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FLAME STRUCTURE 2014
8th International Seminar on Flame Structure

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(TU Berlin)**

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Abstract.

Re-ignition and re-initiation mechanisms of quenched detonation waves passing over a backward facing step are studied numerically using a high-order Discontinuous Galerkin method with detailed thermo.chemistry. A stoichiometric Hydrogen/Oxygen mixture with di.erent diluents (Argon and Nitrogen) is considered to assess e.ects of mixture composition and reactivity on the initiation process. It is found that the wall reflection of the decoupled shock plays a critical role in controlling the formation and growth of the ignition kernels and the possible transition to detonation. Through parametric studies, it is shown that for more reactive Argon-diluted mixtures, ignition appears first behind the regular shock reflection, which is followed by spontaneous re-initiation. By replacing Argon with Nitrogen, the reactivity reduces and re-ignition through Mach reflection is observed. This ignition phenomenon is a.ected by the adia.batic heating behind the Mach stem and the enhanced mixing along the slip-line due to hydrodynamic instabilities. The present numerical investigation shows good agreement with corresponding experimen.tal measurements and confirms previous postulations regarding the role of the Mach reflection on the re-ignition.

Introduction.

Detonation is a highly energetic combustion process, involving a compression shock and an attachedflame, which provides fast heat release as a driving source. The formation and the quenching of thesedetonation waves exhibits a pronounced sensitivity to the geometry. For example, with abruptlyexpanding geometries, the detonation wave can be significantly delayed or potentially quenched. Thereason for this phenomenon is as follows. As the shock gradually weakens during the expansion, thepost-shock state becomes less favorable for highly sensitive chemical reactions. Thus, the flamegradually decouples from the shock front, which results in the breakdown of the positive feedback.However, since the detached shock is also capable of interacting with downstream geometricboundaries, it has been found that the delay or quenched detonation front can be re-ignited undercertain conditions. The investigation and analysis of the re-ignition has significance for practicalapplications. In fact, the process described above is analogous to those encountered in manydetonation facilities. In pulse detonation engines, for example, detonation, after being initiatedin the initiator section, passes over an expanding nozzle and propagates into the larger combustionchamber. Furthermore, it is also related to the deflagration-to.detonation transition (DDT) inobstructed tubes with periodically arranged obstacles. As such, the further understanding of theseprocesses not only deepens our understanding of detonation physics, but will also provide furtherguidance for practical designs. Although notable progress has been made on identifying re-ignitionmechanisms of quenched detonation waves, conclusions from di.erent studies are sometimesinconsistent and disputable. With interest to the present investigation, the following re-ignitionprocesses are summarized:1) Autoignition and re-initiation by regular shock reflection: The autoignition of a quencheddetonation wave is induced by a regular reflection of the flame-detached shock-wave. Lee pointed outthat this mode exhibits similarities to the triple-point collision in multi-dimensional detonationsystems. Fast autoignition will re-initiate the detonation with a strongly overdriven explosion. Theonset and dynamics of this re-ignition mode have been indirectly deduced from experimental sootfoilrecords, and observed from numerical simulations using one-step chemical mechanisms.2) Autoignition and re-initiation by Mach reflection: When the incident shock angle exceeds acritical value, Mach reflection can occur. This results in the formation of a high-temperature regionbehind the Mach stem, which promotes ignition and re-initiation. This mechanism was deduced fromexperimental investiga.tions of detonation waves passing over a backward-facing step. Even insubsequent experiments, however, the distinction to ignition by regular reflection could not beisolated due to the limited spatio-temporal resolution of the measurement method. Ignition by Mach-heating was also emphasized in a computational study on DDT in channels with periodically positionedobstacles. These simulations showed that by varying the spacing between obstacles to promote Machreflection, the heating of the fresh mixture by the collision of the strong Mach stem with thedownstream obstacle leads to the onset of detonation. Ignition by Mach heating was also observed incomplex wave interactions. However, by excluding these confinement effects and geometric interactions,it remains unclear whether and how transitions to detonation is facilitated.3) Re-initiation by hydrodynamic instabilities: This mechanism, first postulated by Teodorczyk etal., emphasizes the effect of enhanced mixing between reaction products and unburned gases byKelvin-Helmholtz (KH) or Richtmyer-Meshkov (RM) instabilities. This is similar to the ignitionmechanism proposed by Radulescu et al. in irregular detonation waves. Recently, a more detailedstudy has been conducted by Bhattacharjee et al., who studied the re-ignition process of a quencheddetonation behind a circular obstacle. At certain conditions, they found that the occurrence of arapidly burning mixture is strongly coupled to the presence of a wall jet, which enhances the mixingand growth of the flame front behind the Mach stem. As postulated, this might lead to the onset oftransverse detonation waves. However, the transition to detonation from hot-spot ignition appearsnon-deterministic under these operating conditions since the re-initiation could not besystematically reproduced. The objective of this work is to provide a better characterization ofre-ignition events of quenched deto.nation waves. Since the shock reflection plays an important role,an analytic model will first be purposed to analyze shock reflection based on quasi-steadyassumptions. This low-order model allows us to evaluate the thermodynamic state and ignition delayof the shock-compressed mixture. These theoretical investigations are complemented by detailedsimulations using a high-order Discontinuous Galerkin approach. A detailed chemical kinetics modelis employed to provide an accurate representation of rate-controlling quenching and ignition events.The geometric configuration under consideration is identical to the experiment by Ohyagi et al. Afteridentifying and discussing relevant physics, the simulation results will then be used to assess thevalidity of the reduced-order model.

