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Effect of Fuel Distribution on the Onset of Detonation in Gaseous Octane-air Mixture

Sunil Bassi*, Sanjay Kumar Soni, and Shashank Chaturvedi

Institute for Plasma Research, Gandhinagar- 382428, India
**E-mail: sunil.bassi@ipr.res.in*

ABSTRACT

Formation of detonation waves in a tube is a complex phenomenon and depends upon many factors like ignition energy, presence of a deflagration to detonation transition (DDT) enhancement device and spatial distribution of fuel, etc. In the present study, gaseous octane-air mixtures have been examined by varying the equivalence ratio linearly along the axial direction of the detonation tube though the overall stoichiometry was maintained in the tube. Three different conditions have been modelled and studied, which includes small, moderate and large, fuel density gradient in axial direction with equivalence ratio ranging from 1 to 2 near the ignition zone. A series of simulation study have been conducted and the analysis of simulation results reveal that the DDT onset is significantly affected by the initial fuel distribution at the ignition zone as well as on fuel density gradient in a detonation tube. It has been observed that a moderate gradient in the fuel density distribution is favourable for onset of detonations. From the study of pressure plots for above mentioned conditions it has been found that the presence of large gradients in fuel density has adverse effect on the stability of detonation wave.

Keywords: Deflagration to detonation transition; DDT; Equivalence ratio; ER

1. INTRODUCTION

Detonation is a mode of combustion, in which fuel burns at almost constant volume condition. The thermodynamic efficiency of detonation is theoretically higher than deflagration mode of combustion[1]. The phenomenon of detonation has many applications like pulse detonation engine (PDE), in which thrust is produced by repetitive detonations in stoichiometric mixture of fuel and oxidiser. The PDE has a simple design, which is a long cylindrical tube, open from one side and closed from other side. A turbulence enhancement device, such as spiral is mostly employed to accelerate the deflagration to detonation transition (DDT) process. Each detonation cycle consists of the four steps[2], i.e. filling of fuel in PDE tube, Ignition to initiate deflagration and DDT, propagation of detonation wave in tube, exhaust of the detonation wave followed by purging to start a fresh cycle. During exhaust of detonation waves from the cylindrical tube, gas comes out at high pressure and with high velocity and therefore, thrust is generated. The key factor that determines the length of the PDE tube is the deflagration to detonation transition distance, which depends upon a large number of variables like temperature of the fuel and air, presence of the DDT enhancement devices, ignition energy and spatial distribution of fuel density.

Many studies have proved the significance of spatial distribution of fuel density on various detonation parameters. Nakawatase[3]*, et al.* have experimentally studied the effect of DDT equivalence ratio on distance in hydrogen-air mixture with and without shchelkin spiral. They have reported significant reduction in deflagration to detonation transition distance within the range of equivalence ratio of 1 - 1.2 and gradual rise in the DDT run up distance as the equivalence ratio moves away from this range. This increase is however less sensitive in the presence of spiral, where DDT occurs at much smaller distances. A similar experimental study was performed by Srihari[4]*, et al.* In this study, experiments were performed with C_3H_8 fuel in air at equivalence ratios 0.8, 1.0, 1.2, 1.4, 1.6 and the minimum deflagration to detonation transition distance has been reported at the equivalence ratio of 1.2 in the tube. Meyer[5]*, et al.* and Boeck[6]*, et al.* have performed similar studies. Boeck and team analysed the detonation wave characteristics in rectangular tube with a concentration gradient in transverse direction. They have reported the reduction in detonation wave velocity from Chapman-Jouguet detonation velocity in presence of concentration gradients. Many simulations such as[7,8] have been performed to study the effect of equivalence ratio on detonation wave characteristics. A few other studies are also referred where effect of equivalence ratio on DDT onset distance and thrust is observed.

Under realistic fuel injection conditions, when injection occurs near the closed end, the fuel distribution is non-uniform, having gradients in axial and radial directions and generally the fuel concentration gradient is highest near closed end and lowest near the other end of the tube. Therefore, variation in concentration gradient of fuel has taken into account in this study and it is assumed linear in axial direction. In simulation, Octane gas was taken as fuel and air as an oxidiser and the total mass of octane gas was chosen such that the mixture remains stoichiometric according to the combustion reaction of octane

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and oxygen. To the best of author's knowledge, a systematic numerical study of the effect of spatial gradients in fuel density distribution on the DDT process has not been reported earlier. This is the focus of the present work.

