Comparison of Detailed Mechanisms for the Numerical Simulation of Unsteady Shock-Induced Combustion

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1 Introduction

Experimental and theoretical studies of Shock-Induced Combustion(SIC) have been extensively reported since 1960's[1-3]. Numerical simulation of such complex flow was reported and validated by various researchers[4-13] from as early as 90's. It has regained its interest in the last decade because of its application to aerospace such as in the studies of Oblique Detonation Wave Engine(ODWE), Shock-Induced Combustion Ramjet Engines(SCHRAMJET). The combustion flowfield in SIC is characterized by the complex coupling and interaction of the shock wave and reaction front and depending on the flowfield conditions, distinctive features are obtained. Numerical simulation of SIC poses various challenges. 1) Accurate prediction of the induction zone 2) Numerical approach to capture the bow shock - an inaccurate numerical approach may result in additional release of chemical energy from different reaction rates resulting in "Spurious runaway reactions"[14]. One of such challenges is the selection of detailed reaction mechanisms to predict accurate combustion flowfield. Various researchers have used different reaction mechanism in the simulation of complex combustion flowfield such as SIC, Scramjet applications and detonation. In this study, the performance of some of the selective hydrogen-air reaction mechanisms was analyzed for unsteady Shock-Induced Combustion flowfield.

2 Reaction Mechanisms for the analysis of SIC

More than 25 reaction mechanisms are available from various research groups for hydrogen-air combustion. But still there exists uncertainty and no one mechanism can predict accurate result for all combustion systems at all conditions. Comparing all the reaction mechanisms for complex combustion flows, such as SIC, is computationally expensive and hence only few reaction mechanisms, that were widely used for high speed combustions, were considered in this study. Jachimowski Reaction mechanisms [15, 16] was widely used in the SIC flows. GRI reaction mechanism[17] was used in detonation and Supersonic combustion studies and other combustion flowfields. Dryer model[18] was modeled especially for high pressure combustion and were also used in detonation simulation. The elementary reactions of hydrogen combustion are a core part of any hydrocarbon mechanism such as syngas or methane combustion

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mechanisms. Reaction mechanism from Combustion Kinetics Laboratory, University of Southern California (USC model)[19] and Combustion Research Group, University of California, San Diego (UCSD model)[20] were regularly updated and reported to predict combustion with high accuracy. Hence reduced mechanism of these combustion models was also considered in this study.

3 Numerical Setup

More detailed description on the numerical approach and modeling of the chemistry were documented in previous papers [12, 13]. For this study, a second order time accurate and third order Weighted Essential Non-Oscillatory(WENO) scheme were employed with AUSMDV flux splitting scheme. An unsteady case of Lehr's experiment in which, when a hemispherical projectile on a cylindrical body of diameter 15mm fired into combustible mixture at Mach number 4.48 results in an unsteady mode of combustion and oscillates regularly at a frequency of 425 KHz. The combustible mixture includes premixed Hydrogen-Air in stoichiometric ratio at initial temperature of 293K and pressure of 320 mmHg with sonic velocity of 403 m/s. There are other cases also, where the projectiles fired at Mach 4.18 and 4.79 results in oscillation frequencies of 148 and 725 KHz respectively. But considering the length scale and computational cost to simulate such complex case for various grid resolutions, only the case with Mach 4.48 was considered in this study.

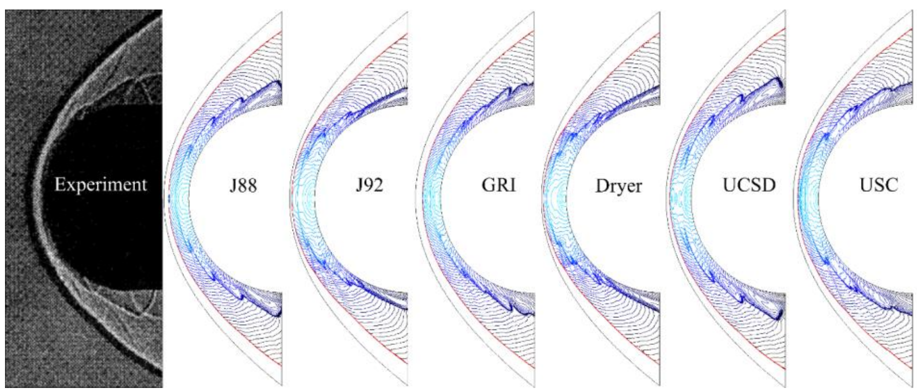

Figure 1 Experimental shadowgraph of Lehr's Experiment[1] and Instantaneous view of Mach distribution for the Various Reaction Mechanisms

4 Results and Discussion

In our previous study[21], we compared the basic characteristics of the reaction mechanism such as Ignition delay times, Laminar Flame Speeds at various initial conditions and SIC flowfield for short period. In this study, the simulation was performed for quite a long time to study the effect of the reaction mechanisms. Four type of grid sizes which are equally spaced along the stagnation streamline were used in this study as listed in table 1. The time scale and length scale were scaled sufficiently enough to capture all the gradients in the flowfield. Initially, from the results of J88 mechanisms, it was observed that the shock wave oscillates far away from the projectile with Grid1 systems than the other cases and predicts a regular oscillation. The shock location for other grids oscillates almost around the same location as shown in Fig. 2. Hence in the further analysis, results of these grid systems will be discussed. Also, it is observed that the shock location was uniformly oscillating for grids Grid2 whereas with grid3, the shock location tends to oscillate slightly with low frequency oscillation with very low amplitude. With further increase in spatial resolution, the amplitude of the oscillation increases.

