Combustion and Flame 179 (2017) 185–198

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

The influence of acoustic impedance on gaseous layered detonations bounded by an inert gas

Ryan W. Houim*, Robert T. Fievisohn

Department of Aerospace Engineering, University of Maryland, College Park, MD 20742, USA

ARTICLE INFO

Article history:
Received 27 May 2016
Revised 3 February 2017
Accepted 3 February 2017
Available online 6 March 2017

Keywords:
Detonation
Layer
Shock wave
Acoustic impedance
Numerical simulation

ABSTRACT

Gaseous detonations propagating through a layer of reactants that is bounded by an inert gas were simulated by solving the two-dimensional reactive Euler equations. A single-step chemical reaction model was used with thermochemical properties that are representative of a highly reactive fuel–oxidizer mixture, such as stoichiometric ethylene and oxygen. A series of cases with varying acoustic impedance ratios between the inert and reactant gases, Z, were studied to explore the influence of acoustic impedance mismatch on the propagation of a detonation through the reactant layer. The detonation failed when $Z \sim 1$ due to a loss of triple points at the interface. The detonation propagated stably when Z is high and the impedance of the inert gas is much higher than the reactants. Reflected shocks are produced from the interaction of the Mach stem of a detonation cell with the interface between the reactant and inert gases. These reflected shocks, in turn, detach and generate new triple points that are necessary to propagate the detonation. The detonation was also stable when the acoustic impedance of the inert gas is much lower than the reactants. A gas dynamic structure forms that involves a detached shock in the inert gas and a series of oblique shocks and slip lines in the reactants. A small local explosion is triggered when the Mach stem of a detonation cell interacts with the compressed reactants behind one of these oblique shocks. The resulting retonation wave produces a new Mach stem and a new triple point that leads to a stable detonation. These results suggest that the acoustic impedance and shock structure in the inert gas can have a significant influence on the stable propagation of a layered gaseous detonation.

1. Introduction and background

Detonations propagating through uniform mixtures of fuel and oxidizer in confined areas have been studied extensively [1]. Relatively little attention has been given towards understanding the fundamental propagation mechanisms of layered gaseous detonations, where the reactants are semi-confined into a layer by an inert gas [2,3]. Layered gaseous detonations have practical importance in both explosion safety and propulsion. For example, hydrogen may accumulate on the ceiling of large structures [2], high molecular weight fuels can accumulate near the ground in vapor cloud explosions [4], and detonations propagate though a layer of reactants bounded by combustion products in rotating detonation engines [5–10].

The first experiments examining detonations propagating through a layer of gaseous reactants that is bounded by an inert gas were conducted by Sommers and Morrison [11]. The general features of a gaseous layered detonation, when the acoustic impedance of the inert gas is high, are shown in Fig. 1. Here, a detonation propagates through the layer of reactants and transmits an attached oblique shock into the inert gas. This oblique shock also turns a hydrodynamically unstable contact surface between the detonation products and the inert gas.

Sommers and Morrison [11] also developed an analytical model to calculate the angles of the transmitted oblique shock and the turned contact surface. They found that the oblique shock and contact surface angles were a function of the acoustic impedance ratio between the reactant and inert gas mixtures. An inert gas with a low acoustic impedance exhibits poor confinement and can cause the detonation to fail. An inert gas with a high acoustic impedance, however, behaves more like a solid wall and can promote a stable detonation. They also found that the transmitted oblique shock would detach for detonations propagating through a hydrogen–oxygen layer that is bounded by helium. As a result, the transmitted shock wave in the inert gas propagated ahead of the detonation. Similar detached shock structures have been observed in numerical simulations of rotating detonation engines [5,7,9,12] and in the experimental work of Adams [13].

* Corresponding author.
E-mail addresses: rhouim@umd.edu, ryan.houim@gmail.com (R.W. Houim).

http://dx.doi.org/10.1016/j.combustflame.2017.02.001
0010-2180/

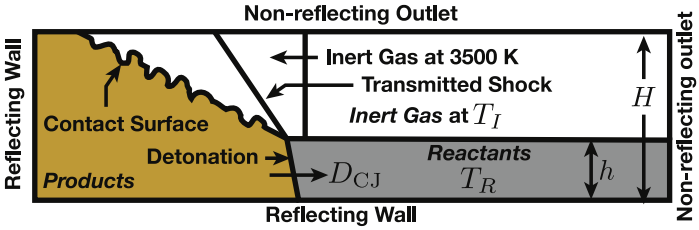

Fig. 1. Initial and boundary conditions for the two-dimensional simulations of a detonation propagating through a layer of reactants bounded by an unconfined inert gas.

Follow-on work of gaseous layered detonations focused on the development of phenomenological models [14–18]. Some of these models were used to predict and analyze the detonation velocity deficit [14,15]. It was found that inert gases that have high acoustic impedance produce detonations that propagate close to the Chapman–Jouguet (CJ) detonation velocity (D_{CJ}). Inert gases with a low acoustic impedance produce lower detonation velocities. Other models were developed to predict the minimum height of the reactant layer needed to support a stable detonation [16]. The detonation of gaseous reactant layers has received relatively little attention in the recent literature with the exception of [2,3].

