Study of Combustion pattern in Oblique Detonation Engine

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ABSTRACT

Oblique detonation engines are being a centre of multiple kinds of research. Likewise, this paper provides the simulation at various Mach numbers to observe the pattern of combustion in an oblique detonation engine. Considering Rahul et al paper[5] as a reference same conditions of pressure, temperature and wedge angles were used in this paper. Yet, a different model of a chemical designed by M.O Conaire and H.J Curran[7] was used and simulation was performed at several Mach numbers until a fully developed combustion had been achieved.

Keywords: Oblique detonation engines, Chapman-Jouguet, SCRAMJET engines, non-heat-conducting.

1 Introduction

Over the years, researchers have been studying the ways of making propulsion more efficient. Oblique detonation wave engines are one among them where detonation plays a key role. It is a mode of combustion which propagate supersonically and it is highly preferred due to its better thermodynamic cycle efficiency than constant pressure cycle or constant volume cycle. This makes detonation highly suitable for the supersonic and hypersonic propulsion system. Looking back into the researches provided in David et al[1] paper, Roy[2] introduced the concept of stabilized normal detonation wave(NDW) in 1946 for hypersonic aircraft. However, to stabilize NDW in steady flow it required variable engine geometry. Then, normal detonation meaning flow downstream would be sonic or subsonic which in turn results in high static temperature which can be the reason for the dissociation of combustion products. NDW could not be suggested beyond Mach number 6 as performance falls steeply.

Ferri[3] suggested the use of deflagration or diffusive combustion to preserve the supersonic flow in the combustor so this new concept was preferred more than NDW since then. Next, Dunlap et al[4] came up with the use of stabilized oblique detonation wave for hypersonic ramjet propulsion. According to Dunlap, the only normal component of flow leaving an ODW is sonic or subsonic. Hence, supersonic flow can be preserved throughout the combustor. It is of great importance because if the incoming Mach number is less as compared to Chapman-Jouguet Mach number, an unstable normal detonation wave is experienced in the combustor. On the other hand, exceeding incoming Mach number as compared to CJ Mach number will lead to oblique detonation. Further, to stabilize wave variable geometry is not required as it is done solely by a wedge.

Not only this, but ODWEs are also more advantageous than SCRAMJET engines owing to the fact that it gives short combustor length and less inlet diffusion. Moreover, these engines can help in delaying the rocket operation because of their performing abilities and the amount of oxygen carried on board could be decreased too. There were experimental attempts made between the 1950s to 1960s but were limited and got the speed only after the Sputnik project in national aerospace research. Since then this has become a vital topic of research. So, this paper is also an effort to study the combustion in ODWE considering Rahul Kumar, Ajay Omprakas and Donald R Wilson [5] paper as a reference. They had provided a detailed analysis of oblique detonation wave using ANSYS Fluent. They used the hydrogen-air mixture, 9 species and 28 steps, chemical reaction model[6], at a specific Mach number 6 and wedge angle 20° respectively. The same air-fuel mixture has been used in the current study with a different chemical model designed by M.O Conaire and H.J Curran (11 species and 19 steps chemical reactions)[7]. The wedge angle is taken 20° from the reference paper but with different Mach numbers to obtain the pattern of combustion using ANSYS Fluent.

2 Computational Fluid Dynamics

As mentioned earlier, the area of focus of this paper will be the pattern of combustion inside the combustor. Let’s zoom into that area and take it as a 2D model (shown into figure 1), an asymmetric channel having a wedge (transition of geometry at the combustor inlet is said to be a wedge for the simplicity of the analysis). The flow enters from the inlet and collides with the wedge. At this point,
oblique shocks are generated and chemical reactions take place due to the high enthalpy of oblique shocks at the wedge. The figure shows the domain of fluid flow where left is combustor inlet and right is the way of exit of combustor towards the nozzle.

![Fig 1: 2D geometry dimensions are in mm](image)

Only half a portion of the geometry had been taken for the flow analysis since the geometry is symmetric. Rahul et al studied the oblique detonation wave at Mach number 6 and wedge angle of 20 deg. Based on their analysis, this paper varied the Mach number keeping the wedge angle fix at 20 deg to observe the pattern of combustion. The conditions such as P1 and T1 were taken from their paper exactly the same, 101325 Pa and 700K respectively. an incoming flow is the premixed hydrogen-air mixture and supersonic flow. At the outlet boundary, the non-reflective boundary condition is imposed. Surface and symmetry plane have slip conditions. Structure grid with different grid spacing is used to mesh various parts of the geometry.

