Combustion and Flame 163 (2016) 414–426

Contents lists available at ScienceDirect

Combustion and Flame

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

On the pressure dependence of ignition and mixing in two-dimensional reactive shock-bubble interaction

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ARTICLE INFO

Article history:
Received 10 June 2015
Revised 8 October 2015
Accepted 12 October 2015
Available online 14 November 2015

Keywords:
Shock wave
Richtmyer–Meshkov instability
Shock-bubble interaction
Detonation
Deflagration

ABSTRACT

We analyse results of numerical simulations of reactive shock-bubble interaction with detailed chemistry. The interaction of the Richtmyer–Meshkov instability and shock-induced ignition of a stoichiometric H_2-O_2 gas mixture is investigated. Different types of ignition (deflagration and detonation) are observed at the same shock Mach number of $Ma = 2.30$ upon varying initial pressure. Due to the convex shape of the bubble, shock focusing leads to a spot with high pressure and temperature. Initial pressures between $p_0 = 0.25 - 0.75$ atm exhibit low pressure reactions, dominated by H, O, OH production and high pressure chemistry driven by HO_2 and H_2O_2. Deflagration is observed for the lowest initial pressure. Increasing pressure results in smaller induction times and ignition, followed by a detonation wave. The spatial and temporal evolution of the gas bubble is highly affected by the type of ignition. The Richtmyer–Meshkov instability and the subsequent Kelvin–Helmholtz instabilities develop with a high reaction sensitivity. Mixing is significantly reduced by both reaction types. The strongest effect is observed for detonation.

1. Introduction

For high-speed reactive flows, such as supersonic combustion, the rapid and efficient mixing of fuel and oxidizer is crucial as the residence time of the fuel-oxidizer mixture in the combustion chamber is only a few milliseconds [1]. The Richtmyer–Meshkov instability (RMI) promotes mixing and thus increases the burning efficiency of supersonic combustion engines [2]. However a discontinuity in thermodynamic properties can cause reaction waves. The reacting shock-bubble interaction (RSBI) allows to investigate the interaction between the RMI and the reaction waves inside the bubble that are initiated by the shock.

1.1. Richtmyer–Meshkov instability

RMI [3,4] is a shock-induced hydrodynamic instability which occurs at the interface between two fluids of different densities. It can be considered as the impulsive limit of the Rayleigh–Taylor instability [5,6], where initial perturbations at the interface grow due to constant gravitational acceleration. In RMI, baroclinic vorticity production at the interface is caused by misalignment of pressure gradient, ∇p, associated with a shock wave and density gradient, $\nabla \rho$, at the material interface. For comprehensive reviews the reader is referred to Brouillette [7] and Zabusky [8]. RMI occurs for a wide range of physical phenomena ranging from extreme large scales in astrophysics [9], to intermediate scales in combustion [1,10] and to very small scales in inertial confinement fusion [11].

1.2. Shock-induced chemistry

A shock-induced change in thermodynamic properties can cause ignition, followed by a reaction wave where two types can be distinguished: deflagration and detonation. Deflagration is a subsonic reaction wave that propagates through the gas mixture due to direct transfer of chemical energy from burning to unburned gas, driven by diffusion [12]. Detonation is driven by a fast chemical reaction and the associated large heat release within the reaction wave. A shock wave immediately precedes the detonation wave and preheats the gas mixture by compression [12]. The detonation wave propagates up to 10^8 times faster than the deflagration wave [13]. Due to the large differences in the characteristic reaction time scales, the type of the reaction wave is crucial for flow evolution.

Limits between deflagration and detonation for a hydrogen-oxygen (H_2-O_2) gas mixture are shown in Fig. 1 as functions of temperature and pressure. The chain branching exceeds the rate of chain breaking on the right side of the reversed-S curve. Due to pressure dependent intermediate reactions, the type of ignition can change several times at constant temperature. Some intermediate products and

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http://dx.doi.org/10.1016/j.combustflame.2015.10.016

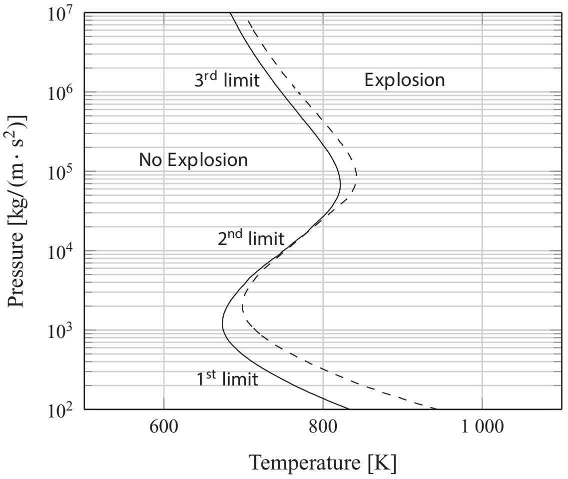

Fig. 1. Explosion limits for a stoichiometric pure hydrogen-oxygen mixture (solid line) and for a stoichiometric hydrogen-oxygen mixture with inert gas (2/1/4) (dashed lines) [15].

reactions are inactive at low pressure and become active at higher pressure, affecting the chemical reaction process significantly [14]. The solid line represents the explosion limit for a pure stoichiometric H_2-O_2 mixture. Wang and Chung [15] added an inert gas to dilute the stoichiometric mixture and observed a distinct shift of the explosion limit to higher temperatures. The dashed line shows a molar ratio of 2/1/4 (H_2/O_2/inert gas), which is close to the gas composition in this work (2/1/3.67).

