Parametric study for performance optimization of pulse detonation engines
by Hasan Zakaria Rouf

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Mechanical Engineering
Montana State University

Abstract:
The Pulse Detonation Engine (PDE) has recently drawn significant attention in the aero-propulsion community for its potential advantages in performance and inherent simplicity over current propulsion concepts. It is an unsteady propulsion device based on the detonation mode of combustion. 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. Numerical modeling has a major role in the development of this technology. This research presents a systematic parametric investigation of PDE performance using an unsteady numerical simulation model which is second order accurate in space and first order accurate in time. The numerical modeling was performed using an automated Java based computational fluid dynamics (CFD) software written with modem objected-oriented programming technique. One- and two-dimensional transient CFD models were employed in a systematic manner to study the propulsive performance characteristic of the PDE under different operating conditions. Effects of PDE combustor length, fill pressure, initial temperature, ambient conditions, and equivalence ratio were examined through numerical simulations. Both uniform and non-uniform fuel-filling schemes were investigated. Systematic computations were also performed to investigate the effects of nozzle length and nozzle expansion ratio.

This study reveals that the addition of a nozzle to the PDE combustor has the potential for a significant improvement in the PDE performance. The obtained results indicate that the presence of a divergent nozzle enhances the impulse generation rate, whereas the presence of a straight nozzle or a convergent nozzle leads to a slower impulse generation. The cycle time was also found to be considerably affected by the nozzle geometry. It was observed that for very high altitude cruises when the ambient pressure is very low, the presence of a nozzle significantly increases the specific impulse of the PDE. The results suggest that a variable geometry nozzle, capable of adapting with the cycle-time and the ambient conditions, is suitable for PDE performance optimization. This study also confirms that the specific impulse can be considerably increased through mixture control; it was found that the use of a leaner mixture dramatically increases the specific impulse of the PDE.

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APPROVAL

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Hasan Zakaria Rouf

This thesis has been read by each member of the thesis committee and has been found to be satisfactory regarding content, English usage, format, citations, bibliographic style, and consistency, and is ready for submission to the College of Graduate Studies.

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF FIGURES–continued

LIST OF FIGURES–continued

LIST OF FIGURES–continued

Figure | Page

NOMENCLATURE

Symbol	Description
A	thrust-wall area
A_{exit}	nozzle exit area
A_{tube}	cross-sectional area of PDE tube
C	frequency factor
C_p	specific heat at constant pressure (per unit mass)
C_v	specific heat at constant volume (per unit mass)
E	total energy
E_{int}	internal energy
$\boldsymbol{F}$	vector of fluxes in x direction
$\boldsymbol{G}$	vector of fluxes in y direction
I	single cycle impulse
Isp	specific impulse
Imp_final	final impulse at the end of a pulse
Imp_max	maximum impulse during a single pulse
Isp_final	specific impulse computed from the final impulse at the end of a pulse
Isp_max	specific impulse computed from the maximum impulse during a single pulse
Iv	impulse per unit volume
k	Boltzmann constant

NOMENCLATURE – continued

k_r	reaction rate
L_{pde}	PDE tube length
L_{nozzle}	nozzle length
m_s	molar mass of specie s
$\overline{M}$	average molar mass
M_{fuel}	fuel mass
N	number of molecules per unit volume
N_s	number density variable of specie s
P	pressure
$\boldsymbol{Q}$	vector of conserved variables
R	gas constant
R_{pde}	radius of PDE tube
R_{exit}	exit radius of nozzle
S	surface area
t	time
T	absolute temperature
u	mean flow velocity (in x direction)
v	mean flow velocity (in y direction)
V	volume
V_{pde}	PDE combustor volume

NOMENCLATURE – continued

Z_s	electric charge of specie *s*
β	fit parameter
θ	activation energy
ρ	density
ρ_s	mass density of specie s
γ	ratio of specific heats
$\bar{\gamma}$	adiabatic index for real gas
$\dot{\omega}_s$	rate of production of specie *s* per unit volume
ν_s	stoichiometric coefficient of specie *s*
η	cycle efficiency

