# Numerical Investigation on the Effects of Nozzle Geometry on the Performance of a Pulse Detonation Engine

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#### **Abstract**

A numerical study is presented on the effects of various nozzle geometries and operating conditions on the performance of a Pulse Detonation Engine (PDE). An unsteady numerical simulation model, which is second order accurate in space and first order accurate in time, using an automated Java based computational fluid dynamics (CFD) software is presented. One- and two-dimensional transient CFD models were employed in a systematic manner to study the propulsive performance characteristics of the PDE under different operating conditions. Preliminary studies of the effects of nozzle geometry on the performance characteristics of a generic PDE are presented. The results indicate that an expanding nozzle, capable of adapting with the cycle time and the ambient pressure, is very suitable for optimizing the PDE performance. Addition of a straight, diverging or converging nozzle improves the performance. However, it is observed that there is an optimum value of the exit area of a divergent nozzle for performance improvement. At low ambient pressure addition of a nozzle increases the specific impulse of the PDE tube. It is also seen that a diverging nozzle is more effective than a converging-diverging nozzle at low ambient pressure. The study indicates that increased volume of the reacting fuel mixture has a negative effect on the PDE performance. The results show that a 25% reduction of the reacting fuel mixture leads to approximately 18% increase in the value of the specific impulse.

# 1. Introduction

The Pulse Detonation Engine (PDE) has recently received considerable interest in the aero-propulsion community due to its potential advantages in performance and inherent simplicity over current propulsion concepts. It is a very promising propulsion concept for aerospace transportation. The operation of the PDE is based on the detonation mode of combustion, which involves the burning of a reactive gas mixture at high pressure and high temperature behind a propagating shock wave. The high-pressure combustion products, acting on the thrust plate at the front end of the engine, produce the forward thrust. The PDE is an unsteady propulsion device, which operates in an intermittent manner governed by a cycle frequency. Fig. 1 shows a schematic of a typical airbreathing pulse detonation engine, which consists of a simple straight cylindrical tube. The details of the operating principle can be seen elsewhere [1, 2]. The design and optimization of a PDE propulsion system are complex due to the unsteady nature of the propulsion cycle and the strong coupling of the propulsive flow with the vehicle configuration and the ambient environment.

A nozzle may significantly affect the performance of a PDE and hence nozzle design is one of the key issues to be resolved. Due to the complexity of the diffraction of detonation wave through a nozzle, the effects of a nozzle on PDE performance are not yet fully understood. The presence of a nozzle may affect the time required to drop the pressure inside the PDE combustor to a certain level at which time the next cycle can be started. Therefore, the effects of the nozzle geometry on the cycle time and PDE performance need to be investigated.

Cambier and Adelman [3] reported a numerical study of a pulse detonation wave engine (PDWE) using quasi one-dimensional computations. The computations were carried out with a shock-capturing total variation diminishing (TVD) algorithm (second order accurate in

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Nomenclature			
$A_{exit}$	Nozzle exit area, m <sup>2</sup>	$m_s$	Molar mass of specie s, kmol
$A_{tube}$	Tube exit area, m <sup>2</sup>	P	Pressure, Pa
E	Total energy, J/m <sup>3</sup>	t	Time, sec
Isp	Specific impulse, sec	T	Absolute temperature, K
Isp_final	Specific impulse final, sec	и	Mean flow velocity, m/sec
Isp max	Specific impulse maximum, sec	$\rho$	density, kg/m <sup>3</sup>
$L_{nozzle}$	Nozzle length, m	$\rho_{s}$	mass density of specie s, kg/m <sup>3</sup>
$L_{pde}$	PDE tube length, m	$\dot{\omega}_{s}$	rate of production of specie s
$l_{propellant}$	Length of the propellant mixture, m		per unit volume, kg/m³ sec kmol