2. NUMERICAL MODEL AND GEOMETRY OF PDE TUBE

Computational Fluid Dynamics equations for the conservation of mass, momentum and energy are solved using finite differencing scheme. A single step chemical reaction model for the combustion of octane is taken and reactions between other species present in air are considered as per details provided ahead. The 2nd order governing equations are solved on a 2D mesh and cylindrical symmetry is assumed in the code. Eulerian mesh is used for this study. Time interval in this time marching code is determined implicitly and maximum time step 1 μs is set to avoid errors due to larger time steps. This code can take into account gas phase reactions. It can handle droplet vaporisation and droplets-fluid interactions for liquid droplet fuels which are not used as here fuel is only in gaseous form. Mass conservation equation for k^{th} species is written as:

$$\frac{\partial \rho_k}{\partial t} + \frac{1}{R}\nabla.(R\rho_k \underline{u}) = \frac{1}{R}\nabla.[R\rho D\nabla(\frac{\rho_k}{\rho})] + \dot{\rho}_k^c + \dot{\rho}_k^s \tag{1}$$

In this equation, the change is density ($\dot{\rho}_k$) within each cell is calculated from the spatial density dependent diffusion and rate of production of species due to chemical reactions ($\dot{\rho}_k^c$).The last term ($\dot{\rho}_k^s$) shows the rate of production of species ' k ' due to droplets evaporations, which is not used in the present study. The rate of production of k^{th} species in chemical reactions is given by the rate law:

$$\dot{\rho}_k^c = W_k \sum_{r=1}^{n} (b_{kr} - a_{kr}) r \tag{2}$$

$$r = k_{fr} \prod_k (\rho_k / W_k)^{a'_{kr}} - k_{br} \prod_k (\rho_k / W_k)^{b'_{kr}} \tag{3}$$

where b_{kr} and a_{kr} are the stoichiometric coefficients of k^{th} species in r^{th} reaction. b'_{kr} and a'_{kr} are the rate law coefficients of k^{th} species in r^{th} reaction. Forward and backward reaction rates coefficients k_{fr} and k_{br} are in form of generalised Arrhenius rate coefficients. W_k is the molar mass of the k^{th} species. The set of chemical reactions modelled in this study include kinetic reactions:

$2C_8H_{18} + 25O_2 \rightarrow 16CO_2 + 18H_2O$
$O_2 + 2N_2 \rightarrow 2N + 2NO$
$2O_2 + N_2 \rightarrow 2O + 2NO$
$N_2 + 2OH \rightarrow 2H + 2NO$

Along with these kinetic reactions, six equilibrium reactions were modelled:

$H_2 \rightleftharpoons 2H$
$O_2 \rightleftharpoons 2O$
$N_2 \rightleftharpoons 2N$
$O_2 + H_2 \rightleftharpoons 2OH$
$O_2 + 2H_2O \rightleftharpoons 4OH$
$O_2 + 2CO \rightleftharpoons 2CO_2$

The Momentum balance equation is:

$$\frac{\partial}{\partial t}(\rho u) + \frac{1}{R}\nabla.(R\rho \underline{uu}) = -\nabla p + \frac{1}{R}\nabla.(R\underline{\sigma}) - \frac{(\sigma_o - \rho\omega^2)}{R}\nabla R + \underline{F} + \rho\underline{G} \tag{4}$$

This equation takes care of viscous stresses along with pressure gradient. Artificial viscosity term of Von Neumann-Richtmyer[9] type is used in the momentum equation for capturing the shock formation. Aerodynamic drag and Stoke's drag terms ($\underline{F}$) are used to calculate the momentum exchange between droplets and gas which are not used in the present study as there are no droplets. $\rho\underline{G}$ is body force which is zero in this case.