3 Theory and Calculation

To ease the analysis, geometry is considered to be symmetrical and 2D. Further, Euler equations are applied considering the flow to be inviscid, non-heat-conducting and reacting gas flow which will help in getting a stable oblique detonation wave. Cartesian form of these equations is described as follows 1-4 equations.

\[
\frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = S
\]

\[
F = \begin{bmatrix}
\rho_s u \\
\rho u^2 + p \\
\rho u v \\
\rho E + p u
\end{bmatrix}
\]

\[
G = \begin{bmatrix}
\rho_s v \\
\rho u v \\
\rho v^2 + p \\
(\rho E + p) v
\end{bmatrix}
\]

\[
S = \begin{bmatrix}
0 \\
0 \\
0 \\
R_s
\end{bmatrix}
\]

Where
F and G-convective fluxes, S-Source term vectors
Subscript \( s=1,2,3...N_s \) (Ns-number of species)
Species continuity is represented by the First \( N_s \) rows. Next, two rows are of momentum equations. \( u \) and \( v \) are velocity components in \( x \) and \( y \) directions respectively.
\( \rho = \sum_{s=1}^{N_s} \rho_s \) mixture, \( \rho_s \) shows species density.
\( E \)-total energy per unit mass,
\( R_s \)-net rate of production of species of chemical reactions.
Governing equations of continuity, momentum, energy and species transport ANSYS Fluent’s set up, density-based solver with the implicit formulation. Advection Upstream Splitting Method (AUSM)(second-order) was applied to get the flux vectors. This method is chosen in order to get the absolute resolution of contact and shock discontinuities because it is oscillations free at stationary and moving shocks. Second-order Upwind scheme with Green Gauss Cell-based method was used for spatial discretization.

4 Chemical kinetics

The combustion phenomenon is modeled using finite rate chemistry model. It uses Arrhenius expressions to calculate the chemical source. To calculate Rs following equation can be used.

\[ R_s = M_{w,S} \sum_{r=1}^{N_r} \tilde{R}_{S,r} \] ........................5

\( M_{w,S} \) –Molecular weight of species S
\( N_r \)–Number of reactions
\( \tilde{R}_{S,r} \) – Arrhenius Molar Rate of production of species s in reaction r.

\[ \tilde{R}_{S,r} = \Gamma [v'_{S,r} - v'_{r}] \left[ k_{f,r} \prod_{j=1}^{N_s} (C_{jr})^{n_{jr}'} - k_{b,r} \prod_{j=1}^{N_s} (C_{jr})^{n_{jr}''} \right] \] ........................6

Here
\( C_{jr} \)– Molar concentration of species j in reaction r(kmol/m³)
\( v'_{S,r} \) and \( v'_{r} \) - stoichiometric coefficients of the reactant and product s respectively in reaction r
\( n'_{jr} \) - rate exponent of the reactant species j in reaction r.

Further, \( r^{th} \) reaction’s general form can be written as follows.

\[ \sum_{s=1}^{N_s} v'_{S,r} M_s \rightarrow \sum_{s=1}^{N_s} v''_{S,r} M_s \] ........................7

where
\( M_s \) –species s

Arrhenius expression can be used to calculate Forward rate constant.

\[ k_{f,r} = A_r T^{\beta_r} e^{-\frac{E_r}{RT}} \] ........................8

Here, \( A_r \) represents the pre-exponential factor
\( \beta_r \) is for temperature exponent
\( E_r \) represents activation energy for the reaction
\( R \) is the universal gas constant.

\[ k_{b,r} = \frac{k_{f,r}}{k_r} \] ........................9

\( k_r \)–equilibrium constant of \( r^{th} \)reaction.