Table 1: A simple table

Type	Grid systems	Mesh size along the stagnation streamline (in μm)	Time Scale for the calculation (in ns)
Grid1	150x200	13.50	3.90
Grid2	200x300	8.90	2.68
Grid3	300x450	6.00	1.79
Grid4	400x600	2.40	1.34

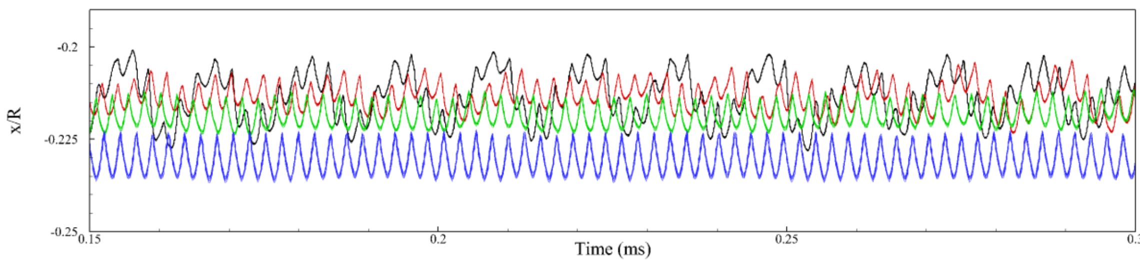

Figure 2. Location of Shock wave over a period of time with different grid systems simulated using J88 model. Grid1 – Blue lines; Grid2 – Green lines; Grid3 – Red lines; Grid4 – Black lines.

Performance of various reaction mechanisms

The x-t graph, taken along the stagnation streamline of the projectile surface over a period, can be one of the viable ways to compare the flow features of SIC for various reaction mechanisms. Temperature profile taken along the stagnation streamline in a well-developed flow is plotted over a period of 200μs for all the reaction mechanisms. With Grid2, as shown in Fig.3, UCSD, USC and J88 models predicts a regular flow whereas, with J92 model, there is a slight disturbance in its regular oscillation. With Dryer model, the flow feature is greatly disturbed which results in high amplitude low frequency oscillation. GRI model results in an unphysical oscillating phenomenon with low frequency. It is also observed that the induction zone for the GRI model is relatively long compared with the other models which results in reaction front being closely attached to the projectile for this case. At high grid resolutions, even the Jachimowski models develops such instability as seen in Fig.4. The flow features of UCSD and USC models gets disturbed slightly at times, but that does not develop into an instability, while the Dryer and GRI model remains same but was completely unphysical.

Investigation of Low frequency instability phenomena

Basically, in a shock-induced combustion, a compression wave called as 'retonation wave' is generated behind the reaction front after a mild explosion, moves through the combusted mixture and gets reflected from the projectile surface. At the same instant, a compression wave is created which moves towards the shock wave, thereby compressing the combustible mixture in the induction zone and accelerates the combustion. This acceleration further strengthens the compression wave and pushes the shock wave far away from the projectile surface. Later the strength of this compression wave decreases and the shock wave moves towards the projectile surface, thereby creating a contact discontinuity which runs through the induction zone. At the same time, the retonation wave gets reflected towards the reaction front after hitting the projectile surface. These two waves meet near the reaction front and creates a mild explosion causing new retonation wave and contact discontinuity. This cycle repeats in a regular cycle in a periodically oscillating SIC. But when the strength of these waves is not consistent, it leads to an instability phenomenon as observed here. For instance, when the strength of the retonation is increased slightly in the flowfield, then the strength of the compression wave, which moves in the induction zone, also increases and pushes the shock wave further.

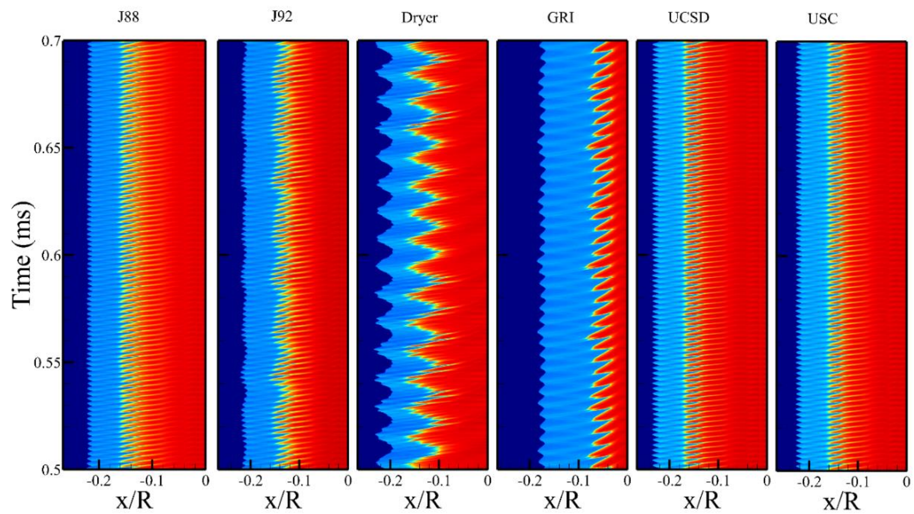

Figure 3. x-t graph of temperature contour for various reaction mechanisms for Grid2