The energy equation consists of energy release in chemical reactions ($\dot{Q}_c$), energy exchange due to various viscous stresses σ and ω. Also heat conduction is taken into account using heat flux $\underline{J}$ term. These terms have been explained in Cloutman[10], *et al.* The form of energy equation is:

$$\frac{\partial}{\partial t}(\rho I) + \frac{1}{R}\underline{\nabla}.(R\rho I\underline{u}) = -\frac{p}{R}\underline{\nabla}.(r\underline{u}) + \underline{\sigma} : \nabla\underline{u} + \tau.\underline{\nabla}(\omega / R) + \sigma_o\underline{u}.\underline{\nabla}R - \frac{1}{R}\underline{\nabla}.(R\underline{J}) + \dot{Q}_c \tag{5}$$

Ideal gas equation is used as equation of state. PDE tube is a 4 m long cylindrical tube with 2.5 cm radius. Ignition point is 5 cm away from closed end. Free slip wall boundary condition is used at cylindrical walls. A schematic of the PDE is as shown in Fig. 1.

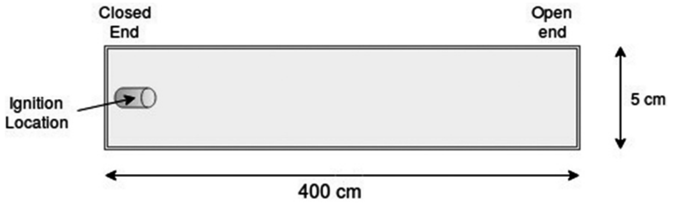

Figure 1. Schematic of cylindrical PDE in 2D.

3. MESH SENSITIVITY AND VALIDATION

Simulations were run for mesh of 4 mm, 2 mm, 1 mm, 0.8 mm, and 0.5 mm sizes and it has been observed that results tend to converge when mesh size is 1 mm or less. The detonation wave parameters such as detonation pressure and detonation speed is nearly constant in all the cases, however the axial location and time of onset of detonation is found to be mesh sensitive above mesh size of 1 mm. The detonation wave velocity and detonation pressure values match very well with the theoretical values from NASA CEA[11]. For octane at initial temperature 300 k and initial pressure 1 atm in stoichiometric conditions NASA CEA gives detonation speed as 1792 m/s and Chapman Jouguet pressure as 20 bar. Tucker[12]*, et al.* have shown in their experiments that in case of iso-octane the onset of detonation occurs within the duration of 3.5 ms to 4 ms, which has been observed in the present simulations.

4. SIMULATIONS RESULTS AND DISCUSSIONS

Simulation were carried out for different cases of spatial distributions of the fuel. Equivalence ratio was varied linearly in the axial direction. However, the overall stoichiometry for fuel-air mixture was maintained in the tube. As radial dimension is very small as compared to axial dimensions, fuel distribution is taken uniform in radial direction.

4.1 Formation of Detonation Wave

Pressure-axial plots were formed to locate the onset of detonation wave in all cases. The plots at various time intervals for one such case, when equivalence ratio near closed end was 1.06 are shown in figures. Initially, a cylindrical region of length 4 mm and radius 5 mm is kept at 1500 K to model initiation of combustion. This time is taken as reference time $T_o = 0$ ms and then system is let to evolve due to CFD and chemical reactions. The transient phenomena that occur during the beginning phase of DDT are presented in plots as shown in Fig. 2.

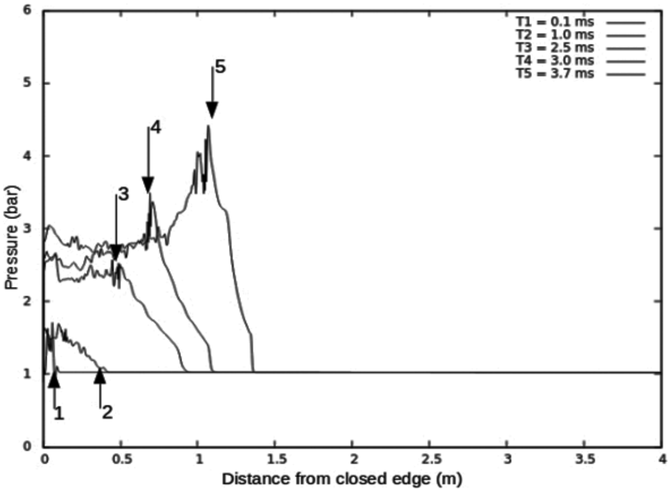

Figure 2. Pressure build up in the initial phase of DDT onset.

