Numerical Study of Unsteady Detonation Wave Propagation in a Supersonic Combustion Chamber

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Abstract. Propagating detonation waves in a supersonic flow in one-dimensional tube and two-dimensional wedged chamber are numerically investigated using detailed chemical mechanisms. A premixed stoichiometric hydrogen and air mixture is used in this study. In the one-dimensional case, various flow conditions are used to examine their effects on the propagation of the detonation wave. In the two-dimensional case, an incoming gas mixture is compressed by wedges and ignited by an arc midway along the wedges, simulated as a number of cells with high parameters. Various features including a vortex are observed.

1 Introduction

Detonation wave propagation in a duct is a classical gasdynamics problem that is the subject of theoretical, experimental and, lately, numerical study. This problem is still fascinating, being rich with multiple length and time scales. Recently, a novel multi-mode detonation wave based propulsion concept was proposed by Wilson and co-workers for space access or hypersonic flight [1,2]. As shown in Fig. 1, the concept consists of four modes, of which each mode has unique features and operation ranges: an ejector augmented pulsed detonation rocket (PDR) mode, a pulsed normal detonation wave engine (NDWE) mode, an oblique detonation wave engine (ODWE) mode and a pure pulsed detonation rocket mode. One of main advantages of this concept is that it can be operated over a wide range of flight Mach number from takeoff to hypersonic speeds. Furthermore, all of the modes are integrated into a single flow path, which should substantially reduce the weight and volume of the vehicle.

A detailed analysis on the pulsed detonation wave engine mode is necessary since most of the thrust is generated in this mode to reach hypersonic speed. The NDWE mode is designed to provide thrust at flight Mach numbers of 3 to 10, which corresponds to combustion chamber Mach numbers less than the Chapman–Jouguet Mach number. A numerical investigation is performed on how the detonation wave is initiated and propagated into a supersonic flow in the combustion chamber since the initiation and propagation of the detonation wave in the supersonic flow is a critical issue for this mode. In this study, the detonation wave is initiated by an arc, represented numerically as an initially small region of high energy.

Two-dimensional, multi-species, Euler equations are used to develop a computational code. The numerical method involving the chemical reactions is more complicated than that for a non-reacting flow due to stiffness arising from chemical reactions. A time-operator splitting method is used to handle the stiffness. Two different chemical mechanisms extracted from GRI-Mech [3] for a hydrogen–air mixture are used.

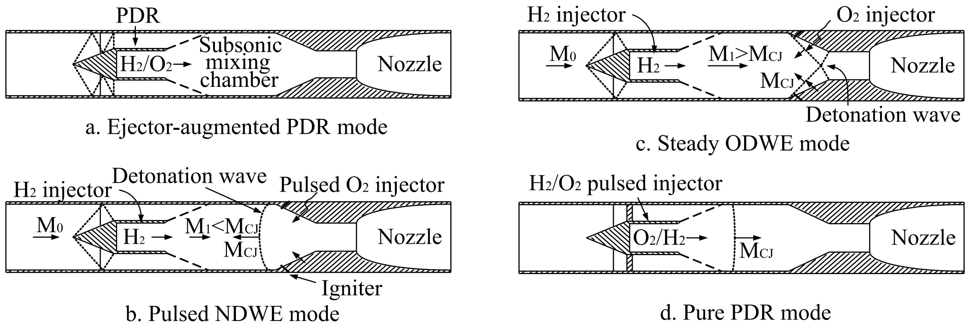


Fig. 1. Multi-mode PDE concept.

2 Formulation of Physical and Numerical Models

2.1 Governing Equations

The governing equations for a two-dimensional, inviscid, multi-species, chemically reacting flow are given as [4,5]

$$\frac{\partial \boldsymbol{Q}}{\partial t} + \frac{\partial \boldsymbol{F}}{\partial x} + \frac{\partial \boldsymbol{G}}{\partial y} = \boldsymbol{S} \tag{1}$$

where

$$\boldsymbol{Q} = \begin{bmatrix} \rho_i \\ \rho u \\ \rho v \\ \rho E \end{bmatrix}, \ \boldsymbol{F} = \begin{bmatrix} \rho_i u \\ \rho u^2 + p \\ \rho uv \\ (\rho E + p)u \end{bmatrix}, \ \boldsymbol{G} = \begin{bmatrix} \rho_i v \\ \rho uv \\ \rho v^2 + p \\ (\rho E + p)v \end{bmatrix}, \ \boldsymbol{S} = \begin{bmatrix} W_i \dot{\omega}_i \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{2}$$

In the above equations, $i = 1 \cdots N_s$, N_s is the number of species, ρ_i is the density of species i, E is the total energy, p is the pressure, u and v are the velocity components, W_i is the molecular weight of species i, and $\dot{\omega}_i$ is the mass production rate of species i. A thermally perfect gas is assumed for each species so that the specific heats, enthalpy and internal energy are functions of temperature only. These thermodynamic properties are evaluated using a thermodynamic database given in the CEA code [6].