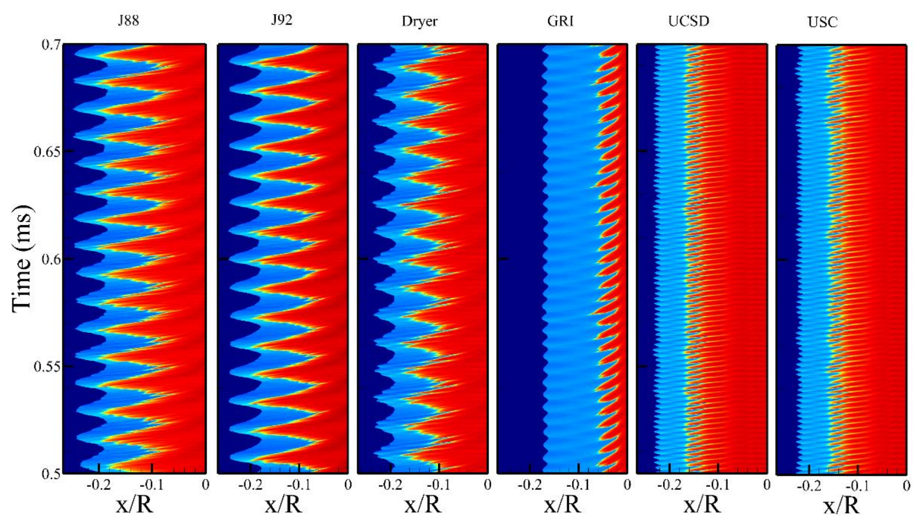

Figure 4. x-t graph of temperature contour for various reaction mechanisms for Grid4

When the shock wave moves away from the projectile surface, then the new compression wave should move a long distance compared to the previous compression wave. This delays the oscillation and the shock wave starts to move towards the projectile surface in the consequent cycle during which the new waves moves a short distance and gets reflected from the shock wave and meets the retonation wave. The resulting detonation will be high in intensity compared to the previous cycle and will lead to a stronger compression wave, which pushes the shock wave further. This instability slowly grows and finally leads to irregular low frequency oscillation rather than just the regular high frequency oscillation as observed in experimental observations. Since all the parameters were kept constant and only the reaction mechanisms were changed during this study, these discrepancies can be attributed to the difference in the reaction rates of different reaction mechanisms. However, detailing more on the reaction rates were beyond the scope of this study and are not discussed more in here.

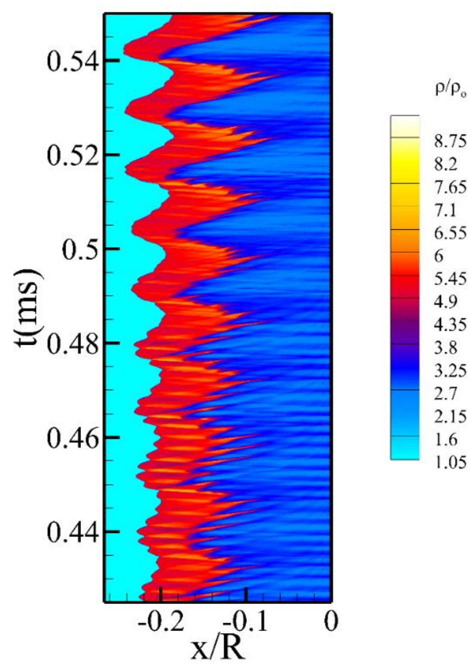

Figure 5. x-t graph of density ratio distribution with J88 model at Grid4 resolution

5 Conclusion

An attempt was made to analyse the performance of the reaction mechanism for combustion in SIC applications. The differences in the results can be attributed to the discrepancies in the rates of the reaction mechanism, as only the reaction mechanism modified in this analysis. However, detailing on the reaction step for this cause was beyond the scope of this study. Through this study, we observed that Jachimowski models are highly sensitive to grids and hence the combustion is accelerated at higher grid resolutions. Dryer model is grid-insensitive but has faster reaction rates which results in high amplitude low frequency oscillation at all grid levels whereas GRI is also grid-insensitive but predicts unphysical oscillation because of low reaction rates. UCSD and USC mechanisms cannot be completely termed as grid-insensitive, but that grid sensitiveness does not affect the flow physics for this case. For SIC related combustion studies, UCSD can be highly relied since it is less sensitive to grids, predicts the SIC flowfield quite well compared to the other models and are updated frequently.

Acknowledgement

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