NUMERICAL STUDY ON STRUCTURE OF OBLIQUE DETONATIONS 
IN HYDROGEN-AIR MIXTURES WITH VARIOUS NITROGEN 
DILUTION

Muhammad Mubashir 1, Nan CHEN 2, Seyed Amin Esfehani 3, Sudip Bhattrai 4 & Hao TANG 1,*  
1,2,3 Jiangsu Province Key Laboratory of Aerospace Power System, College of Energy and Power Engineering,  
Nanjing University of Aeronautics and Astronautics, Nanjing 210016, China  
4 Department of Mechanical Engineering, Institute of Engineering, Lalitpur, Nepal

ABSTRACT
Oblique detonation waves are investigated by numerical simulations, to study the structure and formation of ODW over a wedge with a different amount of nitrogen dilution in hydrogen-oxygen-nitrogen mixtures. The Euler equations are solved numerically for 2-D unsteady reactive flow and the kinematic mechanism for the H2-air reactive mixture considers a 9-species reaction mechanism with 19-reversible elementary reactions. In the result of numerical simulations a range from (H2: O2: N2/2:1:3.76) to (H2: O2: N2/2:1:2) mixtures having a same structure but from (H2: O2: N2/2:1:5) to (H2: O2: N2/2:1:0) mixtures, a new X-shaped shock structure is occurred under the formation of ODW. If a part of flow behind the structure is subsonic and the specific energy release is too high, the entire structure may become detached from the wedge. ODW angle is gradually increasing with decreasing the amount of nitrogen dilution. The position of triple points is varying in mixtures but especially in the (H2: O2: N2/2:1:0) mixture, triple point position suddenly moved away from the trace. Firstly induction length decreases to critical nitrogen value, after (H2: O2: N2/2:1:2) mixture it is gradually increasing.

Keywords: Detonation, Hypersonic, Nitrogen, ODW, Shock-induced combustion

1. INTRODUCTION
In the recent time, hypersonic air crafts have attained a huge attention in the aircraft industry. One of the major challenges is to evolve novel propulsion systems because high Mach flights need high power and conventional aircraft engines are not able to generate require power. Oblique detonation wave engines (ODWE) and the Ram Accelerators are based on the concept of the oblique detonation wave [1]. This sort of modified Scramjet, ODWE is also known as shock-induced combustion Ramjet, having main advantages of Scramjet. Such kind of propulsion system achieves high thermal cycle efficiency and rapid combustion rate [2, 3]. Hence the oblique detonation propulsion attained much attention in hypersonic air crafts due to its potential application. Firstly, it needs to induce the structure of oblique detonation waves to acquire the ODWE. The former researcher’s, oblique detonation waves are clarified to be the oblique shock waves and post-shock release region [4, 5]. The structure of an ODW connected to a wedge was explained by Li et al [6]. He studied the oblique detonation numerically and perceived the structure composition. The structure composed of a nonreactive oblique shock wave, an induction region behind oblique shock wave, a set of deflagration waves and the oblique detonation surface. At the end of the induction zone, exothermic reactions are activated, sending compression waves to strengthen the oblique shock wave. In a one-dimensional gas phase detonation, the energy release creates an increase in pressure and temperature that propagates the shock and the shock creates the increase in pressure and temperature that is the reason to trigger the chemical reaction. Ensuing studies focus on two objects. One is the formation of oblique detonation wave and the other is about the structure of the ODW in the stoichiometric hydrogen-air mixture. If a detonation could be stabilized in a high speed, fuel-oxidizer mixture, the high pressure generated by the detonation could give high thrust. Teng and Jiang propose a model, which is the basis of numerical results and theoretical study. This pattern provides a fine but influential tool to augur the wave structure [7]. On the stability studies, the entire structure of ODW is found to be stable to inflow disturbances [8-10]. But the inner instability of oblique detonation, defined by good scale structures on oblique detonation surfaces, has been studied latterly.

In previous studies both the formation and structures have been studied vastly. Chi-ping Li, K. Kailasanath, and Elaine S. Oran discussed the nitrogen dilution effects on ODW [11]. That was not enough to understand the whole facets. In the further study, we will analyze the ramp-stabilized ODW formation and structure in different hydrogen-oxygen-nitrogen mixtures.

This work was supported by the National Natural Science Foundation of China (NSFC No. 51576098).
2. PHYSICAL AND NUMERICAL MODEL

The schematic representation of oblique detonation wave induced by the wedge in the ignitable gas mixtures is shown in figure 1. Supersonic ignitable gas mixture reflects on the two-dimensional wedge and originates an oblique shock wave. The shock wave stimulates the exothermic chemical reaction and then a complex detonation structure will form downward.

