Detonation Wave Diffraction Through Compositional and Geometrical Discontinuities in Pulse Detonation Engines.

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Abstract

The motivation for this work emerges from the recent interest in obtaining the high theoretical thermodynamic and propulsive efficiencies that pulsed detonation engines (PDEs) can achieve. In practical applications it is desirable for PDEs to use fuels that have already gained acceptance/approval by the military and/or aviation industry, such as JP-5 or JP-10. Unfortunately, the use of such fuels makes the fuel-air mixtures difficult to detonate. To solve this problem, various research teams are currently investigating the use of a detonative initiator also known as a "pre-detonator," which utilizes a small tube filled with a very sensitive mixture that can be easily detonated and discharged into the main combustor tube. Hence, the importance of detonation diffraction from the small tube into the main combustor tube arises. The present paper studies such detonation diffraction processes where the main combustor tube is filled with a stoichiometric ethylene-air mixture and the initiator tube is filled with mixtures of varying equivalence ratios of ethylene-air enriched with varying amounts of oxygen. Moreover, the oxygen enrichment leads to a detrimental effect in the specific impulse of the PDE. This work highlights the importance of minimizing and/or eliminating oxygen enrichment by characterizing the effects to the specific impulse of the PDE.

Introduction

Recent PDE research teams are utilizing a detonative initiator system to initiate the detonation in the main combustor tube, in essence this system is a detonation-to-detonation initiator. The concept is to use a small tube, on the order of 5% or less of the main combustor's volume, filled with a highly sensitive mixture, such as a fuel-rich Ethylene/O_2 mixture. A detonation is rapidly initiated in this small tube and discharged into the main combustor. The goal is to successfully transmit the detonation wave initiated in the highly sensitive mixture into a less sensitive mixture such as Ethylene/Air. Thus an effective detonation transmission from the initiator tube into the main combustor is extremely important. The key issue in this process is on "effective transmission" in other words, a successful transmission is one in which the detonation wave exiting the small tube overcomes the diffraction process and continues propagation into the less sensitive mixture as a detonation wave. Also, an "effective transmission" refers to a process in which the detonation wave exiting the pre-detonator tube fails to transition as a detonation wave due to the diffraction process and continues as decoupled shock and deflagration waves, but due to reflection and implosion processes which dominate the gasdynamic flow downstream of the initiator tube, a detonation re-initiation process occurs and thus an "effective" transmission occurs. The concept of a re-

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initiation process can be conceptualized due to the non-uniform energy distribution that exists during the diffraction process, which is created by shocks colliding with each other and thus producing local hot spots where detonation re-initiation can occur.[1]

The main limitation in using this type of initiator is the reduction to the specific impulse of the PDE. The initiator tube must be filled with a very sensitive mixture in order to generate a detonation wave strong enough to overcome the diffraction process. And thus, it is necessary to use oxygen as the oxidizer. In air-breathing engines, the requirement to carry a small amount of oxygen on board requires to account for such mass when calculating the fuel based specific impulse, I_{spf}. Therefore, it is clear that the fuel specific impulse is inversely proportional to the auxiliary mass of oxygen used for each cycle of the PDE.

$$I_{spf} = \frac{I_T}{m_f \cdot g_0} \tag{1}$$

$$I_T = A_{HW} \int_{t_1}^{t_2} P_{HW}(t)\, dt \tag{2}$$

where:
I_T = the total impulse in *N-s*
$m_f = m_{fuel} + m_{oxygen}$ in *kg*
$g_0 = 9.81\ m/s^2$
A_{HW} = Area at the Head Wall = Thrust Wall Area in m^2
$P_{HW}(t)$ = Pressure evolution at the head wall in *Pa*

Diffraction Process:

Although the detonation diffraction process can be considered as a "classical" area of detonation research, most of the previous work (until recently) focused on detonation suppression rather than effective transmission. As it was pointed out by Li and Kailasanath [2], an important result from the "classical" diffraction work is the concept of a critical diameter, d_c. The critical diameter indicates the minimum tube diameter for a successful detonation transmission into an unconfined space for a given fuel-oxidizer mixture. Hence, if the detonation wave is traveling in a tube with a diameter d, which is less than the critical diameter, $d < d_c$, and it encounters a sudden expansion into an unconfined space, the detonation diffraction process will cause the energy release zone to decouple from the leading shock wave and thus the detonation wave fails to transition into the unconfined space. The critical diameter, d_c, is usually expressed in terms of the detonation cell size, λ. Knystautas et al. [3] have an excellent paper with further details on critical tube diameters and detonation cell sizes for different hydrocarbon-air mixtures. More recently, Kaneshige and Shepherd [4] have reported cell sizes for stoichiometric C_2H_4-Air and C_2H_4-O_2 at 24 mm and 0.8 mm respectively.

Shepherd et al. [5] and Schultz [6] have shown that detonation waves experiencing diffraction over sharp convex corners can be categorized into three regimes: a) supercritical, b) critical, and c) subcritical. As a detonation wave propagates from a confined tube into an unconfined space diffracts at the exit plane and has to overcome the sharp convex corners. From gasdynamic theory we know that at these corners, expansion waves originate to inform the rest of the flow filed about the existence of the convex corners. These expansion waves interact with the detonation wave and are responsible for the curvature induced to the detonation wave. Also, due to the expansion waves behind the curved detonation wave, both temperature and pressure are reduced. Hence, from chemical kinetics we can infer that the reaction rates of the chemical reactions responsible for the energy release behind the detonation wave are also reduced due to their dependence on temperature and pressure [7].

With that in mind, the supercritical regime encompasses detonation waves which successfully transmit into the unconfined space, and this occurs when the energy release rate overcomes the effects of

the expansion waves. In the subcritical regime, the detonation fails and the leading shock wave decouples from the reaction zone and we end up with a shock wave followed by a deflagration wave. In the critical regime the detonation wave fails but a detonation re-initiation process is observed due to shock to shock interaction produced by the transverse waves.

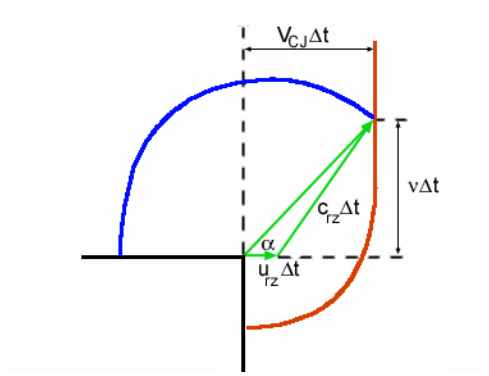

Figure 1: Schultz's extension of Skews' construction to disturbance propagating into a detonation front. red=detonation wave, blue=head of expansion wave, green=expansion wave interacting with detonation wave, and α = disturbance angle.

Knowing that the expansion waves can weaken a detonation wave undergoing diffraction to the point where the expansion waves prevail over the energy release rate. Therefore attention to when and where the expansion waves interact with the detonation waves can serve us as a geometrical tool to better understand detonation diffraction. Skews [8, 9] first came up with a geometrical model of the expansion wave interacting with a non-reacting shockwave undergoing diffraction, but it was Schultz [6] who first extended Skews' model for a detonation wave undergoing diffraction by applying Skews' model to the ZND detonation model. The resulting disturbance angle, α, can be expressed in terms of the Chapman-Jouguet detonation velocity, V_{CJ}, the speed of sound within the reaction zone, c_{rz}, and the flow velocity within the reaction zone, u_{rz}, as follows:

$$\alpha = \arctan\left(\frac{\sqrt{c_{rz}^2 - \left(V_{CJ} - u_{rz}\right)^2}}{V_{CJ}}\right) \tag{3}$$

Since the present paper studies the detonation diffraction process through compositional and geometrical discontinuities, a modified version of Schultz' geometrical model is employed to take into account the compositional discontinuities, such as the diffraction of Ethylene/O_2 detonation wave into a Ethylene/Air mixture. In order to better understand the effects that the highly energetic mixtures have on successful detonation diffractions, the Ethylene/O_2 mixture will be diluted with varying amounts of N_2. Furthermore, this paper will investigate the correlations between detonation diffraction processes in 2D channels and in 3D axisymmetric tubes. Here a quasi-confined environment exists because the detonation exiting the small 3D axisymmetric tube or 2D channel with critical dimensions, D_0 or Y_0, encounter a sudden expansion into the larger tube/channel with finite critical dimension, D or Y. In this situation wall effects will come into play as has been observed by Vasileev [10].