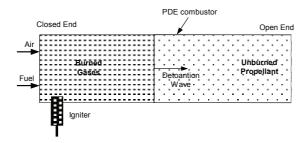


Fig. 1. Schematic of a typical air-breathing pulse detonation engine

space) for multiple species and multi-step finite-rate Eidelman et al. [4] performed a twodimensional simulation of a detonation tube using a second-order Godnunov solver on unstructured grids. A detailed description of the basic operations of a PDE was provided by Bussing and Pappas [1]. The authors concluded that a detonation combustion process is thermally more efficient than a traditional constant pressure combustion process. In a subsequent study performed by Bussing et al. [5], a comparison between open- and closed-end initiations was provided. In recent years Cambier and Tenger [6] reported a computational study of nozzle effects on PDE performance. In the following year Eidelman and Yang [2] reported the effects of adding a nozzle on PDE efficiency. Their results indicate a drastic increase of engine efficiency in the presence of a nozzle. Based on experimental investigations, Cooper et al. [7] reported that the addition of a divergent nozzle has negligible effect on PDE performance; while, the addition of a straight nozzle is very much effective to improve PDE performance. Recently, Mohanraj and Merkle [8] reported multi-cycle performance analysis of a PDE using a quasi onedimensional model. In this research, results of a systematic study on various nozzle geometries, effects of ambient pressure and the tube fill fraction are presented.

# 2. Mathematical Formulation and Numerical Methodology

# 2.1 Governing Equations

The following assumptions were made in the formulation of the transient combustion process in a pulse detonation engine: (i) no species diffusion, (ii) no heat conduction, (iii) heat flow due to density gradient is neglected, (iv) bulk viscosity is neglected, (v) diffusion due to pressure gradient is ignored, (vi) heat capacities are a function of temperature (real gas), (vii) thermal equilibrium (single temperature), (viii) viscous dissipation and viscous work are neglected, and (ix) no body forces.

The time-dependent conservation equations governing the dynamics of the inviscid, non-heat conducting, reacting gas flow, are being solved. The fundamental set of governing equations for the system is:

• Conservation of Mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0 \tag{1}$$

• Conservation of momentum:

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + P)}{\partial x} = 0 \tag{2}$$

Conservation of Energy:

$$\frac{\partial E}{\partial t} + \frac{\partial (uE + uP)}{\partial x} = 0 \tag{3}$$

Here  $\rho$ , u, P, and E are the density, velocity, pressure and total energy respectively. The physical and chemical effects of combustion are modeled by solving the chemical kinetics equations. The general form of the conservation equations for the mass densities of chemical species (index s) is given by the following reaction kinetics equation:

$$\frac{\partial \rho_s}{\partial t} + \vec{\nabla} \cdot (\vec{u}\rho_s) = m_s \dot{\omega}_s \tag{4}$$

where  $\vec{u}$  is of course the mean flow velocity,  $m_s$  is the molar mass and  $\dot{\omega}_s$  is the rate of production of species s per unit volume respectively.

#### 2.2 The CFD Model

The combustion in a PDE is unsteady in nature. Onedimensional and two-dimensional unsteady CFD computations are used to get realistic approximations of the unsteady processes associated with a PDE operation. The CFD code Café-Vienna, developed by Dr. J.-L. Cambier was used to perform the unsteady computations. Café-Vienna is a Java version of the Mozart CFD code [9], that computes inviscid flow field using the Euler equations. An inviscid, two-dimensional numerical scheme coupled to the detailed reaction kinetics of the combustion is employed. The PDE environment is characterized by multiple shocks in the flow field. The scheme used here is that of Harten [10], generalized to multiple species; it is second-order accurate in space, total variation diminishing (TVD), and first order accurate in time. The chemical kinetics and the inviscid transport process are coupled via an operator-splitting method.

