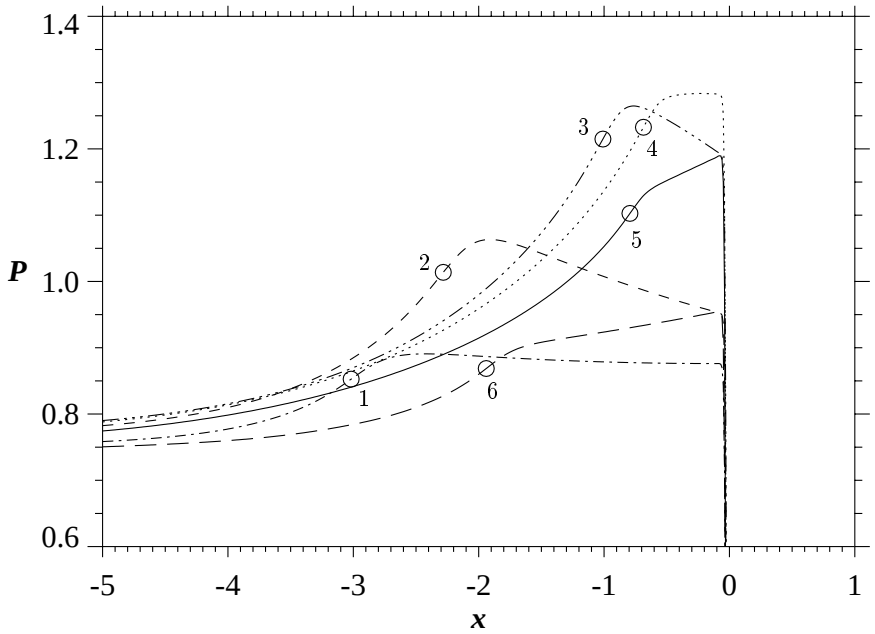


Figure 1: (a) Points in the regular detonation shock pressure cycle at which the snap-shot profiles of the variation in (b) pressure are taken during one cycle of the regular pulsating instability.

for fuel F, chain-radical Y and product P. The chain-initiation, chain-branching and chain-termination rate constants are given by k_I, k_B and k_C respectively. The inverse activation energy for the initiation reaction is ϵ_I and for the chain-branching reaction ϵ_B. The chain-initiation and chain-branching cross-over temperatures are given by T_I and T_B respectively and are the values at which the chain-initiation and chain-branching rates are equal to the chain-termination rate. Consumption equations for fuel and radical are

$$\frac{\mathrm{D}f}{\mathrm{D}t} = -r_I - r_B, \quad \frac{\mathrm{D}y}{\mathrm{D}t} = r_I + r_B - r_C, \tag{4}$$

where

$$r_I = f \exp\left(\frac{1}{\epsilon_I}\left(\frac{1}{T_I} - \frac{1}{T}\right)\right), \quad r_B = \rho f y \exp\left(\frac{1}{\epsilon_B}\left(\frac{1}{T_B} - \frac{1}{T}\right)\right), \quad r_C = y, \tag{5}$$

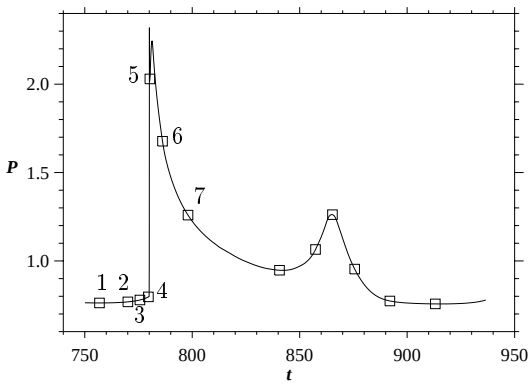
and f and y represent mass fractions of fuel and radical. The chemical energy q is defined as

$$q = Q(1-f) - (Q+R)y, \tag{6}$$

where $Q > 0$ represents the total chemical energy available in the unreacted mixture and R represents the amount of endothermic energy absorbed by the initiation and chain-branching reactions in breaking down the reactant F into the energetic radical Y. In order to mimic the typical reaction dynamics of chain-branching chemistry, in addition we assume that

$$T_I > 1, \quad T_B < 1, \quad \epsilon_I \ll \epsilon_B \ll 1, \quad R = 0. \tag{7}$$

2(a)



2(b)