Experimental Set-up

The following figure (Figure 2) shows the 3D axisymmetric test section and the 2D channel test section. The optical access window (i.e. our field of view) is highlighted in the diagrams below. These windows were used to interrogate the flow field by using a high-speed laser shadowgraph system capable of taking images at up to 150,000 frames per second. Furthermore, CH chemical luminescence images

were also recorded simultaneously with the shadowgraph images. These optical diagnostic systems have been discussed in greater detail by Sinibaldi et al. in references [11, 12].

For the axisymmetric cases the D/D_0 expansion ratios tested varied from 2.0 to 4.0. Meanwhile for the 2D channels, the Y/Y_0 expansion ratios varied from 1.0, which indicates no expansion, to 4.0. Also, the equivalence ratio of the Ethylene/Oxygen mixtures within the initiator tube was varied from 0.7 to 2.6. The equivalence ratio of the Ethylene/Air mixture within the large tube/channel was kept constant at 1.0.

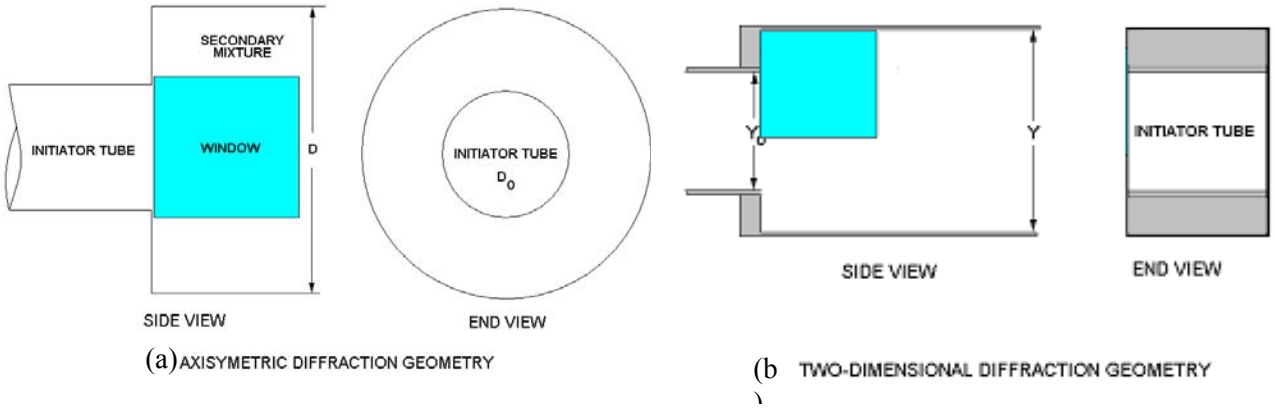

Figure 2: Optical Access Test Section Configurations Used for Imaging Studies (a) Axisymmetric Test Section (b) Two-Dimensional Test Section.

Results and Discussion

Diffraction:

The results shown in Figures 3a and 3b are still quite preliminary, as it is indicated in Figure 3a, due to mixing and diffusion phenomena, interface gradients between the ethylene-oxygen and ethylene-air mixtures appear to severely affect our results. Nonetheless, one can identify that these interface issues are predominant at higher expansion ratios, thus indicating the limits of successful detonation transitions.

