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Effect of Fuel Inhomogeneity in 2-D Simulation of a Rotating Detonation Combustor (RDC)

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Abstract: One of the key advantages of the detonation based engine is the increased thermodynamic efficiency over the traditional constant pressure combustor. These detonation-based engines are also known as Pressure Gain Combustion systems (PGC) and Rotating Detonation Combustor (RDC) is a form of PGC, in which the detonation wave propagates azimuthally around an annular combustor. In most RDCs, fuel and oxidizer are injected discretely from separate plenums, and combined with the inherent turbulent nature of the flow; the fuel-oxidizer mixture is rarely premixed and results in inhomogeneous mixing within the domain. Due to the discrete fuel injection locations, fuel/oxidizer will stratify to form local pockets of rich and lean mixtures. Unmixedness, which is defined as the standard deviation of equivalence ratio normalized by the mean global equivalence ratio, is a measure of the degree of fuel-oxidizer inhomogeneity. The objective of the present study is to investigate the impact of unmixedness on the performance of an RDC. To model this effect, a lognormal distribution of the fuel mass fraction is generated with a mean equivalence ratio of 1 and varying standard deviations at the inlet boundary as a numerical source term. Moreover, instead of using complete randomizations of fuel mass fraction at the inlet boundary, cells are bundled for a given length scale, and the mass fractions for these bundles are updated based on the lognormal distribution after every three-time steps. Using this methodology, a numerical analysis is carried out to predict the flow physics, flow structure, and detonation cell size for H2-air mixture.

Keywords: Rotating Detonation Combustor (RDC), 2-D Simulation

1. Introduction

Detonation based combustion has an advantage of rapid energy release that need to be exploited for the propulsion application as compared to the conventional deflagration based combustion system. The mixing effects, dynamics of a detonation wave, efficient injection system design, and managing heat loss/heat transfer in a detonation-based engine are some of the major challenges posed to the propulsion industry. One key feature of a detonation process is rapid burning of fuel-air mixture, which occurs much faster than deflagration and can lead to a more compact and efficient system design. In addition, due to the small chemical time scales, there is not enough time for the pressure to equilibrate and thus the overall process is thermodynamically closer to a constant volume process rather than constant pressure process, typical of conventional propulsion system. The constant volume cycle is thermodynamically more efficient than a constant pressure Brayton cycle. PGC is expected to increase thermal efficiencies 5% to 10% higher than any other technological advancement in the field of power and propulsion [1]. Zel’ dovich [2] was the first to show that the detonation process under the same condition is more beneficial than the
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deflagration process, because the reaction products in detonation based combustion have lower entropy than in deflagration. After a few decades of minimal development, heightened interest in PGC, namely, pulse detonation engine (PDE) began around 1990 [3]. PDE is based on pulsating detonation wave in a tube with a frequency of 20-100 Hz. One of the drawbacks of PDE is that it is an intermittent or pulsed based detonation rather than a continuous mode of detonation. Due to this, it is difficult to couple PDE with the downstream of the turbine section. Because of these inherent problems associated with PDEs, the concept of Rotating Detonation Combustor (RDC) gained popularity as it provide a quasi-steady source of thrust, and doesn’t require repeated initiation of detonation. In an RDC, combustion or the detonation chamber is annular, and continuous supply of fuel and air mixture is injected axially at the base of the combustion chamber, and once initiated; a detonation wave propagates circumferentially around the annulus of the combustor. The detonation wave propagates at a frequency ranging from 1-100 KHz depending upon the design and the fuel/air mixture composition. Simple and compact design of RDC makes them an attractive option to couple with turbines for future power and propulsion application.

