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Shock Mach number influence on reaction wave types and mixing in reactive shock–bubble interaction

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ABSTRACT

We present numerical simulations for a reactive shock–bubble interaction with detailed chemistry. The convex shape of the bubble leads to shock focusing, which generates spots of high pressure and temperature. Pressure and temperature levels are sufficient to ignite the stoichiometric H_2–O_2 gas mixture. Shock Mach numbers between $Ma = 2.13$ and $Ma = 2.90$ induce different reaction wave types (deflagration and detonation). Depending on the shock Mach number low-pressure reactions or high-pressure chemistry are prevalent. A deflagration wave is observed for the lowest shock Mach number. Shock Mach numbers of $Ma = 2.30$ or higher ignite the gas mixture after a short induction time, followed by a detonation wave. An intermediate shock strength of $Ma = 2.19$ induces deflagration that transitions into a detonation wave. Richtmyer–Meshkov and Kelvin–Helmholtz instability evolutions exhibit a high sensitivity to the reaction wave type, which in turn has distinct effects on the spatial and temporal evolution of the gas bubble. We observe a significant reduction in mixing for both reaction wave types, wherein detonation shows the strongest effect. Furthermore, we observe a very good agreement with experimental observations.

1. Introduction

The interaction between high-speed reactive flows and shock waves is a generic situation present in many combustion systems. Controlled application can promote mixing; uncontrolled interactions, however, can lead to undesirable heat release and thermomechanical loads. Especially in supersonic combustion, where 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], mixing can be enhanced sufficiently by shock-induced instabilities. The selected generic configuration of reacting shock–bubble interaction (RSBI) is representative for a large range of hydrodynamic instabilities and different reaction wave types occurring in application, and allows us to study the interaction between different effects in detail.

1.1. Hydrodynamic instabilities

Two hydrodynamic instabilities dominate in a RSBI: the Richtmyer–Meshkov instability (RMI) and the Kelvin–Helmholtz instability (KHI). RMI can enhance mixing in high-speed reactive flows, promote turbulent mixing and thus increase the burning efficiency of supersonic combustion engines [2]. The instability occurs at the interface between two fluids of different densities. Theoretically stated in 1960 by Richtmyer [3] and experimentally verified by Meshkov [4] in 1969, RMI can be considered as the impulsive limit of the Rayleigh–Taylor instability [5,6]. The misalignment of pressure gradient, ∇p, associated with a shock wave and density gradient, $\nabla \rho$, at the material interface causes baroclinic vorticity production at the interface. For comprehensive reviews the reader is referred to Brouillette [7] and Zabusky [8]. RMI occurs on a wide range of highly reactive environments from extremely large scales in astrophysics [9], to intermediate scales in combustion [1,10] and down to very small scales in inertial confinement fusion [11].

RMI induces velocity shear and small perturbations at the interface of the bubble, which are necessary preconditions for KHI [12]. The perturbations are amplified, eventually generating vortices at the interface accompanied by the appearance of smaller scales [7]. KHI drives the breakup of large-scale structures [13] and forces mixing [14]. Both effects are the main hydrodynamic drivers in RSBI.

1.2. Shock-induced ignition and reaction waves

Independently of the scale, RMI is accompanied by a second phenomenon in reactive gas mixtures: the shock-induced variation

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of thermodynamic properties, which can lead to ignition, followed by a reaction wave. Two reaction wave types can be distinguished: deflagration and detonation. Deflagration is a subsonic diffusion-driven reaction wave that propagates through the gas mixture due to direct transfer of chemical energy from burning to unburned gas [15]. 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 [15]. The detonation wave propagates up to 10^8 times faster than the deflagration wave [16]. Due to the large differences in the characteristic reaction time scales, the reaction wave type has a crucial influence on the flow evolution.

Under certain circumstances a deflagration wave can transform into a detonation wave. Deflagration-to-detonation transition (DDT) is one of the most interesting unresolved problems in combustion theory. Generally, a self-propagating deflagration wave is unstable and tends to accelerate. Under specific conditions the continuous acceleration can suddenly transition into a detonation wave [17]. Liberman et al. [18] proposed a mechanism mainly driven by flame acceleration divided into three stages. The reaction front accelerates and produces shock waves far ahead of the flame. Thereafter, the acceleration decreases, shocks are formed on the flame surface and pockets of compressed and heated unburnt gas emerge (preheat zone). In the final stage the transition to detonation happens: the flame propagates into the preheat zone and produces a large amplitude pressure pulse. Increasing pressure enhances reaction rates and the feedback between the pressure peak and the reaction leads to a growth of the pressure peak, which steepens into a strong shock that, coupled with the reaction zone, finally forms an overdriven detonation wave.

Furthermore, the flame front can propagate into regions of gas that already have been compressed and preheated by preceding shock waves such as in shock–bubble interactions (SBI). The reaction rates and the heat release are enhanced in these regions, which in turn increases the pressure pulse and accelerates the transition to detonation. In general, DDT can occur in two regions: it develops from the preheated, compressed gas mixture between the leading shock wave and the flame or it arises from within the flame [19]. The latter transition process is relevant for the presented study as RSBI contains regions of irregular compression by the initial shock wave.