As it is observed in the plots within time $T_o = 0.1$ ms to $T_o = 3.7$ ms, a primary shock front develops after ignition and it travels forward axially with. It leaves behind the region in which chemical reactions are occurring. As rate of reactions increase with time due to temperature increase in the region where exothermic combustion reactions are going on. Pressure keeps on building in the reaction zone and it accelerates along axial direction and finally reaction zone gets coupled with primary shock. As a result of coupling between shock front and reaction zone, fuel-air mixture at that location gets compressed leading to onset of detonation wave. This Onset of DDT is observed at $T_o = 3.9$ ms in this case as presented in Fig. 3.

At the onset of detonation an initial overpressure is observed as observed in experiments[14]. This overdriven detonation relaxes after $T_o = 3.9$ ms and pressure gradually becomes constant as shown in Fig. 4.

Detonation wave is found to have approximately CJ velocities as calculated by time of flight method. In this case, onset of detonation was observed at 1.23 m from the closed end. A slight overpressure is observed initially, after which pressure stabilises to a nearly constant value which is 20 bar. The velocity of stabilised detonation wave has been observed to be nearly 1765 m/s .These values match well within the theoretical values for the mixture calculated from NASA CEA open tool. A slight decrease of 1.5 per cent from CJ detonation wave velocity was observed, same has been reported in the studies[15,16].

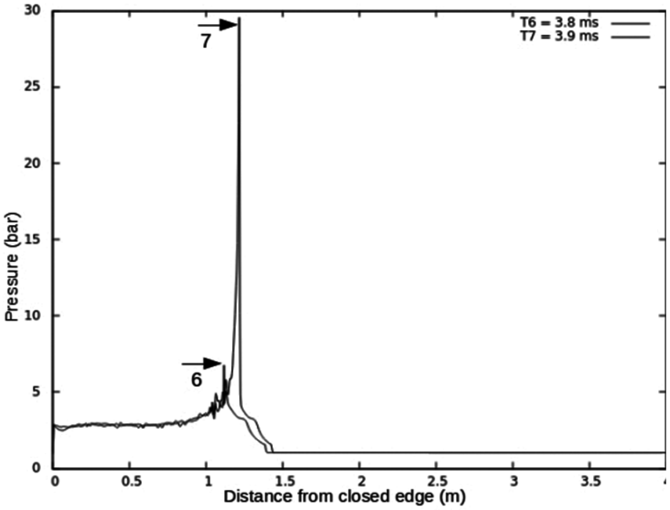

Figure 3. Onset of detonation.

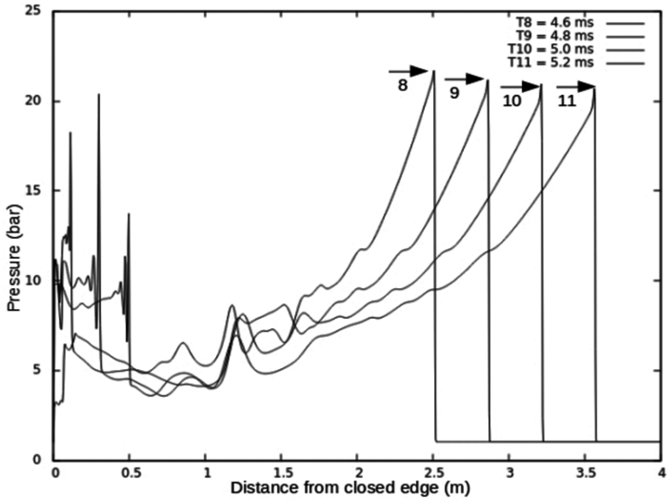

Figure 4. Detonation wave stabilisation.

4.2 Variation of DDT Distance with Fuel Concentration

A series of simulations were carried out for different cases of axial fuel distribution inside DDT tube. Variation in DDT distance with equivalence ratio near the closed end was of the tube is as presented in Table 1.

These values were plotted as shown in Fig. 5 and it is observed that fuel distribution has significant effect on the DDT distances in gaseous fuel-air mixtures. For nearly uniform distribution, onset of DDT occurs at about 150 cm for octane-air mixture. Smallest distance for onset of DDT is observed in the case when equivalence ratio at closed end is 1.18 and near the other end is 0.82. As the axial gradient becomes higher, i.e. in case of more fuel accumulated near closed end DDT onset occurs at larger values.