In the last decade, numerous research groups have investigated the concept of RDC using both numerical and experimental techniques, to understand the overall flow field structure, effect of geometry, fuel and injection technique on the performance of the RDC, all of which are summarized in papers [4-6]. Among all the performance parameters which were investigated in these studies, one major parameter, which has a profound effect on the performance of a rotating detonation combustor, is the complex distribution of fuel-air mixture within the combustion chamber. Detonation chamber features a complex distribution of fuel-oxidizer mixture with regions of varying equivalence ratio and this non-homogeneity within the annulus of an RDC causes reduction in wave speed [7], skewed wave front and irregular detonation cell structure [8], and loss of performance [9], as compared to a perfectly premixed mixture. Much of the computational research in the field of RDC utilizes full scale 3-D numerical simulation, to understand the flow physics and performance of RDC, including the effects of inhomogeneity. However, the stumbling block in using high fidelity 3-D simulation to model RDC is the large difference in length and time scales between the flow field and the chemical reactions. Thus in order to capture the detailed flow physics, very fine grid cells of the order of 10 to 100 microns and time steps on the order of 10s of nanoseconds are required, which makes 3-D simulations computationally expensive. To overcome this, 2-D numerical simulations are often utilized to gain basic and qualitative understanding of RDCs. Recently, Sathya et al [10], developed a novel approach to incorporate the effects of inhomogeneity in 2-D simulation by extracting a Probability Density Function (PDF) of fuel mass fraction from a non-reacting 3-D simulation and using it as an inlet boundary condition in the 2-D analysis. The present study utilizes a similar approach as used in [10], to model the effects of fuel inhomogeneity.

The objectives of the current research work is to determine the impact of fuel-air inhomogeneity on RDC performance by modeling inhomogeneity of fuel-oxidizer mixture in a 2-D domain using a lognormal distribution as a Probability Density Function (PDF) of fuel mass fraction. The mean equivalence ratio is held constant while the standard deviation is varied.
2. Computational Method

The geometry used for the 2-D domain of an RDC (Fig. 1), is obtained by unwrapping the 3-D combustor design which is based on the experimental setup presented by Shank et al in [11]. The length of the 2-D domain is equal to the mean circumference of the coaxial cylinders used in the 3-D domain (459.6 mm) and the height of the 2-D domain is equal to the height of the combustion chamber (101.6 mm) in 3-D geometry.

The effects of fuel-oxidizer inhomogeneity in 2-D domain are model using numerical source terms at the inlet boundary. Multiple probes points are placed at different axial locations similar to [12], in order to analyze the flow parameters such as detonation wave speed, peak pressure and temperature. 4 sets (90° apart in the circumferential direction) of 11 probe points are used in axial direction, with each probe point 6.35 mm apart axially and the first probe point is located at 6.35 mm from the inlet of the 2-D domain. These 4 sets of 11 probe points are used to measure the time-averaged static pressure in the 2-D domain (Fig. 1). In addition, 4 probes are placed (90° apart in the circumferential direction) at an axial distance of 2.54 cm from the inlet boundary to measure the instantaneous peak pressure and temperature. Reynolds-Averaged Navier Stokes (RANS) equations are solved, and the source terms in the species mass transport equations are determined using detailed chemical kinetics, Arrhenius form for the rate coefficient, and ideal gas equation of state via the commercial software package STAR-CCM+, which utilizes the finite volume discretization method to solve a system of governing equations.

The current work uses a structured mesh grid for the discretization of the 2-D domain, such that the grid size up to the height of the detonation wave front is 0.1 mm and gets progressively coarser towards the exit plane up to a maximum of 0.15 mm. Time step of $2.5 \times 10^{-8}$ seconds is used in our simulation. All the subsequent analyses were carried out once the detonation wave reaches a quasi-steady state. 2-D simulation is carried out under a specific operating condition [12], where the inlet plenum pressure is maintained at 4.12 bar and the mass flow rate of fuel and air injected is 0.0093 kg/s and 0.32 kg/s respectively, with mean global equivalence ratio maintained at unity. Fuel-oxidizer injection is modeled as a numerical source terms and is applied to the first row of the 2-D domain. The injection of fuel-oxidizer mixture is dependent on the downstream pressure of the detonation chamber. In the absence of the detonation wave, the amount of mass flow rate entering the 2-D domain is calculated using the isentropic relation presented in Equation (1)

$$\dot{m} = \frac{P_o A \sqrt{T}}{\sqrt{RT_o}} M(P) \left(1 + \left(\frac{\gamma-1}{2}\right) \frac{M(P)^2}{\gamma^{(\gamma+1)}}\right)^{\frac{\gamma-1}{\gamma+1}}$$