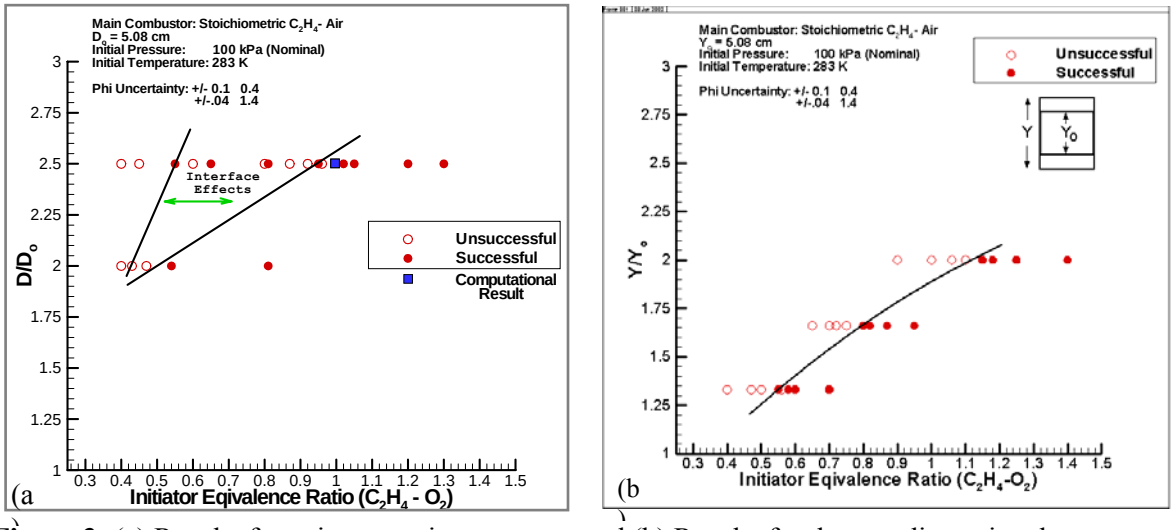

Figure 3: (a) Results for axisymmetric geometry; and (b) Results for the two dimensional geometry.

The results for the 2D channel tests are shown in Figure 3b, one can easily see that the effects of mixture sensitivity are clearly demarked. The trends shown indicate that as the expansion ratio is increased from $Y/Y_0 = 1.3$ to 2.0, the minimum equivalence ratio required in the initiator (small channel) increased from 0.55 to 1.15, respectively. This behavior ties into the reduction of the chemical kinetics reaction rates by the stronger expansion wave produced at the higher expansion ratios. Further analysis is required to correlate expansion ratios to detonation cell sizes, which are a relative measure of the chemical kinetics reaction rates.

Although interface effects were not characterized during the 2D channel tests, further optical diagnostics, such as the diode-laser based absorption spectroscopic diagnostics developed by Hanson et al. [13] will be needed to properly quantify the interface gradients in both the 2D channels and the 3D axisymmetric tubes.