## 2.3 Code Validation and Grid Independency Test

The code validation was performed by comparing the computed results with the experimental results of Schauer et al. [11]. In order to demonstrate the numerical accuracy of the present numerical scheme, comparisons were also made with the analytical results of Wintenberger et al. [12] who developed a simple analytical model to approximate the PDE performance. In order to minimize the computation time with a desired level of accuracy, the grid independence test is essential. The grid resolution should ensure that the main detonation features such as detonation speed, temperature, and pressure distribution behind the detonation shock are grid independent, as well as ensure that the computational cost is minimum. In this test, the system configuration is a straight cylindrical tube with constant cross-section, 20 cm in length and 2 cm in radius. The PDE tube is uniformly filled with a stoichiometric hydrogen-air mixture. Both the ambient pressure and the initial fill pressure are chosen to be 1 atm and the initial temperature of the PDE chamber is set at 300 K. Using four different uniform grid sizes onedimensional simulations were carried out to establish the grid independence. The different grid sizes are: 1, 0.8, 0.4, and 0.2 mm. The initial conditions were kept the same for all the cases. It was observed that for the different grid spacing, all the simulations show very similar detonation behavior. In general, the results with the coarsest grid (grid size 1 mm) fall within 7% of the results obtained using the finest grid (grid size 0.2 mm), except near the region of peak pressure. Therefore, the

grid with 1 mm element size was chosen for the current study. Details of the code validation and grid independency test are reported in Cambier et al. [13] and Rouf [14].

#### 3. Results and Discussions

A reference PDE tube, 30 cm in length and 2 cm in radius, is uniformly filled with a stoichiometric hydrogen-air mixture. Both the ambient pressure and the initial fill pressure are chosen to be 1 atm. Initial temperature of the PDE chamber is 300 K. Detonation initiation is assured by having a large amount of energy deposition near the closed-end (thrust wall) of the tube. This is achieved by creating a high pressure and high temperature region near the closed-end. Computations were performed for a single pulse in a two-dimensionalaxisymmetric configuration. Three basic nozzle configurations were investigated: diverging nozzle, straight nozzle, and converging nozzle. It was observed that addition of a nozzle increases the performance of the PDE. In this paper the effects of different length of the straight nozzle, exit area of the divergent nozzle, ambient pressure and tube fill fraction are presented.

# 3.1 Length of Straight Nozzle

Several cases were run to study the effects of the length of a straight nozzle connected with the PDE tube. The nozzle length was systematically varied, whereas the tube length was held constant. The length of the straight nozzle was varied from 5 to 50 cm, giving a range of the length ratio  $L_{nozzle}/L_{pde}=0.17$  to 1.67.

Fig. 2 shows the maximum specific impulse during a single pulse (Isp-max) and the final specific impulse at the end of a single pulse (Isp-final) as functions of the nozzle length. It can be observed that both Isp-final and Isp-max increase nearly linearly with the increase of the nozzle length. Alternately, the observations suggest a higher specific impulse for a longer straight nozzle. To explain this behavior the "no-nozzle" case needs to be considered first. As reported by Li et al. [15] and Li & Kailasanath [16], in the no-nozzle case, when the detonation wave leaves the combustion chamber, it expands very quickly as a spherical wave. In contrast, in the straight nozzle case, when the detonation wave leaves the PDE tube it enters the nozzle section, and therefore, the wave is still confined by the nozzle wall. This is the reason why the shock does not decay as quickly as in the no-nozzle case. This results in an increase in pressure relaxation time and prolongs the thrust generation.

Fig. 3 represents the thrust generation during a single pulse as a function of time for different nozzle lengths. It can be observed that with the increase of the straight nozzle length the thrust generation time is prolonged. A close observation of the thrust profile reveals that in the case of 10 cm long nozzle the thrust becomes negative at around 1.2 ms; meanwhile for the 20 cm long nozzle the thrust takes on a negative value at around 1.5 ms; this means that the thrust generation time is approximately

25% longer for the 20 cm long nozzle. Due to the prolonged thrust generation, a higher impulse is obtained for a longer straight nozzle.