(1)

Where $P_o$ & $T_o$ are the total pressure and total temperature at the inlet and are set to 4.12 bar and 300 K respectively. The throat area $A$ is calculated from geometry of the RDC presented in [11]
and is found to be $3.973 \text{cm}^2$. The Mach number $M(P)$ is dependent on the cell static pressure $P$ immediately downstream of the inlet domain and is calculated using the Equation (2)

$$M(P) = \sqrt{\left(\frac{2}{\gamma - 1}\right)\left(\frac{P}{P_0}\right)^{\frac{\gamma}{\gamma - 1}} - 1}$$ (2)

The downstream static pressure $P$ determines the flow of mixture into the combustion chamber. The mass flux source term at the inlet boundary is calculated using equation 3.

$$S_m = \frac{\dot{m}}{lw}$$ (3)

Where $l$ represent the detonation channel height and $w$ represent the channel width. Similarly, momentum and energy source terms are obtained using equation 4 and 5 respectively.

$$S_{mom} = \frac{\dot{mu}}{lw}$$ (4)

$$S_e = \frac{\dot{mq}}{lw}$$ (5)

Effects of mixture inhomogeneity are accomplished using a predefined lognormal distribution with a mean equivalence ratio of 1. The justification for choosing this distribution is based on the extracted PDF obtained from the 3-D simulation presented in [10], and it is bounded from 0 to 1. Since the distribution in 3-D simulation is positively skewed and lognormal distribution closely matches the distribution obtained from it. To reproduce this generated PDF on the 2-D domain, a Java macro is developed to generate random numbers that follows the lognormal distribution and subsequently these generated random numbers are provided as fuel mass fraction at the inlet boundary of the 2-D domain. The degree of inhomogeneity of fuel/oxidizer mixing is varied by changing standard deviation of the PDF while maintaining the mean value as the global equivalence ratio of unity.

The outlet boundary condition is set to atmospheric condition, and the other two boundaries of the 2-D domain are periodic boundary condition, to model the detonation wave propagation in circumferential direction.

3. **Results and Discussion**

The present study utilizes a lognormal distribution as a PDF of fuel mass fraction for the inlet boundary in order to model the effects of mixture inhomogeneity. Unmixedness, in our case is defined as the standard deviation of the fuel mass fraction divided by the mean fuel mass fraction and is presented by Equation 6

$$q = \frac{\sigma_i}{y_{mean}}$$ (6)
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Fig 2: Distribution plots of fuel mass fraction for varying level of unmixedness

Four cases are considered to represent varying levels of unmixedness \((q = 0.033, 0.056, 0.067 \text{ & } 0.078)\) with a constant mean (global equivalence ratio =1) of the distribution (Fig. 2).

Fig 3: Contour plot of equivalence ratio. Top Left-Premixed case; Top Middle-Non-Premixed \(q=0.033\); Top Right-\(q=0.056\); Bottom Left-\(q=0.067\); Bottom Right-\(q=0.078\)
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The variation in local equivalence ratio obtained due to the induction of unmixedness in the flow field is shown in comparison with a perfectly premixed case in Fig. 3. The contour plot of equivalence ratio shows how the mixture inhomogeneity creates localized pockets of fuel rich and lean mixture region within the domain and in subsequent section it is shown that these localized pockets of lean and rich mixture region affects the performance of an RDC.

A. Detonation Wave Velocity

Theoretical Chapman-Jouguet (CJ) velocity is obtained, using the analytical method presented in [10], whereby a system of non-linear equations is solved for H2-air mixture. Further to this, the four cases of varying unmixedness were taken into consideration and the detonation velocity for each of the cases were obtained using the multiple probe points shown in Fig. 1 at different time steps. Table 1 contains the mean detonation velocity for the four cases considered in our analysis along with that of the perfectly premixed and experimental value along with CJ velocity obtained from the analytical solution.