**Figure 1 Schematic of wedge-induced oblique detonations in the combustible gas mixtures**

In the prior results showed that the viscosity and the boundary layer have little effects on the structure exclude slightly varying in boundary layer thickness and use the inviscid calculation in most of the results[12-13]. The Euler equations are solved numerically for 2-D unsteady reactive flow and the conservation form of the governing equations can be written as

**Continuity:**  \[ \frac{\partial \rho}{\partial t} + \nabla (\rho \phi) = 0 \]  

**Momentum:**  \[ \frac{\partial (\rho U)}{\partial t} + \nabla (\rho \phi U) = -\nabla p \]  

**Energy:**  \[ \frac{\partial (\rho E)}{\partial t} + \nabla (\rho \phi E) = qR \]  

**Species:**  \[ \frac{\partial (\rho Y_i)}{\partial t} + \nabla (\rho \phi Y_i) = \omega_i W_i \]  

Where,  \( E = \frac{1}{2} U^2 + \frac{p}{\rho} \) and  \( \phi = \rho U \) is the convective face flux. For the perfect gas mixture,  \( p = \rho RT \), these equations are solved in combination with the equation of state to completely define the inviscid reactive flow field. In the species conservation equation,  \( Y_i \) the mass fraction of chemical species  \( i \) and  \( \omega_i W_i \) is the reaction source term where  \( W_i \) is the molecular weight of the species,  \( i \) and  \( \omega_i \) are the molar production rate obtained as the summation of the rate of creation or destruction of each species from the reaction steps. The reaction rates are calculated from the Arrhenius law,

\[ k = AT^\alpha \exp(-E/RT) \]  

The AUSM+ flux discretization method is used to calculate the face convective flux values [14]. The cell-to-face extrapolation of the primitive variable is attained by extrapolating the cell centered variables to face centers using a second-order Taylor series expansion. The kinematic mechanism for the H\(_2\)-air reactive mixture considers a 9-species [O\(_2\), H, OH, O, H\(_2\), H\(_2\)O, N\(_2\), H O\(_2\), and H\(_2\)O\(_2\)] reaction mechanism with 19-reversible elementary reactions, from [15]. A description of the reactions and thermodynamic data of the involved species are supplied using the CHEMKIN format. The thermodynamic data related to heat capacity and enthalpy for the individual components is supplied as piece-wise polynomial functions of temperature [16]. For scalar field variables, both the lower and upper walls of the combustor were modeled as adiabatic boundaries with zero-gradient. Inlet flow is modeled as a mass flow inlet with the stoichiometric premixed H\(_2\)-air mixture. Zero-gradient extrapolated boundary conditions were used for all flow variables at the outlet boundary.

In this study, the inlet flow parameters are temperature796K, pressure35040Pa, and mach5.95. The ramp angle is fixed to be 15° in these simulations and computational domain is 0.1mx0.06m. All the simulation results are independent of the mesh. Inflow mixtures are stoichiometric and the fuel-air equivalence ratio is 1.
3. NUMERICAL RESULTS AND DISCUSSION
The simulation shows the same fundamental wedge-induced detonation structure. This structure is shown in figure 2, taken from a simulation of an oblique detonation on a 15° wedge with the incident Ma 5.95 in the stoichiometric hydrogen-air mixture (H₂: O₂: N₂/2:1:3.76).

Figure 2 Temperature contour plot showing the stable wedge-induced detonation structure

The oblique shock has two different parts that have distant shock angles are shown in figure 2. The shock angle in the zone near the leading edge of the wedge corresponds to non-reactive shock, through which the incoming flow turns 15° parallel to the wall. Behind the region of this shock is called induction region. In induction region, all fluid properties remain constant except induction parameter. The value of induction parameter increase from left to right in the induction zone. At the end of induction zone, the chemical reactions are triggered and generate deflagration waves. The deflagration waves define incremental changes in pressure and temperature generated by the energy release in a chemical reaction. The deflagration waves propagate upward at local Mach angle, intersect and steepen the original oblique shock wave. After a certain ignition delay, the initial shock wave and deflagration waves coincide at one point on OSW, this point is called triple point, which is associated with the divergent shock below. From this point, the ODW ensures together with a slip line that separates the two regions, detonation region, and lower combustion region. The slip line can be seen clearly in figure 2. The fluid parameters are different behind the two different parts of shock structures due to different shock strength.