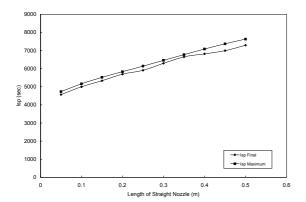


Fig. 2. Specific impulse versus length of straight nozzle

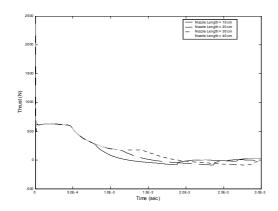


Fig. 3. Instantaneous thrust profiles for different lengths of straight nozzle

As mentioned earlier, reducing the cycle time can optimize the PDE performance. Fig. 4 shows the blowdown time (time when pressure inside PDE chamber reaches 1 atm) as a function of the nozzle length. The results indicate that the increase in length of a straight nozzle leads to an increase in the blow-down time. In other words, the cycling would be faster if the nozzle is shorter.

Fig. 5 shows the average temperature inside the PDE tube as a function of time for different straight nozzle geometries. The results show that when the straight nozzle is longer, the temperature inside the PDE tube drops at a slower rate. This can be explained by the fact that increased nozzle length causes a delay in the arrival of the expansion waves. This delay in turn causes the temperature inside the PDE to drop at a slower rate.

### 3.2 Exit Area of Diverging Nozzle

To study the effects of the exit area of a divergent nozzle, a cylindrical PDE tube, 30 cm in length with an internal radius of 2 cm, was attached with various geometries of the divergent nozzles. The divergent nozzle

was also 30 cm in length and connected at the open-end of the PDE tube. The throat area of the nozzle is equal to the PDE tube area, which means there is no constriction between the tube exit plane and the nozzle exit plane. The exit area of the nozzle was systematically varied, whereas the PDE tube area was held constant. The nozzle exit radius was varied from 2.5 to 7 cm, giving a range of the nozzle expansion ratio ( $A_{exit}/A_{tube}$ ) of 1.56 to 12.25. The initial amplitude of the oscillatory impulse profile was observed to increase with the increase of the nozzle expansion ratio (i.e. nozzle exit area). Rapid impulse generation was also observed with the increase in nozzle expansion ratio.

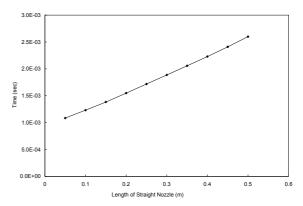


Fig. 4. Blow-down time versus length of straight nozzle

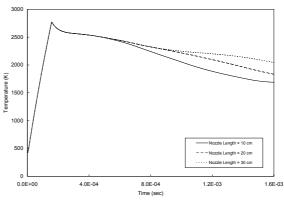


Fig. 5. Effect of straight nozzle length on PDE temperature

In Fig. 6 *Isp-final* (computed from the final impulse at the end of a single pulse) and *Isp-max* (computed from the maximum impulse during a single pulse) are plotted as functions of the expansion ratio. The results indicate that initially both *Isp-final* and *Isp-max* increase with the nozzle expansion ratio. The *Isp-final* reaches a maximum value at an optimal value of the expansion ratio and then it gradually decreases. Whereas the *Isp-max* shows a monotonic behavior, that is, it keeps increasing with the nozzle expansion ratio.

It can be recalled that the PDE performance should be optimized in terms of cycle time also. Fig. 7 shows the blow-down time as a function of the nozzle expansion ratio. It can be observed that the blow-down time

decreases with the nozzle expansion ratio. This means that the cycling would be faster if the nozzle expansion ratio is larger. Therefore, the impact of adding a variable area divergent nozzle with the PDE tube appears potentially attractive. Comparing Figs. 4 and 7, it can be concluded that shorter nozzles with a higher expansion ratio may be an attractive option due to lower values of blow-down time.

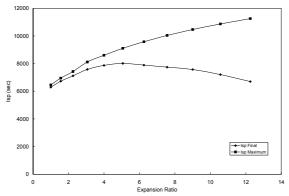


Fig. 6. Specific impulse as function of expansion ratio of a divergent nozzle

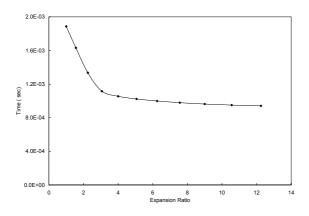


Fig. 7. Blow-down time versus expansion ratio

## 3.3 Effects of Ambient Pressure

In this section, the effects of the ambient pressure on the performance of a PDE are investigated. This investigation will help to observe the PDE performance at different altitudes. Four different geometries are considered: (i) a straight PDE tube, 10 cm in length and 2 cm in radius; (ii) a straight PDE tube, 30 cm in length and 2 cm in radius (iii) a diverging nozzle, 10 cm in length and 4 cm in exit radius, attached at the open end of the PDE tube (10 cm in length and 2 cm in radius), and (iv) a 10 cm long converging-diverging nozzle, having a throat radius of 1.4 cm and an exit radius of 4 cm, connected with the PDE tube (10 cm in length and 2 cm in radius). Computations were performed for values of ambient pressures as 0.25, 0.50, 0.75, and 1 atm. Like the previous investigations, here the PDE tube is uniformly filled with a stoichiometric hydrogen-air mixture. Here the ambient pressure was varied, while the initial fill pressure was kept constant (1 atm).

Fig. 8 shows the variation of the specific impulse with the ambient pressure for all the four different configurations. From this figure it is evident that with the decrease in the ambient pressure, the specific impulse increases. The performance gain is due to the fact that a reduction in the back-pressure results in a higher pressure difference between the chamber and the ambient. This leads to an increase in the momentum flow rate of the exhaust products directed towards the ambient. Therefore, decreasing the ambient pressure increases the net thrust, which increases the impulse, and hence the specific impulse is increased.

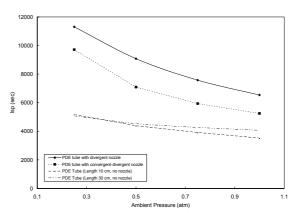


Fig. 8. Specific impulse versus ambient pressure for different configurations

A closer look at Fig. 8 reveals that when a divergent nozzle or a convergent-divergent nozzle is present with the PDE tube, more performance gain can be obtained at lower ambient pressures than the configurations without any nozzle. For the first configuration, where the PDE tube 10 cm long and no nozzle is attached to the tube, a 50% reduction of the ambient pressure increases the specific impulse by 24.4%. For the diverging and the converging-diverging nozzle cases, the same reduction of the ambient pressure leads to an increase of the specific impulse by about 38% and 35% respectively. The observations suggest that at lower back-pressures the presence of a nozzle is very much beneficial. Fig. 8 also implies that a diverging nozzle is more effective than a converging-diverging nozzle at low ambient pressures.

# 3.4 Effects of Tube Fill Fraction

Several cases were run to study the effects of the size of the propellant mixture in the PDE tube. Fig. 9 shows a schematic of the computed configuration where the PDE tube (of length  $L_{pde}$ ) is not completely filled with the propellant mixture. The propellant mixture occupies the length  $l_{\text{propellant}}$  of the PDE tube and the remaining portion is filled with air. The tube fill fraction (TFF =  $l_{\text{propellant}}/L_{pde}$ ) is the ratio of the volume of the propellant mixture to the volume of the PDE tube. Numerical

results were obtained for a range of values of tube fill fraction from 0.2 to 1.0.