ANSYS Fluent’s function mixing law was employed in getting the mixture specific heat at constant pressure. Every species could be said a function of temperature. In this case, M.O Conaire and H.J Curran[7] hydrogen-air combustion mechanism of 5 species \( \text{N}_2, \text{O}_2, \text{H}_2, \text{H}_2\text{O} \) and \( \text{OH} \) and 2 reactions is applied. This technique was chosen due to its accurate global results with fewer reaction steps. In the chemical reactions, \( \text{N}_2 \) is not involved as the highest temperature is still not equal to the dissociation temperature of nitrogen. Nevertheless, it exists as a collision partner.
5 Mesh Convergence

In order to obtain an optimal design mesh convergence test was performed on sizes $10^{-05}$ m and $8 \times 10^{-06}$ m. Mesh convergence was done on the geometry shown above in fig 1. Below fig 3 and 4 conveys the mesh convergence graph at $10^{-05}$ m and $8 \times 10^{-06}$ respectively. It can be seen that results do not change on the stated values which proves them to be optimal values. Then, $10^{-05}$ m mesh size is considered in all the further works in this paper.

![Graph 1: Convergence plot](image1)

6 Results and Discussion

The starting point for this simulation was chosen to be Mach 4 and it is performed for various Mach numbers to observe the pattern of combustion and till proper combustion is achieved in the combustion chamber. Images of pressure, temperature and H$_2$O mass fraction at Mach numbers are provided below to understand clearly. Inlet mole fractions of N$_2$, O$_2$, H$_2$ are 0.556, 0.148 and 0.296 respectively.

6.1 Mach 4

Oblique shock is generated at the entry of combustor but seeing H$_2$O figure it is clear combustion is happening somewhere at the extreme left.

![Fig 2: Pressure contour at Mach 4](image2)
Fig 3: Temperature Contour at Mach 4

Fig 4: H$_2$O mass fraction contour at Mach 4

Graph 2: H$_2$O mass fraction
6.2 Mach 5

Increasing Mach number by one, did not show many changes into the pattern of combustion in the H₂O mass fraction picture.
Fig 5: Pressure contour at Mach 5

Fig 6: Temperature Contour at Mach 5

Fig 7: H$_2$O mass fraction contour at Mach 5

Graph 5: H$_2$O mass fraction
6.3 Mach 6

Here, combustion can be seen in the figures. At Mach 4 and 5, it was happening at the extreme end but at Mach 6 it is also occurring in the middle portion. The combustion still did not develop fully which could be seen in the Rahul et al paper[5] at Mach 6. With this chemical model, the flow is not completely developed. Further analysis will reveal which Mach number gives desirable combustion.
Fig 9: Temperature Contour at Mach 6

Fig 10: H$_2$O mass fraction contour at Mach 6

Graph 8: H$_2$O mass fraction
6.4 Mach 8

Combustion is taking place early at Mach 7 and Mach 8, in the combustor as compared to previous cases.
Fig 12: Temperature Contour at Mach 8

Fig 13: H$_2$O mass fraction contour at Mach 8

Graph 11: $H_2O$ mass fraction
6.5 Mach 9

Results of Mach 9 show improper combustion inside the combustor. The desirable combustion is not achieved even at this point.
Fig 15: Temperature Contour at Mach 9

Fig 16: H$_2$O mass fraction contour at Mach 9

Graph 14: H$_2$O mass fraction
After Mach 9, Mach 10 does not display significant improvements. However, at this Mach number combustion is seen to be fully developed and as it was desired to be at CJ conditions. Figures below show proper combustion is achieved at Mach 11 with the chosen chemical model.

6.6 Mach11

Graph 15: $H_2$ mass fraction

Graph 16: $O_2$ mass fraction

Fig 17: Pressure contour at Mach 11
Fig 18: Pressure contour at Mach 11

Fig: H$_2$O mass fraction contour at Mach 11

Graph 17: H$_2$O mass fraction
7 Conclusions
Using M.O Conaire and H.J Curran designed chemical model, the analysis was done. Conditions from Rahul et al. [5] paper were taken except chemical model and Mach numbers. For simulation Mach numbers were chosen from 4 to 11. At Mach 11, desired fully develop combustion can be seen in the combustor at CJ conditions. To advocate, pressure, temperature and H2o Mass fraction images are provided with the specified Mach numbers.

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Not applicable

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Not applicable

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11 Authors' contributions

Dheeraj Kumar Namala and Kajal Mishra did literature review. Dheeraj Kumar Namala conceived idea and worked on ANSYS simulations. Kajal Mishra verified the simulations and contributed to the final manuscript.

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Not applicable

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