ABSTRACT

The Pulse Detonation Engine (PDE) has recently drawn significant attention in the aero-propulsion community for its potential advantages in performance and inherent simplicity over current propulsion concepts. It is an unsteady propulsion device based on the detonation mode of combustion. 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. Numerical modeling has a major role in the development of this technology. This research presents a systematic parametric investigation of PDE performance using an unsteady numerical simulation model which is second order accurate in space and first order accurate in time. The numerical modeling was performed using an automated Java based computational fluid dynamics (CFD) software written with modern objected-oriented programming technique. One- and two-dimensional transient CFD models were employed in a systematic manner to study the propulsive performance characteristic of the PDE under different operating conditions. Effects of PDE combustor length, fill pressure, initial temperature, ambient conditions, and equivalence ratio were examined through numerical simulations. Both uniform and non-uniform fuel-filling schemes were investigated. Systematic computations were also performed to investigate the effects of nozzle length and nozzle expansion ratio.

This study reveals that the addition of a nozzle to the PDE combustor has the potential for a significant improvement in the PDE performance. The obtained results indicate that the presence of a divergent nozzle enhances the impulse generation rate, whereas the presence of a straight nozzle or a convergent nozzle leads to a slower impulse generation. The cycle time was also found to be considerably affected by the nozzle geometry. It was observed that for very high altitude cruises when the ambient pressure is very low, the presence of a nozzle significantly increases the specific impulse of the PDE. The results suggest that a variable geometry nozzle, capable of adapting with the cycle-time and the ambient conditions, is suitable for PDE performance optimization. This study also confirms that the specific impulse can be considerably increased through mixture control; it was found that the use of a leaner mixture dramatically increases the specific impulse of the PDE.

CHAPTER 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 PDE uses detonation waves that are initiated at the end of a combustor and propagate through a propellant mixture with a supersonic speed and produce very high pressure and temperature to trigger the chemical reactions. Due to the rapid detonation process, nearly constant volume combustion is achieved, which has a higher thermal efficiency than a traditional constant pressure combustion process [Bussing and Pappas (1994)].

The Pulse Detonation Engine is an unsteady propulsion device. It is based on the detonation mode of combustion, which involves the burning of a reactive gas mixture at the 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 operation of the PDE is distinguished from the operation of the steady-state standard rocket engine or turbojet by its cyclic operation. The PDE is an unsteady propulsion device, which operates in an intermittent manner governed by a cycle frequency. Following Eidelman et al. (1991), one complete detonation cycle is comprised of mixture loading, detonation initiation, detonation propagation, and purging of the detonation products. Each process is unsteady in nature and interdependent. The interaction and timing of the interdependent processes are crucial for multi-cycle engine efficiency.

The PDE is expected to become the next generation of aerospace propulsion engines. Following Bussing et al. (1997) and Kim (1999), the thermodynamic efficiency of the pulse detonation engine is higher than that of the traditional constant pressure combustion process, standard in conventional aerospace propulsion engines. It is mechanically simple and cost effective. It is suitable for a wide range of flight Mach numbers, regardless of the engine size and shape. Some of the anticipated advantages of the PDE are (a) higher thermodynamic efficiency, (b) higher specific impulse (lower specific fuel consumption), (c) compactness of engine design due to the capability to operate at a very high energy density,(d) very high operating frequency, (e) high combustion chamber pressure, and (f) high thrust per unit weight.

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 vehicle configuration and ambient environment. Numerical modeling and the use of simplified analytical models can play a major role towards the development of this technology. An intensive numerical effort is currently underway in order to quantify the performance characteristics of the pulse detonation engine. This research presents a systematic parametric investigation of the performance of the PDE using an unsteady numerical simulation model, which is second order accurate in space and first order accurate in time. One- and two-dimensional transient CFD models are employed in a systematic manner to elucidate the propulsive performance characteristics of the PDE over a wide range of operating conditions.