4.3 Detonation Wave Stabilisation

For operating the pulse detonation engine effectively, the detonation wave must be stabilised inside the detonation

Table 1. DDT distance values for different fuel density gradients

ER near closed end	ER near open end	DDT distance (cm)
1.02	0.98	145.6
1.04	0.96	118.4
1.06	0.94	124.0
1.08	0.92	131.2
1.12	0.88	122.4
1.18	0.82	110.4
1.20	0.80	116.8
1.40	0.60	153.6
1.60	0.40	192.0
1.80	0.20	230.4
2.0	0.0	244.8

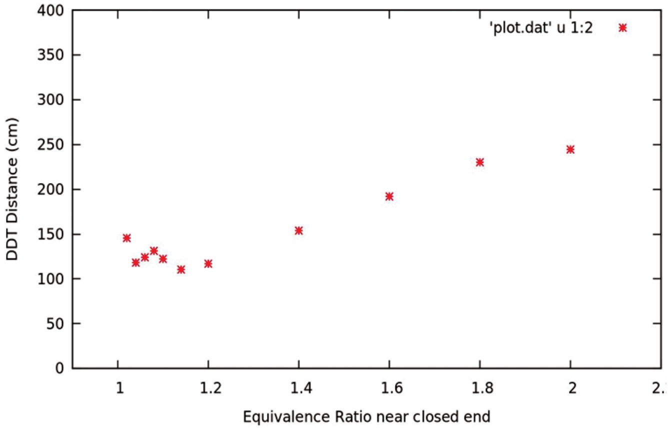

Figure 5. Variation of DDT distance with ER at closed end.

tube. In these simulations, the stability of detonation wave is studied by observing the detonation pressure and velocity of shock front. When these parameters become invariable, the detonation wave is said to become stabilised. It is observed that the detonation wave stabilised within the tube of length 4 m when the equivalence ration near closed end is less than 1.4. While in case when gradient in fuel density is large, detonation pressure does not become stable even after reaching the end of the DDT tube. We can see in the difference in the behaviour of detonation wave when we have a large gradient in fuel density, ER 1.8 near closed end and ER 0.2 near open end, compared to the detonation wave characteristics in the previously shown case.

A stabilised detonation wave propagates in the detonation tube, when equivalence ratio is 1.06 near closed end as shown in Fig. 4. The pressure peaks at various time steps can be seen in the plot. While in case of equivalence ratio 1.8 near closed end and 0.2 near open end, pressure at shock front develops very slowly. The shock front reaches to axial distance more than 2.5 m in 7.2 ms and yet DDT onset is not observed as shown in Fig. 6. The onset of detonation occurs after 2.5 m with some overpressure as shown in Fig. 7. This overpressure does not relax to a constant value even at the end of 4.0 m tube signifying that detonation wave does not gets stabilised . Also, it can be seen that in high gradient case, detonation onset occurs with a larger time delay compared to the first case. These plots reveal that for a stable DDT phenomenon, large gradients should be avoided in the detonation tube.

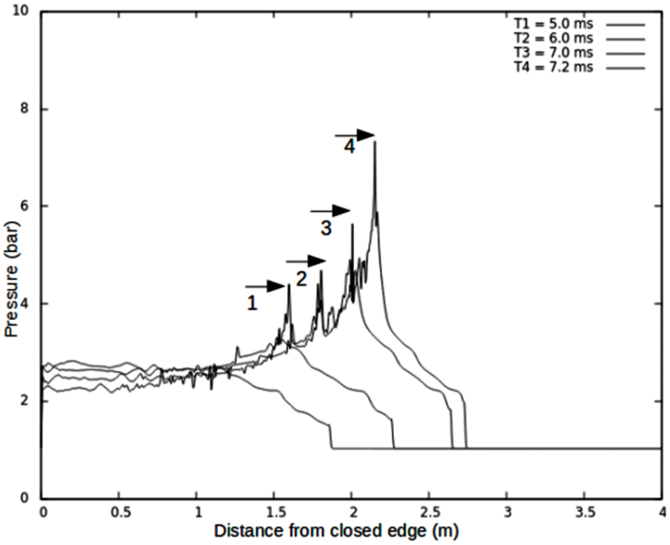

Figure 6. Build-up of pressure at shock front in case of ER 1.8 near ignition location.