Gaseous detonations are unstable to transverse perturbations. A detonation that is planar will have a multidimensional cellular structure produced by transverse shock waves and triple points that interact with the leading shock front. Details of these cellular detonations have been extensively discussed in the literature [19–25]. These transverse waves and triple points are often necessary to propagate a gaseous detonation and, as a result, will fail if too many of these triple points are lost [19,26]. This can occur when a detonation diffracts around a sudden expansion [27].

Criterion on the limiting channel sizes for stable detonation propagation are often based on the detonation cell size because of the importance of transverse waves. For example, the minimum size of a circular tube that can support a detonation is often reported as $d^* > \lambda/\pi$, where d^* is the minimum tube diameter and λ is the detonation cell size [25]. Tubes with porous walls produce much weaker transverse shock reflections in comparison to tubes with rigid walls. The d^* for a porous tube, as a result, is much larger than a tube with rigid walls [26].

Gaseous interfaces do not reflect transverse shocks of detonation cells as effectively as rigid walls. In the worst case, the interaction of these transverse shocks with the surface of the reactant layer may reflect expansion waves if the acoustic impedance of the inert gas is low [28]. As a result, the critical height, h^*, for a layer of reactants that is bounded by an inert gas necessary to support a detonation is much larger than d^*. This criterion has been empirically determined to be $h^* > 3\lambda$ if the inert gas is confined by a solid wall [2] and $h^* > (12 \pm 5)\lambda$ if the inert gas is unconfined [3].

This paper presents two-dimensional numerical simulations that explore the physical mechanisms by which detonations propagate through layers of gaseous reactants bounded by an unconfined inert gas. A single-step chemical model is used with thermochemical parameters that are representative of a highly reactive fuel–oxidizer mixture, such as stoichiometric ethylene and oxygen. The influence of the acoustic impedance of the inert gas is examined in a parametric study.

2. Model and geometrical setup

The effects of viscosity and diffusion are neglected and the flow is simulated by solving reactive Euler equations,

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0, \tag{1}$$

$$\frac{\partial \rho Y}{\partial t} + \nabla\cdot(\rho Y\mathbf{v}) = -\dot{\omega}, \tag{2}$$

$$\frac{\partial \rho\mathbf{v}}{\partial t} + \nabla\cdot(\rho\mathbf{v}\mathbf{v}) + \nabla p = 0, \tag{3}$$

$$\frac{\partial \rho E}{\partial t} + \nabla\cdot[\mathbf{v}(\rho E + p)] = q\dot{\omega}, \tag{4}$$

where ρ is the density, $\mathbf{v}$ is the velocity vector, p is the pressure, E is the total energy, Y is the reactant mass fraction, $\dot{\omega}$ is the mass production rate of the products, and q is the heat release due to chemical reaction. The gas is calorically perfect so that

$$p = \rho R_g T, \tag{5}$$

where R_g is the gas constant. The molecular weight of the reactants, products, and inert gas are assumed to be the same. The total energy is

$$\rho E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho\mathbf{v}\cdot\mathbf{v}, \tag{6}$$

where γ is the ratio of specific heats. The sound speed is defined by

$$c = \sqrt{\gamma p/\rho} \tag{7}$$

and the acoustic impedance is

$$\mathcal{R} \equiv \rho c = p\sqrt{\frac{\gamma}{R_g T}}. \tag{8}$$

A single-step, irreversible, second-order chemical reaction model is adopted [29],

$$\mathrm{R} + \mathrm{M} \rightarrow \mathrm{P} + \mathrm{M}, \tag{9}$$

where R, P, and M represent the reactants, products, and a third body, respectively. (The chaperon efficiency of the products and reactants is unity.) The mass production rate of the products is

$$\dot{\omega} = A\rho^2 Y \exp(-Ea/RuT), \tag{10}$$

where A is the prefactor, Ea is the activation energy, and Ru is the universal gas constant.

The thermochemical parameters are assumed to be constant and are chosen to be representative of a highly reactive fuel–oxidizer mixture similar to stoichiometric ethylene and oxygen. This reaction model has been used to study deflagration-to-detonation transition [30]. The thermochemical input parameters and the resulting Chapman–Jouguet (CJ) and Zeldovich-von–Neumann–Döring (ZND) output detonation properties are listed in Table 1.

The governing equations are solved using the method of lines. A Strang-splitting approach is used to couple the hydrodynamic and the chemical reaction terms. A fifth-order accurate Godunov algorithm [33] with the HLLC approximate Riemann solver [34,35] is used for spatial discretization. The equations are marched in time using third-order strong-stability preserving Runge–Kutta [36] with a Courant–Friedrichs–Lewy (CFL) number of 0.8.