Operating Principle of a Typical Pulse Detonation Engine

The pulse detonation engine operates in a cyclic manner. One complete cycle consists of filling the PDE combustor with unburned propellants, detonation initiation, detonation propagation, and finally exhaust of the combustion products. Figure 1 shows a schematic of a typical air-breathing pulse detonation engine, which consists of a simple straight cylindrical tube. The tube, also called the PDE combustor, is open at one end and closed at the other. At the beginning, fuel and air are introduced in the PDE combustor through the inlet valves. Then the valves are closed and detonation is initiated by electric sparks which in turn produce a large amount of energy near the closed end. After being initiated at the closed end, the detonation wave propagates through the PDE combustor at a supersonic speed. The detonation wave causes enormous rise of pressure and temperature inside the PDE tube which initiates the combustion process. When the detonation wave leaves the PDE tube it is quenched, as there is no fuel outside of the PDE tube. The burned gases are then exhausted, and the momentum of the exhaust gases produces the forward thrust. Detail description of the PDE operation is reported later in Chapter 2.

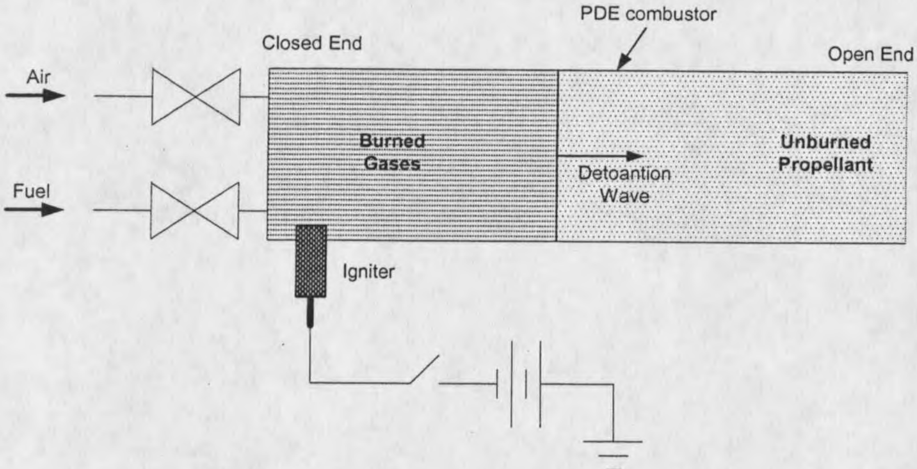

Figure 1. Schematic of a typical air-breathing pulse detonation engine

Background

Eidelman and Yang (1998) reported that Helman et al. (1986) introduced the modern PDE concept in 1986. Subsequently a number of analytical, computational and experimental studies were performed. Performance estimations of the PDE are mostly carried out by the methods of computational fluid dynamics (CFD). The performance estimations by the CFD methods are more accurate than the simplified analytical methods. As reported by Kim (1999), numerical investigations on PDE performance have progressed following the development of computational methods on high-temperature non-equilibrium flows.

Cambier and Adelman (1988) 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 for multiple species and multi-step finite-rate kinetics. The algorithm is second-order accurate in space. A straight cylindrical tube, with a diverging nozzle connected at the aft end of the tube, was considered. Their results indicated that a pulse detonation wave engine can produce a very high specific impulse (of the order 6500 sec). They predicted cyclic frequency 667 Hz. The predicted value of the specific impulse and the cyclic frequency were higher than the experimental observations. The authors identified that a PDWE could be operated in rocket mode with all the oxidizer supply carried on board. In this mode their predicted specific impulse was around 800 sec, which is higher than conventional rocket engines.