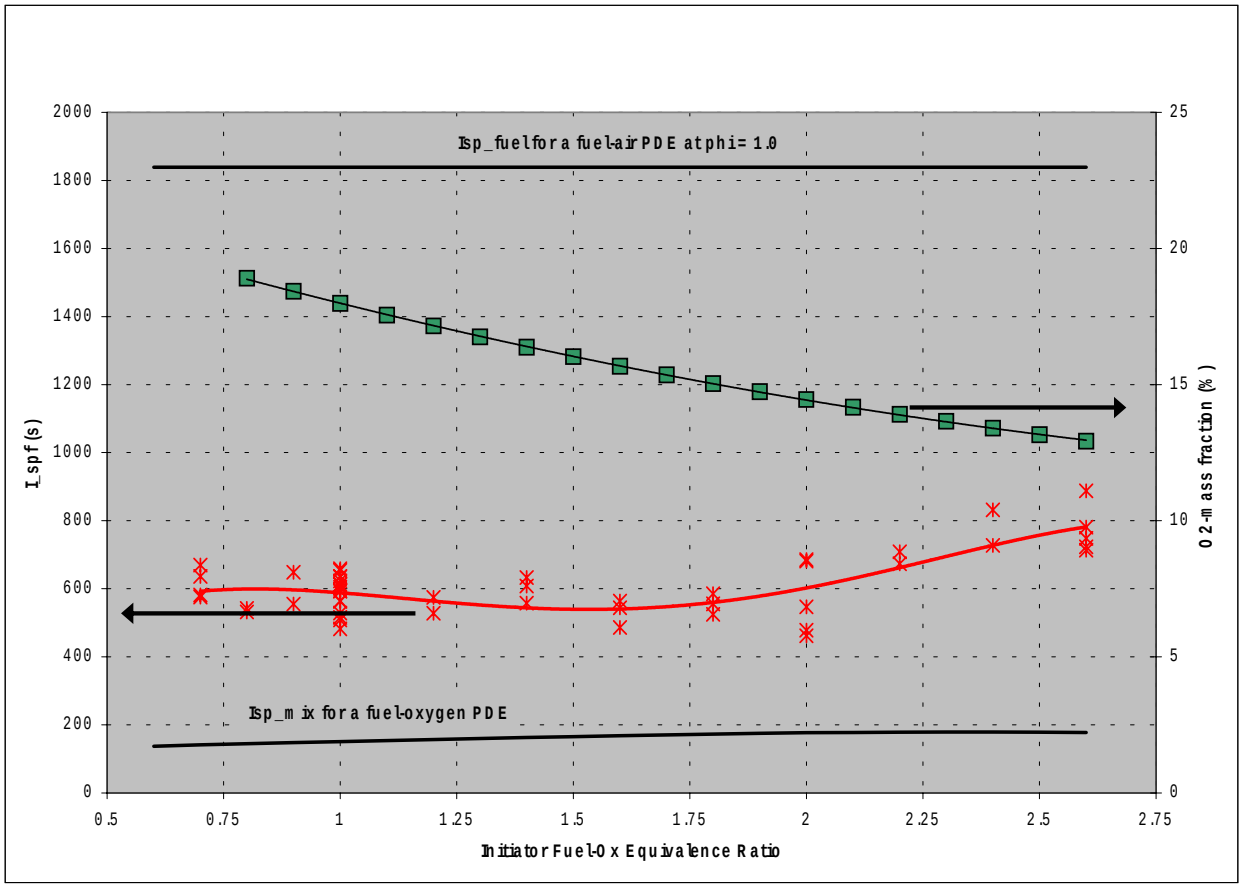

Figure 4: I_{spf} and O_2 mass fraction versus Initiator equivalence ratio

Specific Impulse:

In order to utilize a small initiator tube, oxygen enrichment is used to create a very sensitive mixture that can detonate in a small tube volume. But this oxygen needs to be taken into account when computing the fuel based specific impulse for a PDE. Initial data is shown in figure 4, where the effects of the oxygen enrichment drastically reduce the attainable Ispf compared to an entirely air-breathing PDE. In this case, the initiator was completely filled with an Ethylene – Oxygen mixture at varying equivalence ratios. The results show that at very rich conditions where the equivalence ratios are greater than 1.8, the Ispf values increase directly proportional to the equivalence ratio up to a maximum of 800 s at $\phi = 2.6$. This effect can be partly described by the account that the fuel in use has a molecular weight lower than the oxidizer ($MW_{C2H4} = 28$ kg/kmol and $MW_{O2} = 32$ kg/kmol). In theory, further increase in the initiator

equivalence ratio will yield higher I_{spf} values, but the limits of effective detonation diffraction start to dominate at equivalence ratios greater than 2.6 and lower than 0.7. Figure 4 also shows a mixture based specific impulse for a PDE operating entirely on Ethylene/Oxygen, which varies from I_{sp} = 138 s to 179 s with the maximum value occurring at ϕ = 2.4 obtained from reference [14]. This indicates that with our current set-up, the optimum operating settings are at a ϕ = 2.6 where the I_{spf} is 4.5 times higher than the maximum I_{sp} of a PDE operating on entirely $C_2H_4 - O_2$, and it is 2.25 times lower than a PDE operating entirely on C_2H_4-Air at stoichiometric conditions.[14]