Table 1: Compare wave velocity in Premixed, Non-Premixed, Experimental & CJ Velocity

<table>
<thead>
<tr>
<th>Case</th>
<th>Detonation wave velocity (m/s)</th>
<th>% CJ velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>CJ velocity [37]</td>
<td>1977</td>
<td>-</td>
</tr>
<tr>
<td>Experimental [25]</td>
<td>1630</td>
<td>82.5</td>
</tr>
<tr>
<td>Perfectly Premixed</td>
<td>1957</td>
<td>98.9</td>
</tr>
<tr>
<td>Non-Premixed (q = 0.033)</td>
<td>1945</td>
<td>98.4</td>
</tr>
<tr>
<td>Non-Premixed (q = 0.056)</td>
<td>1881</td>
<td>95.2</td>
</tr>
<tr>
<td>Non-Premixed (q = 0.067)</td>
<td>1872</td>
<td>94.7</td>
</tr>
<tr>
<td>Non-Premixed (q = 0.078)</td>
<td>1790</td>
<td>90.6</td>
</tr>
</tbody>
</table>

The data presented above clearly demonstrate the effects of mixture inhomogeneity on the mean detonation velocity, which is decreasing with an increase of mixture inhomogeneity. This collaborate the hypothesis that inhomogeneity affects the instantaneous wave velocity and in turn the performance of an RDC. Still the mean detonation velocity for the case of q = 0.078 is approximately 10% higher than that of the experimental value. The primary reason for higher detonation velocity as compared to the experimental value is due to the effects of fuel-product stratification and heat loss from an RDC, which are not incorporated in the current CFD simulation. However, the effects of fuel-product stratification and heat loss were explained using an analytical method presented by Sathya et al [10].

B. Pressure Profile

Time dependent peak pressure is obtained from multiple probes points. Data obtained from these probe points for different time steps were used to compare the peak pressure profile for all the four cases of non-premixed simulation along with that of the perfectly premixed simulation. Fig.4 shows the instantaneous peak pressure comparison between premixed and non-premixed cases.
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**Fig 4: Time Depend Peak Pressure Comparison between Premixed & Non-Premixed cases**

The plot demonstrates that the instantaneous peak pressure in between the premixed and non-premixed cases is mostly higher for the case of perfectly premixed simulation as compared to the cases of non-premixed simulations. The sole reason for this higher peak pressure is due to uniform mixture composition within the domain, leading to relatively higher pressure gain as compared to the non-premixed simulation where we have local pockets of varying equivalence ratio ranging from lean mixture to a fuel rich mixture. However, we see few instances in the plot where the instantaneous peak pressure is higher for non-premixed simulation as compared to that of premixed one (circled and marked as point 1, 2, 3, 5, 8, 9, and 11 in Fig.4), due to local region of fuel rich mixture arising from the effect of mixture inhomogeneity in the domain. Similarly, we also see few instances where the peak pressures in the non-premixed cases are way below than that of the corresponding premixed one (circled and marked as point 4, 6, 7, and 10 in Fig.4), because local equivalence ratio in that pocket is relatively lesser than unity, leading to smaller pressure gain in the system.

**C. Detonation Wave structure**

The detonation wave structure is analyzed based on the numerical Schlieren imaging obtained from the 2-D simulation. In order to obtain the Numerical Schlieren plot, equation 7 is used, which is presented in [13].

\[
S = c \exp\left(\frac{-d(\nabla \rho - |\nabla \rho|_{\text{min}})}{(\nabla \rho|_{\text{max}} - |\nabla \rho|_{\text{min}})}\right)
\]

\(\nabla \rho\) Indicates the density gradient between the grid cells and c & d are the scaling constant (c=0.8 and d=1000), to enhance the flow visualization even for the small density gradient in the flow field.