# PDE Combustor

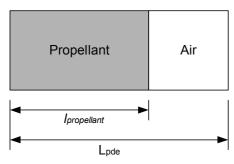


Fig. 9. Schematic of the straight tube PDE with partial tube filling

The variation of the specific impulse (*Isp*) with the tube fill fraction (TFF) is shown in Fig. 10. As shown in this figure, increasing the tube fill fraction ( or, the volume of the reactive gas mixture) plays a negative role on the specific impulse. For the values of tube fill fraction 1, 0.75, and 0.50, the *Isp* values are approximately 5325 sec, 6000 sec, and 7250 sec respectively. The results indicate that a 25% reduction of the propellant mixture size leads to an Isp increase by approximately 18%; a 50% reduction leads to an *Isp* increase by approximately 36%. This trend has been confirmed by the experimental observations of Schauer et al. [11]. One possible reason for this increase in the specific impulse is that when a tube is partially filled with propellant mixture, the remaining portion will act as a straight nozzle for the exhaust of the detonation products. As already discussed in the previous sections, the presence of a straight nozzle with a PDE tube can significantly increase the PDE performance and the performance increases with the length of the straight nozzle.

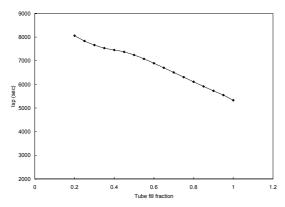


Fig. 10. Specific impulse versus tube fill fraction

Also observed was the pressure profile behind the moving detonation wave while the detonation wave remained inside the PDE tube's non-combustible air section. Fig. 11 shows the pressure profile inside a 10 cm long PDE tube, with a tube fill fraction of 0.6 at times

0.026 ms and 0.064 ms. It can be observed that at 0.026 ms the detonation wave stays approximately 5 cm away from the thrust wall. Since the filling length is 6 cm, the shock front is still inside the propellant mixture. From the pressure profile it can be seen that the peak pressure behind the shock is 13 atm. When the detonation wave enters the non-reactive air section the detonation is quenched, and the shock loses its strength as it no longer receives energy support from the chemical reactions. Fig. 10 shows the pressure profile behind the quenched shock when the shock reaches near the tube-exit at approximately 0.064 ms. It can be seen that the peak pressure behind this quenched shock is only about 8 atm, which is considerably lower than the pressure behind the original shock front.

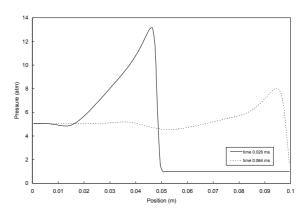


Fig. 11. Pressure profile at two different times for tube fill fraction 0.6

## 4. Conclusion

The results of a systematic numerical investigation of the effects of nozzle geometry and various operating conditions namely ambient pressure and tube fill fraction on PDE performance characteristics are presented. An automated Java-based CFD software designed with modern object-oriented programming techniques was employed to investigate the propulsive performance characteristics of the PDE. Accuracy of the code was tested by comparing the results with other published results and grid independency test was performed. It can be concluded from the current numerical study that addition of a nozzle to the PDE combustor increases the performance which includes: (i) increased impulse, (ii) prolonged duration of thrust, and (iii) reduced cycle time. Adding a straight nozzle delays the arrival of the expansion wave at the thrust wall from the PDE tube exit, hence, the duration of thrust generation is prolonged. A divergent nozzle also delays the arrival of the expansion wave at the thrust wall. It also increases the effective thrust-wall area. A convergent nozzle causes multiple shock reflections in the nozzle section and increases the impulse generation considerably.

An expanding nozzle can provide a better performance in stagnant ambient air. For an expanding nozzle, there is an optimal expansion ratio at which the maximum performance can be achieved. For very high altitude operation, i.e., at very low ambient pressure, addition of a nozzle considerably increases the specific impulse of the PDE. The performance gain is due to the increased momentum flow rate of the exhaust products at a lower back-pressure. It is also observed in this study that increased volume of the reactive gas mixture decreases the specific impulse of the PDE tube. This observation is consistent with other published experimental data.

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