Eidelman et al. (1989) performed two-dimensional simulations of a detonation tube using a second-order Godnunov solver on unstructured grids. Their system consisted of a straight cylindrical tube with uniform cross-section with a converging nozzle connected at the aft end of the tube. The detonation was initiated at the open end and it traveled towards the closed end. In case of open end initiation, the pressure developed due to reflection of the wave at the thrust wall is higher than that during a closed end initiation. They concluded that the best performance can be obtained for open-end detonation initiation, i.e. when the detonation wave proceeds upstream to impact on the thrust wall at the closed end of the tube.

Using the same numerical technique, Eidelman et al. (1990) investigated a different configuration with an inlet near the closed end of the PDE tube and no nozzle with the PDE tube. They concluded that for the best performance, the detonation initiation must take place in the vicinity of the exit plane of the chamber resulting in initial propagation of the wave towards the thrust wall. The results indicated that the internal flow processes (detonation, expansion, intake) are directly coupled with external flow processes (shock formation, stagnation point formation etc).

A detailed description of the basic operations of a PDE was provided by Bussing and Pappas (1994). They described the basic physics associated with the operation of a PDE. The authors concluded that a detonation combustion process is thermally more efficient than traditional constant pressure combustions. They performed some preliminary simulations using the *Mozart* quasi-1D CFD code developed by Dr. J.-L. Cambier. One-dimensional computations of the PDE combustion with both hydrogen-oxygen and hydrogen-air mixtures were performed. Both air-breathing and rocket mode operation of the PDE were discussed. The authors considered closed-end detonation initiation using an energetic initiation region adjacent to the closed end.

In a subsequent study performed by Bussing et al. (1994), a comparison between open- and closed-end initiations was provided. The one-dimensional computations showed an equivalent performance between open-end and closed-end detonation initiation. Equivalent impulse generation and fuel efficiency were observed for both cases. The authors recommended only a diverging nozzle at PDE tube end to fully expand the combustion gases to ambient pressure.

Cambier and Tenger (1997) analyzed the effects of different cycling parameters, fueling strategies, and nozzle geometries on the performance of a PDE. Their results indicated that the presence of a nozzle can significantly affect the performance of a PDE. Five different nozzle shapes were studied; the bell shaped nozzle gave better performance than the shapes with positive curvature. Flow dynamics and phase duration were also reported to be affected by the presence of a nozzle. They identified that the multi-cycle estimations can be significantly different from single pulse estimations. For their configuration, closed-end ignition initiation gave better performance than open-end initiation. The same result was reported by Bussing et al. (1994). They identified the need of a computational scheme that is capable of isolating the contribution of the detonation initiation energy for multi-cycle operation. Their results indicated that the cyclic frequency can be increased by proper selection of injection pressure.

Ebrahimi(1999) performed one- and two-dimensional transient CFD computations for evaluating operational performance of PDEs with hydrogen-oxygen propellants. The Generalized Propulsion Algorithm with Chemical Kinetics and Two-Phase Flow (GPACT) computer program was applied to perform the simulations of the unsteady processes associated with a PDE operation. A kinetic model using 8 species and 16 reactions was employed. Methods of detonation initiation were examined. Comparisons between open- and closed-end detonation initiation processes were reported. The results indicate that the open-end detonation initiation results in a rapid establishment of the detonation wave within a shorter distance compared to the closed-end detonation initiation. It was observed that the elevated wall temperature stimulates some reactions near the wall in case of multi-cycle studies. However, in the grid sensitivity study the authors got unacceptable results with very fine grids.

Mohanraj et al. (2000) studied multi-cycle performance of a PDE using a quasi one-dimensional model with a single progress variable equation to represent chemical reactions. Closed-end detonation initiation was considered. Results of a parametric study to investigate the effects of ambient pressure, nozzle, injection pressure, and upstream stagnation pressure were presented. The results indicated that both divergent and convergent-divergent nozzles can improve PDE performance at low ambient pressures. However, at a very low ambient pressure the presence of a divergent nozzle may cause performance deterioration.