The height of the detonation wave front is same for both the premixed and the non-premixed cases (fig 5), which validate that the height of the detonation wave front is a function of inlet stagnation pressure as presented in [14]. Slip line governs the degree of product expansion and in turn affects...
the thrust or the performance of the RDC [15]. Slip line in the case of premixed simulation is much more dominant as compared to the non-premixed cases (as marked by $\alpha$ in Fig.5), and the dominance of the slip region decreases with the increase of unmixedness. Also due to the effect of mixture inhomogeneity, it develops a vortical structure behind the detonation front and as the effect of inhomogeneity increases, the vortical structure increases in size, providing a more corrugated detonation wave front, as compared to planar wave front in the case of premixed simulation. Moreover, due to large variation in local equivalence ratio, the wave has to travel through a larger patch of lean mixture, causing a separation of shock wave and the reaction zone. This phenomenon affects the wave speed and in turns the performance of an RDC.

![Fig 5: Comparison of wave structure between premixed (Top left) and non-premixed cases Top Middle-q=0.033; Top Right-q=0.056; Bottom left-q=0.067; Bottom right-q=0.078](image)

**D. Detonation cell size**

Another important parameter for RDC design is the detonation cell size, and the geometric dimensions for the RDC, in general, increase with increasing cell size. The detonation cell size is defined as a distance between the two consecutive triple points which originates when there is an interaction of the detonation wave front with that of the transverse wave and the reflected wave. The geometric dimension of an RDC is determined based on a set of guideline put forth by Bykovskii et al. [16] that relates the detonation cell size $\lambda$ with minimum combustor dimension for the stable propagation of the detonation wave within an RDC. Current study investigates the effect of mixture inhomogeneity on the detonation cell size. In order to obtain the detonation cell size for both premixed and non-premixed cases, the contour of the detonation cell size are obtained.
by tracing a region of maximum pressure downstream of the detonation front. Subsequently once the contour plot of the detonation cell size is obtained, we are calculating the individual cell size from the contour plot using the commercial software package called ImageJ and subsequently tabulating the mean cell size for both premixed and non-premixed simulation cases.

It is evident from Fig. 6 that with the increase in unmixedness mean detonation cell size increases. Analyzing the detonation cell size behavior across the different cases of non-premixed simulation as shown in Fig. 7, it is evident that as the effect of mixture inhomogeneity increases, the detonation cell size pattern becomes more irregular which can be seen prominently for the case of q=0.078. As the detonation wave passes through a larger region of inhomogeneity separation of the detonation wave front from the reaction zone occurs due to the triple points extinguishing in the non-detonable mixture which causes the cell size pattern to be more irregular.

Fig.7: Contour of Detonation cell size Premixed (Top Left) & Non-Premixed cases; q=0.033 (Top Middle), q=0.056 (Top Right), q=0.067 (Bottom Left) and q=0.078 (Bottom Right)
4. Conclusions
The current work substituted the expensive 3-D numerical simulation by an inexpensive 2-D CFD simulation to model the effect of fuel/oxidizer inhomogeneity. Based on the comparison study between premixed and different cases of non-premixed simulation, it is found that:

1. The mean detonation velocity shows a decreasing trend with an increase in the mixture inhomogeneity. This validates the hypothesis that unmixedness plays a crucial role in affecting the wave speed and in turn the performance of RDC.

2. The instantaneous peak pressure for non-premixed cases are mostly lower than the premixed simulation due to homogeneous mixing in premixed domain, however there are instances where the peak pressure in the non-premixed are higher than the premixed simulation, owing to local fuel rich mixture pockets in the domain.

3. The height of the detonation front is same for both premixed and all cases of non-premixed simulation. Furthermore the detonation wavefront in non-premixed are corrugated as compared to the planar wavefront in premixed case. Also as the effect of fuel/oxidizer inhomogeneity increases, the vortical structures behind the detonation front increases in size producing a more corrugated wavefront and as the wave moves through a higher region of unmixedness, separation of shock wave and reaction zone occurs causing a reduction in wave speed and in turn affects the performance of an RDC.

4. The mean detonation cell size is higher for non-premixed as compared to the premixed case. With the increase in the mixture inhomogeneity, the mean detonation cell size shows an increasing trend as observed in the cases of non-premixed simulation. Detonation cell size shows a more irregular pattern with increasing unmixedness, due to triple points extinguishing in the non-detonable mixture causing a separation of wavefront from the reaction zone.

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6. References
Journal article:
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Journal article in press:

Symposium Proceedings:

Conference proceedings:


