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Three-dimensional reacting shock–bubble interaction

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ABSTRACT

We investigate a reacting shock–bubble interaction through three-dimensional numerical simulations with detailed chemistry. The convex shape of the bubble focuses the shock and generates regions of high pressure and temperature, which are sufficient to ignite the diluted stoichiometric $H_2{-}O_2$ gas mixture inside the bubble. We study the interaction between hydrodynamic instabilities and shock-induced reaction waves at a shock Mach number of $Ma = 2.83$. The chosen shock strength ignites the gas mixture before the shock-focusing point, followed by a detonation wave, which propagates through the entire bubble gas. The reaction wave has a significant influence on the spatial and temporal evolution of the bubble. The misalignment of density and pressure gradients at the bubble interface, caused by the initial shock wave and the subsequent detonation wave, induces Richtmyer–Meshkov and Kelvin–Helmholtz instabilities. The growth of the instabilities is highly affected by the reaction wave, which significantly reduces mixing compared to an inert shock–bubble interaction. A comparison with two-dimensional simulations reveals the influence of three-dimensional effects on the bubble evolution, especially during the late stages. The numerical results reproduce experimental data in terms of ignition delay time, reaction wave speed and spatial expansion rate of the bubble gas. We observe only a slight divergence of the spatial expansion in the long-term evolution.

1. Introduction

The interaction between a shock wave and a density inhomogeneity induces Richtmyer–Meshkov instability (RMI). The baroclinic vorticity production mechanism and subsequent Kelvin–Helmholtz instabilities (KHI) result in a complex turbulent flow field. The shock–bubble interaction (SBI) is a common setup to study this interaction, which has been done intensively for several decades [1]. An additional degree of complexity can be added by replacing the inert bubble gas by a reactive gas mixture. In the generic configuration of a reacting shock–bubble interaction (RSBI), the increase of pressure and temperature across the shock wave accelerates the chemical reactions. Depending on the shock strength, the stimulation of the reaction kinetics can be sufficient to ignite the reactive bubble gas. The subsequent reaction wave interacts with the hydrodynamic instabilities and affects integral properties of the flow field. By three-dimensional numerical simulation we investigate RSBI of a gas bubble filled with hydrogen (H_2) and oxygen (O_2), diluted with xenon (Xe) in a pure nitrogen (N_2) environment at a shock Mach number of $Ma = 2.83$. The setup is motivated by previous works of the authors [2,3], where the ignition behavior and the early stage bubble evolution of RSBI in two dimensions was investigated. Specific reaction wave types and ignition spots were triggered by the variation of the initial pressure or the shock strength. The subsequent mixing processes and the bubble evolution, including the spatial expansion and the growth of instabilities, showed a high dependence on the reaction wave type. Three-dimensional effects, which are relevant for the long-term evolution are the focus of the current work.

Shock-accelerated flows in reactive environments involve a wide range of scales, from extremely large scales in astrophysics [4], intermediate scales in combustion engines [5], down to very small scales in inertial confinement fusion [6]. Independent of the scale, the misalignment of the pressure gradient, ∇p, associated with the shock wave, and the density gradient, $\nabla \rho$, across a material interface, produces baroclinic vorticity ($\nabla p \times \nabla \rho$) and induces Richtmyer–Meshkov instability (RMI) [7,8], the impulsive limit of the Rayleigh–Taylor instability [9,10]. The RMI promotes turbulent mixing and increases the burning efficiency [11,12]. For a comprehensive review on RMI, the reader is referred to Brouillette [13]. Furthermore, the instability induces velocity shear and small perturbations at the interface of the bubble, which are, besides the initial density mismatch, necessary preconditions for the

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Kelvin–Helmholtz instability (KHI) [14]. The perturbations are amplified and generate vortices at the interface accompanied by the appearance of smaller scales [13]. The breakup of large-scale structures is driven by the KHI [15,16] and forces mixing.

1.1. Shock–bubble interaction

The classical inert shock–bubble interaction (ISBI) describes the hydrodynamic effects induced by a planar shock wave propagating through a gas bubble. 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 the bubble. The transmitted shock wave focuses at the downstream pole of the bubble and collapses into a single shock-focusing point. 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 [13,17].

ISBI was intensively studied over the last decades. The first detailed experimental investigations were performed by Haas and Sturtevant [18] in 1987. They studied gas bubbles filled with either helium or chlorodifluoromethane (R22), surrounded by air, and contributed with their results to a better understanding of the temporal bubble evolution under shock acceleration and established a new class of canonical flow configurations. Quirk and Karni [19] complemented these experimental findings by their detailed numerical results of shock–bubble interaction problems. Shock wave focusing, formation of a jet towards the center of the bubble and the transition from regular to irregular refraction were reproduced. For a detailed review of ISBI the reader is referred to Ranjan et al. [1].

1.2. Reacting shock–bubble interaction

The classical setup of ISBI can be extended replacing the inert bubble gas by a reactive gas mixture. Thus, the compression and temperature increase across the shock wave induce an additional effect: the chemical reaction rates are elevated, radicals form and accumulate. For sufficiently strong shock waves, the mixture ignites and reaction waves propagate through the reactive bubble gas.

Two reaction wave types have to be distinguished: deflagration and detonation. Deflagration is a subsonic diffusion-driven reaction wave that propagates through the gas mixture due to the direct transfer of thermal energy from burning to unburned gas [20]. 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 [20]. Detonation waves propagate up to 10^8 times faster than deflagration waves [21]. The latter reaction wave is observed and studied in our numerical investigation of RSBI.

First experimental studies of RSBI were performed by Haehn et al. [22] in 2012. In their setup, a gas bubble filled with a stoichiometric mixture of H_2 and O_2, diluted by xenon (Xe) is penetrated by a shock wave with shock 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 ignition, followed by a deflagration wave. The reaction wave type changes for higher shock Mach numbers; Haehn et al. [22] observed a detonation wave for $Ma = 2.83$, even before the shock wave has reached the shock focusing point. They conclude, that the post-shock thermodynamic conditions are near the ignition limits. Several chemiluminescence exposures are provided by Haehn et al. [22] to depict the qualitative evolution of the bubble and the reaction processes. The reaction wave has propagated through the bubble gas before the formation of the vortex ring is initiated. 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. [22] 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% of all measurements showed no ignition within the given experimental time frame. Numerical studies are necessary to obtain a deeper understanding of the physics and reaction kinetics of RSBI. Accurate numerical simulations can provide detailed insight into induction times, gas compositions and mixing processes during the shock–bubble interaction.

We presented first numerical results for two-dimensional RSBI [2,3]. Pressure dependent ignition and reaction waves were in agreement with experiments of Haehn et al. [22]. Despite the missing spatial dimension, the simulations reproduced bubble expansion, ignition location and reaction wave types, and explained experimentally particularities, such as the transition from deflagration to detonation and a double detonation. Nevertheless, some important effects, especially for the long-term evolution, were suppressed as the vortex stretching term is absent in two dimensions. The two-dimensional vortex cores remain stable, whereas three-dimensional vortex rings become unstable and may break up into three-dimensional turbulence [23]. In order to obtain accurate predictions for the mixing processes in the long-term evolution of RSBI, an extension to three-dimensional simulations is needed.

1.3. Scope of the present work

The present numerical investigation extends our previous work on two-dimensional RSBI [2,3] and complements the experimental results of Haehn et al. [22] by three-dimensional RSBI simulations with detailed $H_2{-}O_2$ chemistry. At a shock Mach number of $Ma = 2.83$ the mixture ignites ahead of the shock-focusing point. Ignition is followed by a detonation wave that has a distinct effect on the hydrodynamic evolution of the RSBI. We also present results for ISBI to study the influence of the reaction wave on the mixing process, on the vortex ring and on the spatial and temporal bubble evolution. By comparison with two-dimensional simulations, we are able to show how three-dimensional phenomena, such as the decaying vortex ring, destabilized by Widnall-type instabilities, influence the long-term evolution of SBI. The experimental findings of Haehn et al. [22] are confirmed and important quantities such as the ignition delay time, the reaction wave speed, and the spatial and temporal bubble evolution are correctly reproduced.

This paper is structured as follows: Section 2 summarizes the governing equations for fluid dynamics and chemical reaction kinetics. Initial conditions and the computational domain are presented in Section 3. Section 4.1 outlines the results of the three-dimensional simulations, followed by a comparison with two-dimensional data in Section 4.2. In Section 4.3, we compare our results with the experimental work of Haehn et al. [22]. The final Section 5 summarizes the key findings.

2. Numerical model

2.1. Governing equations

We solve the full set of compressible reacting multi-component Navier–Stokes equations in conservative form