Bratkovich et al. (1997) reported an analysis of the PDE cycle. The expansion process of the detonation products was assumed to be isentropic. Based on this assumption the PDE cycle analysis was reduced to the analysis of the Humphrey cycle. The Humphrey cycle is more efficient than the Brayton cycle which is used in conventional rocket engines.

Eidelman and Yang (1998) performed numerical investigations of the pulse detonation engine performance using a Second Order Godunov Method on both structured and unstructured grids. Both fuel-air and fuel-oxygen mixtures were considered as propellant. They indicated that equating the PDE cycle with the Humphrey cycle, as reported by Bratkovich et al. (1997), is an oversimplification that misses the kinetic energy of the detonation products, and does not consider the transient nature of the PDE processes. Their results indicated that the PDE cycle is more efficient than the constant volume cycle. The authors concluded that the PDE cycle can be considered as a valve-less implementation of the constant volume cycle. Their results indicated that a nozzle can significantly increase efficiency of the PDEs.

Zitoun et al. (1999) performed experimental and numerical studies to investigate the propulsive potential of reactive mixtures that use detonative combustion. The experimental setup consists of a straight cylindrical tube as the PDE. The authors computed the specific performance of a multi-cycle pulse detonation engine for various reactive mixtures based on an empirical formula developed from their experimental data. The results indicated that the pressure level inside a PDE combustor is independent of the length to diameter ratio (*l/d*). Moreover, almost linear dependence of maximum impulse levels with the length to diameter ratio (*l/d*) of the PDE was observed. Computational results were obtained by employing a numerical algorithm which is based on the method of the flux-corrected transport (FCT) technique. The experimental and numerical results were in good agreement. The results indicated that the specific performance is independent of the size of the combustion chamber.

Cooper et al. (2001) carried out direct impulse measurements for detonations in a tube, closed at one end and open at the other end, by using a ballistic pendulum arrangement. The results showed a satisfactory agreement with the analytical results reported by the Wintenberger et al. (2001). The effects of various exit treatments on the performance of the PDE were examined. The authors observed that a diverging nozzle had a minor effect on the specific performance and concluded that a straight extension is much more effective than the diverging nozzle in increasing the specific performance. The results suggested an increase in the specific performance if the nozzle length is increased.

Schauer et al. (2001) performed an experimental study to investigate the PDE performance using hydrogen-air fuel. In their experiment the PDE was a cylindrical tube uniformly filled with a hydrogen-air propellant mixture and operated at the cycle rate of

16Hz. Their results indicated that the thrust increases linearly with the frequency. The measured detonation wave speed for stoichiometric hydrogen-air mixture was in excellent agreement with the results of Soloukin (1963). The numerical results in the current research were compared with the experimental results of Schauer et al.

Although analytical methods provide approximate solutions, sometimes they are more suitable for a better understanding of PDE performance. Wintenberger et al. (2001) developed an analytical model for the impulse of a single-cycle pulse detonation engine. The PDE was modeled as a straight tube with a constant cross section; one end of the tube was open and the other end was closed. The results predicted by this model showed satisfactory agreement with the experimental results of Schauer et al. (2001). The specific performances for a wide range of fuel-oxygen-nitrogen mixtures were computed. Effects of equivalence ratio, initial chamber pressure, initial chamber temperature, and nitrogen dilution were investigated. The authors reported that the specific impulse is nearly independent of initial pressure and temperature. The results of Wintenberger et al. (2001) were about 20% lower than the results reported by Zitoun et al. (1999). For stoichiometric hydrogen-air mixture the specific impulse predicted by the analytical model is 4335 sec. The numerical results in the current work were compared with the analytical results of Wintenberger et al.

Endo and Fujiwara (2002) estimated the PDE performance analytically by developing a simple model. It was modeled as a straight tube with a constant cross-section; one end of the tube was open and the other end was closed, and a detonation was initiated at the closed end. Viscous effect and thermal conduction were neglected. They estimated pressure on the thrust wall as a function of time. However, no validation of the analytical model was reported.