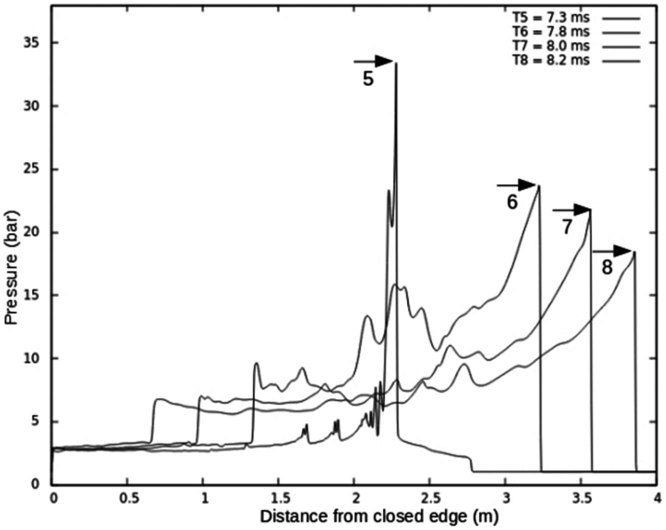

Figure 7. Onset of detonation wave in case of ER 1.8 near ignition location.

5. CONCLUSIONS

The study leads to conclusions given as follows:

(i) It is observed that DDT onset is significantly affected by the initial fuel distribution at the time of ignition. Three regimes have been observed. In the first regime, if the fuel density gradient is very small and equivalence ratio near the ignition location is near to 1.0, corresponding to a nearly uniform mixture, DDT occurs at large distances. In the second regime, with moderate gradients, DDT onset occurs at relatively short lengths for the cases where equivalence ratio near the ignition location is near 1.20. Finally, in mixtures with larger gradients, where equivalence ratio is higher than 1.40, DDT onset occurs at length exceeding 2 m.

(ii) In case of nearly uniform mixture (very small fuel density gradient), pressure plots were studied at different time instants and detonation parameters were estimated. The detonation pressure and velocity turn out to be 20 bar and 1765 m/s, which are comparable with CJ detonation parameters. However, a slight decrease in detonation velocity is observed after formation of detonation wave that may be due to local equivalence ratio effects.

(iii) For the conditions examined in this study, the minimum DDT distance is found when the equivalence ratio is 1.18 at the ignition zone and 0.82 at open end.

(iv) In addition, it is also noticed that if the equivalence ratio near the closed end is kept 1.4 and above, no stable detonation wave is formed even at 4 m distance.

On the basis of these observations, it can be concluded that the fuel density gradient in axial direction of detonation tube has to be moderate while the equivalence ration in the vicinity of ignition zone of detonation tube should be in the range of 1.18 to 1.2.

As a future work, it will be interesting to study the effects of spray like fuel droplet distributions in air and various other parameters related to fuel droplets on the DDT phenomenon.

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CONTRIBUTORS

Mr Sunil Bassi obtained his MSc (Physics) from National Institute of Technology Jalandhar. Presently he is working as Scientific Officer at Institute for Plasma Research, Gandhinagar. His area of interest consists of numerical simulations of reactive flows with computational fluid dynamics relevant to pulse detonation engine.
In the present work, he has carried out the simulation work.

Mr Sanjay Kumar Soni received his BE from Government Engineering College, Bilaspur and MTech in Production Engineering from Indian Institute of Technology, Delhi. His area of interest consists of experimental study of pulse detonation engine operation and CFD simulations of pulse detonation engines.
In the present work, he has provided guidance in result analysis and conclusions of the study.

Dr Shashank Chaturvedi obtained his BTech (Chemical Engineering) from Indian Institute of Technology, Delhi and PhD from Princeton University, Princeton, NJ. His area of interest consists of computational modelling of different fusion reactor configurations, including tokamaks, as well as pulsed-power systems, pulsed electromagnetics, radiation hydrodynamics, MHD simulations and shock waves.
In the present work, he has provided guidance in simulation work and result analysis.