1.3. Reacting shock-bubble interaction

The interaction of a shock wave with a gas bubble containing a reactive gas mixture triggers RMI simultaneously with chemical reaction processes. In classical inert shock-bubble interactions (SBI) the baroclinic vorticity production generated at the interface causes the bubble to evolve into a vortex ring. Upon contact, the incident shock wave is partially reflected and partially transmitted. In case of a convergent geometry (a heavy gas bubble surrounded by light ambient gas with an Atwood number $A = (\rho_1 - \rho_2)/(\rho_1 + \rho_2) < 1$) the transmitted shock wave travels more slowly than the incident shock wave outside of the bubble. The transmitted shock wave focuses at the downstream pole of the bubble. As the shock wave collapses in the shock-focusing point, pressure and temperature increase. This phenomenon is known as the shock-focusing phenomenon. Furthermore, vorticity deposition leads to a growth of the initial interface disturbances. Provided that the initial energy input is sufficient the flow develops a turbulent mixing zone through non-linear interactions of the material interface perturbations [7,8].

The non-reacting setup of SBI was rigorously studied over the last decades. In 1983, Haas and Sturtevant [16] investigated the interaction of shock waves propagating in air with a gas bubble filled with either helium or R_{22}. Through their shadow-photographs, Haas and Sturtevant [16] did not only significantly contribute to a better understanding of the temporal bubble evolution under shock acceleration, but also established an entire new class of canonical flow configurations. Later, Quirk and Karni [17] conducted a detailed numerical investigation of such shock-bubble interaction problems and complemented experimental findings by reproducing the transition from regular to irregular refraction, shock wave focusing and the formation of a jet towards the center of the bubble. For a comprehensive review on SBI please refer to Ranjan et al. [18].

Haehn et al. [19] extended the setup by replacing the gas within the bubble by a reactive gas mixture. As the shock wave propagates through the bubble temperature and pressure increase. This results in a raise of chemical reaction rates up to ignition of the gas mixture. In their experimental investigation, a stoichiometric gas mixture of H_2 and O_2, diluted by xenon (Xe) is compressed by a shock wave propagating at Mach numbers between $Ma = 1.34$ and $Ma = 2.83$. In general, maximum pressures and temperatures are reached when the shock passes the bubble. Subsequently, the gas mixture relaxes and the two main parameters controlling the reaction rate, temperature and pressure, decrease.

At low shock Mach numbers the gas mixture does not ignite within the experimental timeframe, as the compression is not sufficiently high. An increase of shock strength results in an ignition, followed by a deflagration reaction wave. At higher shock Mach numbers the stoichiometric mixture reacts in a detonation wave, even before the shock wave has reached the shock focusing point. Haehn et al. [19] determine Damköhler numbers in the range from 0.25 ($Ma = 1.65$) to 8.00 ($Ma = 2.83$). They conclude that heat conduction plays an important role at lower Mach numbers, and that the Zeldovich mechanism becomes important at higher Mach numbers. This finding is consistent with the two limiting cases of shock-induced combustion, the strong and the weak ignition [20]. Strong ignition leads to a detonation mostly initiated directly by the shock wave, whereas weak ignition is characterized by the occurrence of small flames that can undergo transition into detonation waves. Haehn et al. [19] provide several chemiluminescence exposures to depict the qualitative evolution of the bubble and reaction processes. Beside such visualizations, they present quantitative data for the temporal evolution of the transverse diameter of the bubble as well as for the vortex ring diameter. However, the complex experimental setup of Haehn et al. [19] implies uncertainties. For instance, the uncertainty of the Damköhler number at the highest Mach number ($Ma = 2.83$) is $Da = 8 \pm 4$. At the lowest Mach number ($Ma = 1.34$) 30% of all measurements showed no ignition within the given experimental time frame. Such uncertainties underline the need for a detailed numerical study of RSBI.

1.4. Objectives of the current investigation

The present numerical investigation complements these of Haehn et al. [19] and establishes a numerical framework for further studies. Special emphasis is given on the general temporal and spatial evolution of RSBI, the comparison with SBI, and the dependence of the bubble evolution on the reaction wave type. In our study the initial pressure is varied at a constant shock Mach number. The chemical reaction rates of most gas mixtures simply increase with pressure H_2-O_2 reactions, however, show a different behavior [21], as discussed in Section 1.2. The reaction rates are sensitive to pressure, and a variation of the initial pressure can change the entire reaction process between detonation and deflagration.

The paper is structured as follows: Section 2 outlines the governing equations. Molecular transport properties for multicomponent flows and chemical reaction kinetics, based on the Arrhenius law as well as the validation of the employed reaction mechanism are presented in detail. Section 3 outlines the computational domain and the initial condition of each simulation. Results are discussed in Section 4. First the spatial and temporal evolution of RSBI are presented. The effect of different types of reaction waves on bubble deformation are compared with each other and with their non-reacting counterparts. The chemical reaction process during shock passage until ignition is analyzed in detail. The pressure dependency of H_2-O_2 reactions enables different reaction branches and leads to different gas compositions, and this results in either deflagration or detonation waves. In the following a consistent definition of the dimensionless Damköhler number is used to evaluate if hydrodynamic or chemical reaction time scales dominate the flow field for given initial pressure. Integral quantities, such as enstrophy or the molar mixing fraction, are consulted to determine the effect of the reaction