2.2 Chemical Kinetics

The overall reaction for the combustion of a stoichiometric hydrogen-air mixture is described by the equation

$$2\mathrm{H_2} + \mathrm{O_2} + 3.762\mathrm{N_2} \rightarrow 2\mathrm{H_2O} + 3.762\mathrm{N_2} \tag{3}$$

This overall reaction is a consequence of a large number of elementary reactions. Two elementary reaction mechanisms for the hydrogen–air mixture are extracted from GRI-Mech [3] and utilized through this work. The first mechanism has twenty-eight reversible reactions and nine species (H_2, O_2, N_2, H, HO_2 H_2O, H_2O_2, O and OH) and the second has forty reversible reactions and thirteen species (H_2, O_2, N_2, H, HO_2, H_2O, H_2O_2, N, NO, NO_2, N_2O, O and OH). Third-body reactions and pressure-dependent reactions are also considered in these mechanisms.

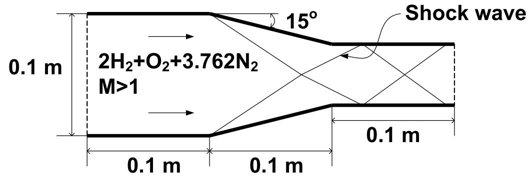


Fig. 2. Schematic of two-dimensional combustion chamber.

2.3 Numerical Methods

The governing equations given in Eq. (1) are discretized by a finite volume method with a cell centered scheme. Time-operator splitting is used to decouple two physical phenomena, the fluid dynamics and the chemical kinetics. This method separates the governing equations into two steps. In the first step, a second-order, two-step Runge–Kutta method is used for time integration, while a second-order Roe scheme with a minmod limiter is used for space integration. Source terms are evaluated in the second step. The equations in the second step become a system of ordinary differential equations and are solved by a VODE code [7]. Whenever the species densities are updated by VODE, the temperature should be also evaluated with updated values of species density and enthalpy. Therefore, the temperature is evaluated twice at each time step, one in the first step and the other in the second step.

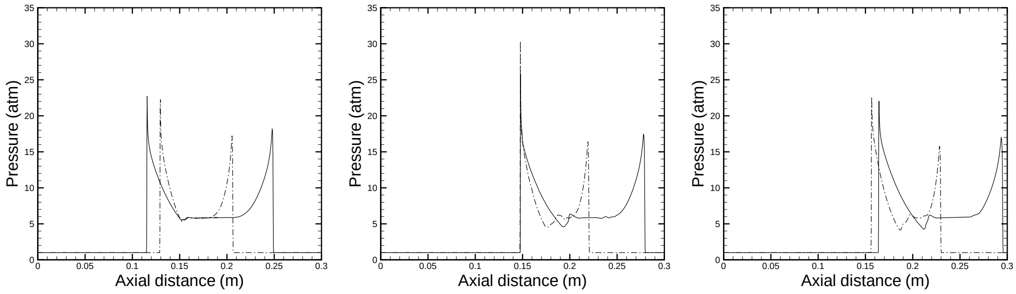
3 Results and Discussion

3.1 Geometric and Physical Configurations

A two-dimensional symmetric combustion chamber is shown in Fig. 2. This chamber is confined by two opposite wedge sections to initiate the detonation induced by the shock wave. This wedged chamber also provides a higher pressure distribution in the detonation wave propagation. The chamber is 0.3 m in length. The left boundary is 0.1 m high and a 15° wedge is located on the top and the bottom. The flow coming into the combustion chamber is a premixed stoichiometric hydrogen-air mixture at different incoming conditions. Twenty-eight reactions with nine species are used for the one-dimensional case, while forty reactions with thirteen species are used for the two-dimensional case. The arc igniter is simulated by an ignition zone of high pressure and temperature, namely, $p = 30$ atm and $T = 3000$ K, respectively.

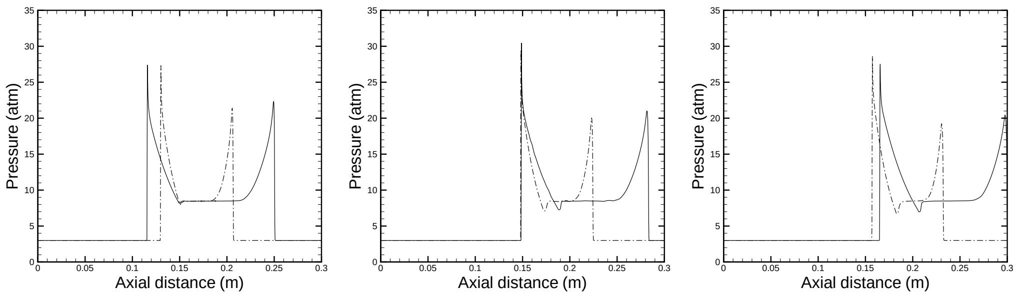
3.2 One-Dimensional, Arc-Ignited Detonation

Two initial flow conditions are used to simulate a one-dimensional detonation tube, one at $p = 1$ atm and $T = 300$ K shown in Fig. 3 and the other at $p = 3$ atm and $T = 700$ K shown in Fig. 4. The mixture is ignited at the center of the tube (0.15 m). The dotted and solid lines in the figures are obtained at about $t = 20$ μs and $t = 35$ μs, respectively. The Chapman–Jouguet (CJ) velocities of the hydrogen-air mixture for these conditions are found to be 1979.33 m/s and 1962.71 m/s, respectively. These values are corresponded to CJ Mach numbers of 4.843 and 3.176.