Kailasanath and Pantik (2000) performed transient CFD computations for evaluating operational performance of PDEs with hydrogen-oxygen propellants. One major objective of this research was to explore the possible reasons for the differences between various performance predictions. They solved compressible, transient conservation equations for momentum, density, total energy, and number densities of species. A comprehensive kinetic model using 8 species and 48 reactions was employed. In this study the system consisted of a straight cylindrical tube with uniform cross-section, which was modeled with a one-dimensional grid. The authors identified that one dimensional simulations could not model fuel-air mixing properly. Therefore, it was assumed that the detonation tube was filled with a premixed stoichiometirc hydrogen-air mixture. A range of values from 4850 sec to 7930 sec (for different pressure relaxation rates) as the specific impulse for a stoichiometric hydrogen-air mixture was obtained. A key observation of this study is that the choice of initial conditions and boundary conditions may significantly contribute to the overall estimated performance. The results of the study suggested that a higher performance can be obtained if the pressure at the end of the tube gradually relaxes to the ambient value.

Li and Kailasanath (2001) performed two-dimensional, transient numerical simulations to study the flow development in a 1350 mm tube. Conservation equations for mass, momentum, energy, and individual species were solved to analyze the flow field inside a PDE tube. All the diffusive transport processes, like thermal diffusion, molecular diffusion, heat conduction, viscosity, and radiation heat transfer inside the flow field, were neglected. However, it was suggested that for multi-cycle operation the effects of heat transfer through the tube wall are important. Therefore, the effects of diffusive transport processes should be considered. The study was focused on the overall flow development inside a PDE tube. The effects of partial tube fill on the pressure history were also reported. It was concluded that for partial tube filling cases the expansion waves, generated at interface between the reactive propellant mixture and the non-reactive air, can significantly affect the pressure evolution and thrust production. An ethylene-air mixture was found more beneficial than an ethylene-oxygen mixture. The results of this research were confirmed qualitatively by experimental results of Sanders et al. (2000) and Jenkins et al. (2000).

Cambier (1999) presented the results of a numerical study of the performance of a generic pulse detonation rocket engine (PDRE) using the *Mozart* Computational Fluid Dynamics code. Computational methods for dealing with the very high chemical stiffness of high-pressure detonations were presented. A comparison between two-dimensional and quasi-one-dimensional simulations was provided. Nozzle performance was reported to be affected by the ambient pressure. Convergent-divergent nozzles with various throat diameters were examined. The results indicated that the cases with larger throat diameters provide much higher thrusts. It was concluded that the thrust and impulse can be estimated on large time scale by an exponential law. The authors identified the need of evaluating the performance in multi-cycle environment and extending the analysis to a realistic environment where the performance is a function of the ambient pressure.

Sterling et al. (1995) analyzed the performance of an air-breathing pulse detonation wave engine (PDWE) over a wide range of Mach numbers. A computational technique to simulate the unsteady operation of a PDWE was presented. One-dimensional numerical simulations were performed to examine the performance of a PDWE operating for multiple cycles. In the analysis the inlet loss and the diffraction of the shock wave at the combustor exit were neglected (by assuming constant pressure boundary condition at the exit) and ideal detonation initiation was assumed. The authors identified that by using controlled gas-dynamics waves the engine can be configured to provide engine aspiration and charge compression. A specific impulse of 5151 sec for a hydrogen-air system was reported.

Kentfield (2000) presented a simple analytical approach to estimate the idealized performance of an air-breathing, hydrocarbon fueled PDE. In this research the system consisted of a straight cylindrical tube with uniform cross-sectional area. Instantaneous flow cut-off valves were assumed to be located at the ends of the detonation tube. A constant volume combustion process was assumed to model the chemical reactions with in the PDE tube. It was concluded that the PDE performance increases with flight Mach number. Another key observation from this study is that initial charge non-uniformities have negligible effect on PDE performance during static operation.