The value of these studies is to optimize the operating conditions of a PDE using a detonative initiator system. Therefore, we must minimize the amount of oxygen enrichment to maximize the fuel based specific impulse. The strategy for the current work is to characterize the I_{spf} as a function of initiator mixture composition, initiator volume, main combustor equivalence ratio, and compositional gradient between the fuel-oxygen to fuel-air interface. This can be accomplished in the following manner:

1. Choose the most sensitive fuel-air mixture for the main combustor. This will lead to the most successful detonation diffraction cases.
2. Identify the lean and rich limits of initiator mixture composition that yield effective detonation diffractions for varying expansion ratios.
3. Use laser absorption diagnostics to characterize the interface compositional gradients at varying fill flow rates.
4. Calculate the I_{spf} values for all the above cases.

Item #1 can be easily obtained for various fuel-air mixtures from reference [4]. For ethylene-air the value is ϕ = 1.2. Figure 3 already shows the trends we need to obtain for item #2, and figure 4 shows initial I_{spf} values required by item #4. Further work is required to characterize the use of Nitrogen dilution in the initiator's mixture. This will effectively simulate a fuel-air initiator mixture with oxygen enrichment.

Acknowledgement

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References

[1] Murray, S.B., Thibault, P.A., Zhang, F., Bjerketvedt, D., Sulmistras, A., Thomas, G.O., Jenssen, A., and Moen, I.O., "The Role Of Energy Distribution On The Transmission Of Detonation," International Colloquium On Control Of Detonation Processes, Moscow, Russia, 2000.

[2] Li, C., and Kailasanath, K., "Detonation Diffraction In Pulsed Detonation Engines," AIAA 2000-3470.

[3] Knystautas, R., Guirao, C., Lee, J.H., and Sulmistras, A., "Measurement Of Cell Size In Hydrocarbon-Air Mixtures and Predictions Of Critical Tube Diameter, Critical Initiation Energy, And Detonability Limits," 9th ICODERS, Pointiers, France, 1983.

[4] Kaneshige, M. and Shepherd, J.E., "Detonation database," Technical Report FM97-8, GALCIT, July 1997. See also the electronic hypertext version at http://www.galcit.caltech.edu/detn_db/html/.

[5] Shepherd, J.E., Schultz, E., and Akbar, R., "Detonation Diffraction," Paper 5410, 22nd International Symposium on Shock Waves, London, UK, 1999.

[6] Shultz, E., "Detonation Diffraction Through An Abrupt Area Expansion," Ph.D. Thesis, California Institute of technology, 2000.

[7] Glassman, I., Combustion, 3rd Ed., Academic Press, 1996.

[8] Skews, B.W., "The Shape of a Diffracting Shock Wave," JFM, v. 29, 1967, pp.297-304.

[9] Skews, B.W., "The Perturbed Region Behind A Diffracting Shock Wave," JFM, v. 29, 1967, pp.705-719.

[10] Vasileev, A.A., "Diffraction Of Multifront Detonation," Combustion, Explosions, and Shock Waves, 24(1), 1988, pp. 92-99.

[11] Sinibaldi, J.O., Brophy, C.M., Li, C., and Kailasanath, K., "Investigation of Detonation Wave Diffraction During the Ignition of Pulsed Detonation Engines," *2nd Joint Meeting of the U.S. Sections Of The Combustion Institute*, Oakland, California, March 25 – 28, 2001.

[12] Sinibaldi, J.O., Brophy, C.M., Li, C., and Kailasanath, K., "Initiator Detonation Diffraction Studies In Pulse Detonation Engines," *37th AIAA/ASME/SAE/ASEE Joint Propulsion Conference*, July 2001.

[13] Hanson, R. K., "Advanced Laser Diagnostics for Reactive Flows", AIAA paper 2002-0169, 2002.

[14] J. M. Austin, E. Wintenberger, M. Cooper, S. I. Jackson, and J. E. Shepherd. ``An analytical model for the impulse of a single-cycle pulse detonation tube." Journal of Propulsion and Power, 19(1):22-38, 2003.