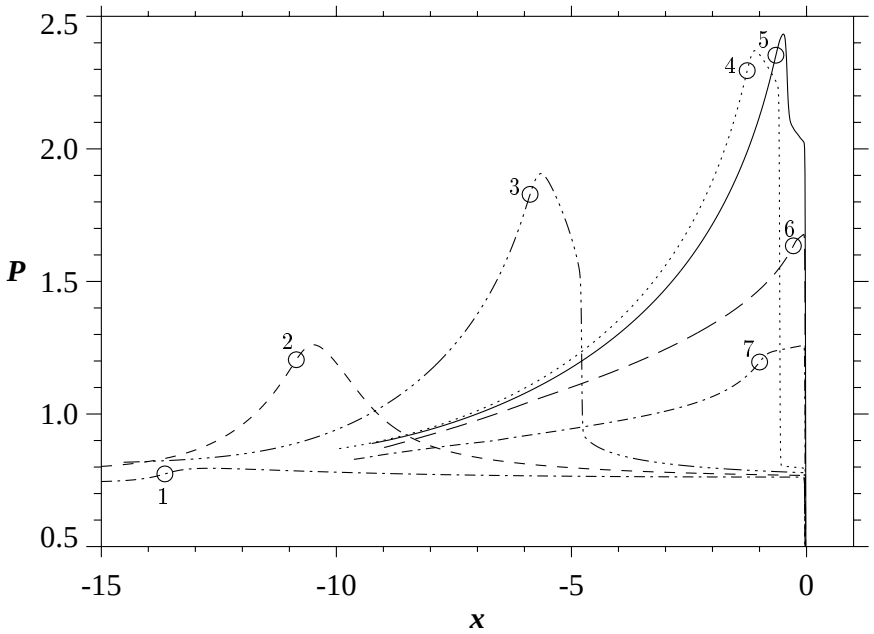


Figure 2: Snap-shot profiles of the mechanisms underlying the large pressure modefound in the detonation shock pressure trace for $T_B = 0.86$ for (b) pressure. Labels 1-7 in figure 2(a) show the points in the irregular detonation shock pressure cycle at which the snap-shots are taken.

For the calculations shown below, $Q = 3$, $\epsilon_I = 1/20$, $\epsilon_B = 1/8$, $T_I = 3$, $\gamma = 1.2$ and the detonation overdrive $d = 1.2$.

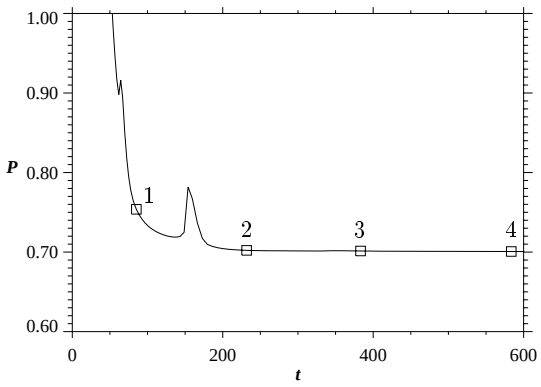
Mechanisms of regular, irregular and failure modes

The chemico-gasdynamic mechanisms driving the regular mode of pulsating instability, observed here for a chain-branching cross-over temperature $T_B = 0.82$, are revealed in figure 1. The instability is driven by periodic low-frequency, finite-amplitude compression and expansion waves in the chain-branching induction zone between the main reaction layer and the detonation shock.

The chemico-gasdynamic mechanisms driving the irregular mode of pulsating instability, observed here for a chain-branching cross-over temperature $T_B = 0.86$, are revealed in figure 2. Unlike the regular mode of pulsating instability, the irregular mode first involves a decoupling between the shock and main reaction layer. Subsequently, the main reaction layer accelerates, drives a compression wave ahead of it, and undergoes a transition to detonation. This internal detonation wave overtakes the lead detonation shock, generating a new high-pressure detonation, which rapidly decays and the instability cycle is repeated.

Figure 3 shows the mechanisms underlying the scenario of detonation quenching, or failure, for $T_B = 0.89$. Here, the shock temperature is observed to drop to the cross-over temperature for the

8(a)



8(b)

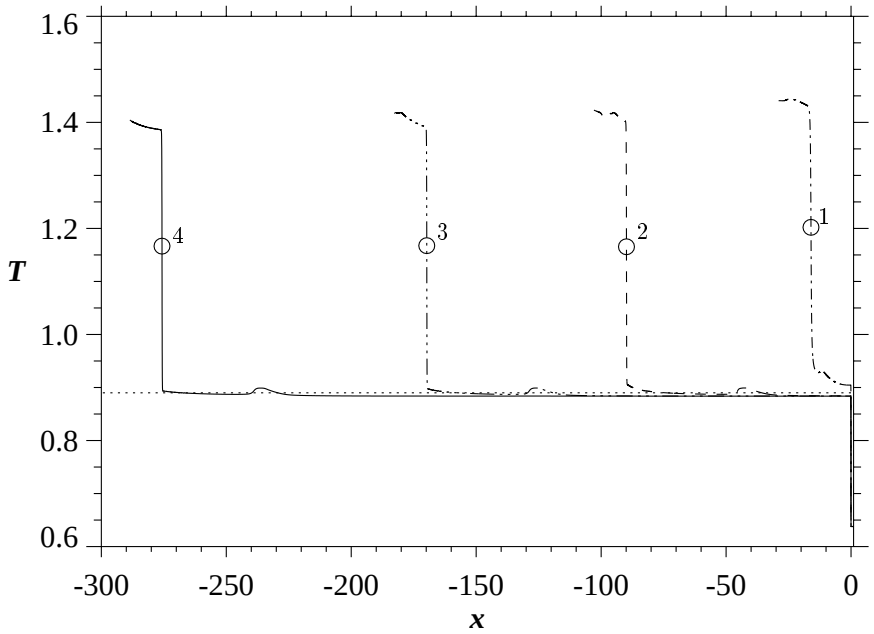


Figure 3: Snap-shot profiles of the flame receding from the detonation front during detonation failure for $T_B = 0.89$ for (b) temperature. The labels in figure 3(a) show the points in the detonation shock pressure cycle at which the snap-shots are taken. The dashed line in figure 3(b) indicates the value of the chain-branching cross-over temperature $T_B = 0.89$.

chain-branching reaction, causing the main reaction layer to decouple and retreat indefinitely from the detonation shock. The criteria for failure is: the shock temperature should fall to the chain-branching cross-over temperature.

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