Kim (1999) reported a numerical model to simulate the time-dependent combustion process in a PDE. An inviscid, two-dimensional numerical scheme coupled to the detailed reaction kinetics of combustion was employed. The governing conservation equations were first discretized using a finite volume algorithm, and a time accurate solution was then obtained by using the Runge-Kutta integration technique. The results of this study were in good agreement with theoretical Chapman-Jouguet data. Different detonation initiation mechanisms were thoroughly examined and the properties of a fully developed detonation wave were found to be independent of the detonation initiation mechanism. A series of shock-induced detonation experiments were performed with a stoichiometric hydrogen-air mixture. The experimental and numerical results agreed well. The numerical results confirmed the postulate that the properties of a fully developed detonation wave are independent of the system geometry whenever the initial conditions and the composition of the fuel-air mixture are the same.

Povinelli and Lee (2001) investigated the effects of flight Mach number on the relative performance of PDE and gas turbine engines. The effects of compression on the inlet temperature and the subsequent sensible heat release were also examined. The results indicated a significant performance benefit during static operation over the gas turbine engine with compression ratio less than 4. They identified that the reduction of sensible heat release due to dissociation of reacting species caucuses a decrease in the PDE performance. The authors indicated that the PDE may be more suitable for combined cycle applications.

Ebrahimi et al. (2002) presented three different levels of analysis to investigate the performance characteristics of a PDE. The results using the three different models (zero-dimensional, one-dimensional, and two-dimensional) mutually supported each other and provided a better understanding of system performance. It was observed that at vacuum conditions the performance of a PDE is similar to that of a rocket engine and at finite backpressures, when the pressure inside the PDE is equal to that in the rocket, the rocket gives better performance than the PDE.

Currently, extensive research is being done at The University of California at Los Angeles guided by Dr. A. R. Karagozian. Mathematical and numerical models have been developed. The research is focused on higher order numerical simulations of the generic PDE configuration with simplified chemical reaction kinetics, so that rapid and straightforward estimates of engine performance can be obtained. Both one- and two-dimensional simulations of the high speed reactive flow phenomena are performed and compared to determine the applicability of one-dimensional simulations for performance characterization. Characteristic engine performance parameters and engine noise estimates within and external to the detonation tube are being investigated.

Motivation

The design and optimization of a PDE propulsion system are difficult, due to the unsteady nature of the propulsion cycle. Numerical modeling can play a significant role towards the development of this technology. A number of computational, analytical and experimental studies were performed to estimate the performance of the PDE. However, the concept of PDE suffers from lack of systematic numerical, experimental, and theoretical studies. As reported by Kaliasanath et al. (1999), there are some disagreements between different performance predictions. For example, the predictions of the specific impulse for a hydrogen-air mixture, reported by different researchers, significantly varied. Sterling et al. (1997) predicted an average value of 5151 sec as the specific impulse for a for a stoichiometric hydrogen-air mixture. Whereas, for the same mixture Bussing et al. (1997) obtained a range of values of 7500 – 8000 sec and Winterber et al. (2001) estimated a value of 4335 sec. Meanwhile, based on experimental results Schauer et al. (2001) reported a specific impulse of 4024 sec for a hydrogen-air system.

A nozzle may significantly affect the performance of a PDE. The optimal PDE nozzle design has yet to be developed. Eidelman and Yang (1998) reported that the addition of a diverging nozzle with a PDE tube can significantly improve the PDE performance. In contrast, based on experimental investigations, Cooper et al. (2001) reported that addition of a diverging nozzle has negligible effect on the PDE performance. Mohanraj et al. (2000) reported that the effect of a diverging nozzle is detrimental at around 1 atm ambient pressure. On the other hand, the results of Eidelman et al. (1998) indicated that at 1 atm. ambient pressure the presence of a divergent nozzle can improve the PDE performance.