(a) $V = 1000$ m/s. (b) $V = 2000$ m/s. (c) $V = 2500$ m/s.

Fig. 3. One-dimensional pressure profiles at $p = 1$ atm, $T = 300$ K and different incoming flow velocities.



(a) $V = 1000$ m/s. (b) $V = 2000$ m/s. (c) $V = 2500$ m/s.

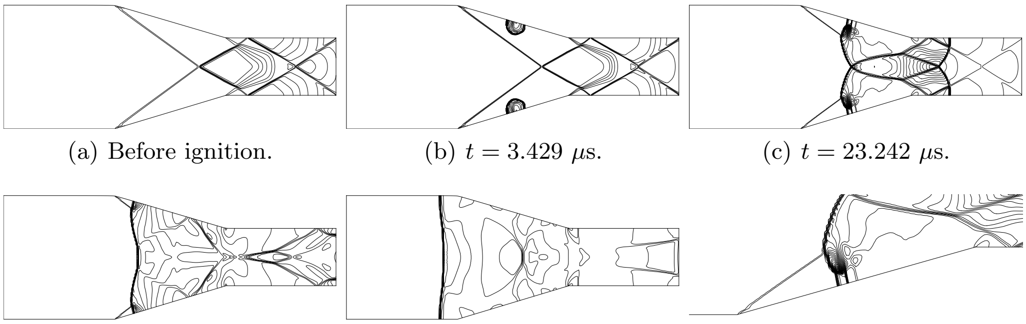
Fig. 4. One-dimensional pressure profiles at $p = 3$ atm, $T = 700$ K and different incoming flow velocities.

Figures 3 and 4 indicate that when the chamber velocity is less than CJ value, as the velocity is increased, the rate of propagation of the upstream moving detonation wave is decreased and the pressure is increased. But the pressure of the downstream moving detonation wave is not significantly decreased. Moreover, the pressure in the region of rarefaction waves is increased to a level of about 5 atm from their initial conditions. When the chamber velocity reaches the CJ value, the upstream moving detonation wave becomes steady. This situation is shown in Figs. 3(b) and 4(b). As the velocity in the chamber is further increased, the standing detonation wave moves downstream and the wave strength is decreased as shown in Figs. 3(c) and 4(c).

3.3 Two-Dimensional, Arc Ignited Detonation

The incoming flow is a stoichiometric hydrogen–air mixture at a pressure of 3 atm, a temperature of 450 K and a Mach number of 2.877. Forty reversible reactions with thirteen species are utilized in this case. An inert air flow past the wedge is shown in Fig. 5(a). Once the shock waves are stabilized, the chemical mechanism is then switched to the hydrogen–air mixture.

The mixture is directly ignited at the center of the wedge surface with a pressure of 30 atm and a temperature of 3000 K. Detonation waves are immediately generated and propagate into the supersonic flow as shown in Fig. 5(b). Figure 5(c) shows two opposite-



(a) Before ignition. (b) $t = 3.429$ μs. (c) $t = 23.242$ μs.

(d) $t = 56.220$ μs. (e) $t = 105.254$ μs. (f) vortex near the wedge surface.

Fig. 5. Pressure distribution for inviscid, arc ignited pulsed normal detonation wave.

facing detonation waves, one moving upstream and the other moving downstream. The pressure behind the detonation wave moving downstream is much higher than that behind the detonation wave moving upstream. At the moment shown in Fig. 5(c), the maximum pressures just behind the upstream and downstream moving detonations are about 63 atm and 104 atm, respectively. This difference in pressure magnitudes is due to the geometry and the incoming flow.

Figure 5(c) and (f) shows a vortex near the wedge surface, which can be attributed to the curved shock via Crocco's theorem. This vortex is generated when the front of the upstream moving detonation wave is merged with the shock wave originated from the wedge corner. The vortex moves to the wedge surface and then hits the surface with the highest pressure encountered in the flow, which is about 187 atm.

4 Conclusions

The one- and two-dimensional propagation of the detonation wave is studied numerically. The ignition of the hydrogen-air mixture is accomplished by a simulated arc igniter. The one-dimensional case shows a natural transition between an unsteady and a steady wave system depending on whether the incoming flow Mach number is below or above the Chapman–Jouguet Mach number of detonation. The simulation showed that the pressure of the upstream moving detonation is higher than that of the downstream moving detonation.

The two-dimensional simulation showed complex wave interactions. The wave strength of the downstream moving detonation is stronger than that of the upstream moving detonation, which is different from that encountered in the one-dimensional case. This difference between the one- and two-dimensional cases is due to the geometry and the subsequent flow produced. It was found that the interaction between a steady oblique shock and a propagating normal detonation wave produced a vortex that moved toward the wedge surface.

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