Approach.

In this work, the 2D reactive Euler equations are solved using a discontinuous Galerkin (DG) method. For this, the computational domain is subdivided into a set of elements. For this, several algorithmic aspects re.quire consideration to enable the application to chemically reacting flows. First, the variable thermodynamic properties, specifically the temperature- and composition-dependent heat capacities introduce spurious oscil.lations for fully conservative flux formulations. To prevent these oscillations, a relaxation method is applied, leading to a framework with quasi-conservation of energy. Second, the detailed chemistry representation introduces a chemically stiff system. A splitting scheme is used for the temporal integration, in which the convection operator is handled explicitly and the reaction source term is advanced implicitly. Finally, the consideration of discontinuities due to shocks and contact interfaces is treated using a WENO-based limiter that was recently proposed by Zhong Shu. This limiter guarantees the positivity of density and pressure based on the entropy minimum principle. More details and verification of the developed computational platform can be found in the work by Lv & Ihme.

Results and discussion.

In this study, we consider the experimental configuration of Ohyagi et al. In this facility, a long initiator section is adopted to ensure fully-developed cellular structures before the detonation wave expands into the combustion section. The height of the combustor section is three times the cross-section of the initiator. All simulations were initialized with a 1D Chapman-Jouguet (CJ) wave near the inlet of the initiator section. Small perturbations were imposed along the shock front to initiate transition to 2D cellular structures. The detonation wave diffracts after entering the combustor section. Low initial pressure and high dilution ratios have been found to be essential in predicting the correct detonation size with detailed chemical kinetics. In the present study, the initial pressure and temperature are set to 26.7 kPa and 293 K, respectively, and the dilution ratio is fixed to 40 For all cases presented, the quenched detonation configurations are observed after the fully established detonation-wave diffracts over the backward-facing step. The decoupled shock front, propagating faster than the flame front, interacts first with the bottom wall. Under different diluent parameters the shock reflection results in a different ignition pattern that can lead to the successful re-initiation or the failure of the detonation. Detailed simulations are performed, showing that the diffraction induces a shock-flame complex, in which shock and flame fronts are completely decoupled. Several ”finger-like” flame segments are observed behind the shock front. After the shock starts to interact with the wall, and subsequently the reflected shock transmits into the burnt mixture. After this reflection occurs, the hot spot is immediately generated around x = 40 mm, followed by an extremely fast transition (on the order of few micro-seconds to an overdriven detonation, which is visible at later time. The new detonation front grows and quickly engulfs the inert transverse wave. After it catches up with the leading incident shock, a reactive Mach stem is formed due to their mutual interactions. The induced hydrodynamic instabilities along the slip line is well resolved in our simulation. The forward wall jetting effect behind the Mach stem is also observed. The new triple point, connecting the reactive Mach stem, reactive transverse wave and inert incident shock, moves along the curved front of the incident shock, and finally re-initiates the whole front. This re-initiation sequence shows very good agreement with that reported in the experimental study by Obara et al.

Conclusions.

Re-ignition events of a quenched detonation wave were investigated through detailed numerical simulations using a high-order discontinuous Galerkin method. A reduced-order model was developed for the parametric investigation of the re-ignition dynamics. The quenched detonation is generated by the diffraction over a backward-facing step. A stoichiometric Hydrogen/Oxygen mixture was considered with variable diluent compositions. A series of detailed simulations was performed to systematically identify ignition mechanisms that are controlled by the coupling between gasdynamic processes and chemical kinetics. It was found that the shock reflection plays an essential role in the formation of ignition spots. Predictions from the reduced-order model are in qualitative agreement with the detailed simulations.

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