1.3. *Reacting shock–bubble interaction*

The impact of a shock wave on a reactive gas bubble allows to investigate the interaction between shock-induced hydrodynamic instabilities and ignition. The shock wave triggers RMI and the pressure and temperature increase leads to the formation of radicals, which accumulate until the gas mixture ignites. RMI, due to the misalignment of the pressure and density gradient at the bubble interface, causes the bubble to evolve into a vortex ring. Provided that the initial kinetic-energy input is sufficient, the flow develops a turbulent mixing zone through non-linear interactions of the material interface perturbations [7,8]. Upon contact, the incident shock wave is partially reflected and partially transmitted. For an Atwood number $A = (\rho_1 - \rho_2)/(\rho_1 + \rho_2) < 0$ (the bubble gas is lighter than the ambient gas), the transmitted shock wave propagates faster than the incident shock wave. $A > 0$ shows the converse effect, the transmitted shock wave travels slower than the incident shock wave outside of the bubble. The transmitted shock wave focuses at the downstream pole of the bubble and collapses into a single point (shock-focusing point).

Classical inert SBI was the subject of several studies over the last decades. Haas and Sturtevant [20] investigated the interaction of shock waves propagating in air with a gas bubble filled with either helium or *R*-22. Their experimental results contributed to a better understanding of the temporal bubble evolution under shock acceleration and established a new class of canonical flow configurations. These experimental findings were completed by the investigations of Quirk and Karni [21], providing detailed numerical results of shock–bubble interaction problems. They reproduced the transition from regular to irregular refraction, shock wave focusing and the formation of a jet towards the center of the bubble. For a detailed review of SBI see Ranjan et al. [22].

A new level of complexity can be added to the setup of SBI by replacing the inert gas with a reactive gas mixture. A strong shock wave can ignite the reactive gas mixture directly at the interface, whereas the additional increase of pressure and temperature in the shock-focusing point is required for ignition at lower shock Mach numbers. Two types have to be differentiated: non-premixed and premixed gas mixtures. Reacting SBI of non-premixed gas mixture was studied by Billet et al. [23]. In their setup a H_2 gas bubble surrounded by air is shocked to study the influence of the volume viscosity on the bubble evolution and vorticity production. Attal et al. [24] verified the results of Billet et al. [23] and furthermore observed the formation of a double diffusion flame in the bridge region of the shocked bubble. Attal and Ramaprabhu [25] studied single-mode reacting RM in a non-premixed setup at different interface thicknesses. They observed shock-induced ignition and mixing enhancement by reshocking the propagating flame. Furthermore shock–flame interaction increases the surface area of the flame and the energy release and therefore the burning rate [26]. Massa and Jha [27] showed that small scales are damped by the shock wave and that the growth of RMI and KHI are reduced.

In 2012, Haehn et al. [28] investigated the interaction of a shock wave with a premixed gas bubble, filled with a stoichiometric gas mixture of hydrogen (H_2) and oxygen (O_2), diluted by xenon (Xe). Besides triggering hydrodynamic instabilities, such as RMI, the shock wave also increases the temperature and pressure, which in turn induces faster chemical reaction rates up to the ignition of the gas mixture. 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. The experiments of Haehn et al. [28] covered both ignition types deflagration and detonation, by varying the shock wave Mach numbers between $Ma = 1.34$ and $Ma = 2.83$.

A weak shock wave with $Ma = 1.34$ does not ignite the gas mixture within the experimental timeframe. Compression is not sufficient to start a self-sustaining chemical reaction. An increase of the shock strength results in an ignition followed by a deflagration wave. The reaction wave type changes for higher shock Mach numbers; Haehn et al. [28] observed a detonation wave for $Ma = 2.83$, even before the shock wave has reached the shock focusing point. Damköhler numbers between 0.25 ($Ma = 1.65$) and 8.00 ($Ma = 2.83$) were determined. Haehn et al. [28] conclude that heat conduction plays an important role at lower shock Mach numbers, and that the Zeldovich mechanism becomes important at higher shock Mach numbers. Their conclusion is consistent with the two limiting cases of shock-induced combustion, the strong and the weak ignition [19]. Strong ignition results in a detonation essentially initiated directly by the shock wave. Weak ignition is characterized by the appearance of small flames that can undergo transition into detonation waves. Several chemiluminescence exposures are provided by Haehn et al. [28] to depict the qualitative evolution of the bubble and reaction processes. Furthermore, quantitative data for the temporal evolution of the transverse diameter of the bubble as well as for the vortex ring diameter are presented. However, the complex experimental setup implies uncertainties. Haehn et al. [28] estimate the uncertainty of the Damköhler number at the highest shock Mach number ($Ma = 2.83$) of up to 50% ($Da = 8 \pm 4$). At the lowest shock Mach number ($Ma = 1.34$), 30%