3.1. Detonation Structure in Different Concentration Mixtures
The simulation explained above show a detonation structure generated by a wedge-induced oblique shock in the stoichiometric hydrogen-air mixture (H₂: O₂: N₂/2:1:3.76). Now we will describe that this basic structure of detonation wave exists in different hydrogen-oxygen-nitrogen mixtures. A set of simulations have been accomplished for different concentration (H₂: O₂: N₂) mixtures ranging from 2:1:0 to 2:1:3.76. The inflow parameters and wedge angle are the same in all simulations, those we discussed earlier. The computational domain for all simulations is 0.1m×0.06m.
When the nitrogen dilution is varied, the production rate of intermediates and the specific energy release are affected and this variation has effects on the detonation structures. In figure 3 shows pressure contours for \((\text{H}_2: \text{O}_2: \text{N}_2)\) mixtures of 2:1:3.76, 2:1:3, 2:1:2.5, 2:1:2, 2:1:1.5, 2:1:1 and 2:1:0. For a mixture ranging from 2:1:3.76 to 2:1:2 having the same detonation structure in these simulations. But for a mixture ranging from 2:1:1.5 to 2:1:0 having the different structure under the oblique detonation wave over a wedge and it is not like a previous structure. When the nitrogen dilution decreases from 2:1:2 to 2:2:1.5, a new shock is generated near the wedge surface and intersect the divergent shock from the triple point. In the result of these two waves intersection, a new structure appears in the form of \(X\)-shaped shock structure. In figure 4 it can be observed and analyzed the composition of a new structure in pressure contours. In the simulation result of 2:1:1.5 the \(X\)-shaped shock structure does not appear clearly but the appearance of \(X\)-shaped shock structure demonstrates with the decreasing amount of nitrogen dilution in the mixture. When the nitrogen is fully eliminated (the stoichiometric hydrogen, an oxygen mixture, \((\text{H}_2: \text{O}_2: \text{N}_2/2:1:0)\) clearly appears on the wedge-induced Oblique detonation structure.
In figure 4, it can differentiate the behaviour of wave formation in 2:1:1.5, 2:1:1 and 2:1:0 mixtures in pressure and temperature contours plots respectively. At the end of induction region, chemical reactions are triggered. As the amount of nitrogen dilution decreases, the energy release increases. This causes the higher temperature, higher speed of sound and lower Mach number of the mixture after combustion. In the result, the reactive shock above the induction region becomes stronger. It can be noticed a small ignition near the wedge surface in figure 4 (H₂: O₂: N₂ /2:1:1.5) mixture. In this region, deflagration waves coupled with an expansion waves and make a new shock wave. With an amount of nitrogen dilution decreases, the ignition near the wedge surface increases and the shock becomes stronger in figure 4 (H₂: O₂: N₂/2:1:1), (H₂: O₂: N₂/2:1:0) mixtures. Temperature continuously increasing near the wedge surface with decreasing of nitrogen dilution in mixtures, it can be seen in figure 4 temperature contour plots. In addition, the whole detonation structure may become detached from the wedge if the specific energy release is too large. Formation of X-shaped shock structure in (H₂: O₂: N₂/2:1:0) mixture at different simulation time steps can be seen in figure 5.
Figure 5 Formation of X-shaped shock structure at different Simulation time steps
3.2. Effect of Nitrogen Dilution on ODW Angle
The reactive shock above the induction region becomes stronger and ODW angle is continuously increasing with decreasing the nitrogen dilution. The steepening in the shock angle can be seen in figure 6. From (H₂: O₂: N₂ /2:1:3.76) to (H₂: O₂: N₂ /2:1:1) mixtures, trace of ODW angle is gradually getting steeper but in mixture (H₂: O₂: N₂ /2:1:0), there is sudden jump in the trace. In this study, Chapman Jouguet detonation angle (CJ ODW) is 37.4º. The highest ODW angle in this study is 52º in (H₂: O₂: N₂ /2:1:0) mixture. In mixture (H₂: O₂: N₂ /2:1:2) ODW angle is 37º and it is close to the CJ ODW angle.

![Figure 6](image.png)

**Figure 6** Angle of standing detonation as a function of dilution for the system (H₂: O₂: N₂ /2:1: X) varies along the horizontal axis

3.3. Effect of Nitrogen Dilution on Triple Point Position
Nitrogen dilution has to effect on triple point position. The position of triple points is constantly varying from (H₂: O₂: N₂ /2:1:3.76) to (H₂: O₂: N₂ /2:1:2) mixtures but from (H₂: O₂: N₂ /2:1:2) to (H₂: O₂: N₂ /2:1:1) mixtures, there is a little variation in the trace. Especially in the (H₂: O₂: N₂ /2:1:0) mixture, triple point position suddenly moved away from the trace. Ignition delay becomes short if the formation of triple point occurs early. In figure 7, the variation of triple point’s position can be observed. Both X and Y axis shows the coordinates of triple points and at points, nitrogen concentration is labelled.

![Figure 7](image.png)

**Figure 7** Variation of triple points for the mixtures (H₂: O₂: N₂ /2:1: X)

3.4. Effect of Nitrogen Dilution on Induction Length
Nitrogen dilution also affects the induction length of the structure. Induction length is varying with an amount of nitrogen dilution in the mixtures. In figure 8, shows the induction length variation against nitrogen dilution. Firstly, induction length decreases from (H₂: O₂: N₂ /2:1:3.76) to (H₂: O₂: N₂ /2:1:2) mixtures but after (H₂: O₂: N₂ /2:1:2) mixture is gradually increased. From (H₂: O₂: N₂ /2:1:3.76) mixture to (H₂: O₂: N₂ /2:1:3) mixture, there is little variation in the trace but after (H₂: O₂: N₂ /2:1:3) mixture to (H₂: O₂: N₂ /2:1:2.5) mixture a sudden drop in trace.
Between (H$_2$: O$_2$: N$_2$/2:1:2.5) mixture and (H$_2$: O$_2$: N$_2$/2:1:2) mixture, there is critical nitrogen value after that its start to increase. In this study lowest induction length gets in (H$_2$: O$_2$: N$_2$/2:1:2) mixture.

![Figure 8 shows the variation of Induction length against the mixtures (H$_2$: O$_2$: N$_2$/2:1: X)](image)

Between (H$_2$: O$_2$: N$_2$/2:1:2.5) mixture and (H$_2$: O$_2$: N$_2$/2:1:2) mixture, there is critical nitrogen value after that its start to increase. In this study lowest induction length gets in (H$_2$: O$_2$: N$_2$/2:1:2) mixture.

In the simulation results of all under study mixtures, (H$_2$: O$_2$: N$_2$/2:1:2) is a most suitable mixture for a fine Oblique detonation wave (ODW) structure. In this mixture, ODW angle is too close to the Chapman Jouguet detonation angle (CJ ODW) and also has the lowest induction length. CJ condition is the ideal condition for supersonic combustion.

4. CONCLUSION

Oblique detonation waves are simulated, to understand the ODW formation and structure in different nitrogen dilution mixtures. In the result of numerical simulations

1) A range from (H$_2$: O$_2$: N$_2$/2:1:3.76) to (H$_2$: O$_2$: N$_2$/2:1:2) mixtures having the same structure but from (H$_2$: O$_2$: N$_2$/2:1:1.5) to (H$_2$: O$_2$: N$_2$/2:1:0) mixtures, a new X-shaped shock structure occurs under the formation of ODW. The formation of X-shaped shock structure is due to the intersection of deflagration waves coupled with expansion waves and the divergent shock from the triple point. As the amount of nitrogen dilution decreases in the stoichiometric hydrogen-air mixture (H$_2$: O$_2$: N$_2$/2:1:3.76), energy release increases.

2) ODW angle is gradually increasing with decreasing the amount of nitrogen dilution. In proposed study, ODW angle is 37º in the (H$_2$: O$_2$: N$_2$/2:1:2) mixture and it is close to the CJ ODW angle.

3) The position of triple points is constantly varying from (H$_2$: O$_2$: N$_2$/2:1:3.76) to (H$_2$: O$_2$: N$_2$/2:1:2) mixtures but from (H$_2$: O$_2$: N$_2$/2:1:2) to (H$_2$: O$_2$: N$_2$/2:1:1) mixtures, there is a little variation in the trace. Especially in the (H$_2$: O$_2$: N$_2$/2:1:0) mixture, triple point position suddenly moved away from the trace.

4) Firstly induction length decreases to critical nitrogen value, that is between (H$_2$: O$_2$: N$_2$/2:1:2.5) and (H$_2$: O$_2$: N$_2$/2:1:2) mixtures. After (H$_2$: O$_2$: N$_2$/2:1:2) mixture it's gradually increasing.
REFERENCES