Research varies in terms of conclusions regarding open-end and closed-end detonation initiation. There seems to be two schools of thoughts regarding the location of the igniter. In the numerical investigation performed by Cambier and Tenger (1999), the open-end detonation initiation gave better performance than the closed-end initiation. On the other hand, Eidelman et al. (1989) identified the closed-end initiation process to be better than the open-end initiation process. The results of the computational study performed by Busssing et al. (1994) indicated that neither initiation scheme offered a clear performance advantage. As discussed by Kailasanath et al. (1999), the disagreements between different studies could be due to a range of factors, for instance the geometry of the specific system, boundary conditions, initial conditions, model assumptions, detonation initiation mechanisms etc.

Although nozzles can significantly affect the performance of a PDE, the requirements for the optimal nozzle are not well understood. Only few investigations have been performed on different nozzle geometries. Therefore, it is important to systematically investigate the nozzle effects on PDE performance. For practical implementation of a PDE, it is very important to simulate the performance of a PDE at different altitudes and ambient pressures. However, only a few studies have been aimed at the effects of the ambient condition on the PDE performance. It is not necessarily advantageous to have a stoichiometric propellant mixture over the entire PDE combustor; the specific fuel consumption can be considerably reduced by an optimum fueling strategy. Sufficient information is not available regarding different fueling schemes. Only a few investigations have been done to observe the effects of initial conditions.

Although numerical analysis of the PDE performance dates back almost two decades [Kalaisanath et al. (1999)], there is a lack of systematic and balanced numerical studies. Additional studies are required to establish the role and performance of a PDE in aerospace applications. To get a better and clearer understanding of PDE operational characteristics, a systematic evaluation of the PDE performance is necessary. The primary objective of this research was to elucidate the propulsive performance characteristics of the PDE over a wide range of operating conditions. The results of a systematic numerical investigation of the PDE performance characteristics have been presented here. PDE performance characteristics were studied over a wide range of operating conditions. The study was performed with an automated Java based CFD software designed with modern object oriented programming techniques. The level of grid resolution and modeling complexity can be varied for each engine component for maximum flexibility and accuracy. One-dimensional and two-dimensional unsteady CFD computations were carried out to get realistic approximations of the unsteady processes of the PDE operation. The numerical scheme used here is second-order accurate in space, total variation diminishing (TVD), and first order accurate in time. Details of this numerical scheme are discussed later.

The Scope of the Current Work

The objective of the work is to utilize Java based automated object-oriented software to perform the parametric investigation for performance optimization of the PDE. The CFD software *Cafe-Vienna*, developed by Dr. J.-L. Cambier, is designed with modern object-oriented programming techniques and implements procedures for automatic cycling. One-dimensional and two-dimensional transient CFD computations were employed to estimate the performance of the PDE. The focus of the study is directed at assessing the overall PDE performance characteristics in a wide range of operating conditions. A systematic study of the performance characteristics of a generic PDE was performed.

The present model is validated by comparing the calculated specific impulse and impulse per unit volume with experimental and analytical results. Computational grid sensitivity was investigated to set the background for the study. Pressure scaling and length scaling were performed. For different conditions of single cycle operation, specific impulse and impulse per unit volume, impulse history, and thrust history were computed and presented.

Computations were performed to investigate the effects of initial temperature, initial pressure, ambient condition, and equivalence ratio. Both uniform and non-uniform fuel filling schemes were investigated. Computations were performed to estimate effects of air temperature in the non-combustion section of the PDE tube in case of partial tube filling. The PDE performance for different ambient pressures was computed. Effects of different nozzle geometries (convergent nozzle, divergent nozzle, straight nozzle, and convergent-divergent nozzle) were studied. Systematic computations were performed to investigate the effects of nozzle length and nozzle expansion ratio.

CHAPTER 2

BASIC CONCEPTS OF A PULSE DETONATION ENGINE

Deflagration and Detonation

Deflagration and detonation are two different modes of combustion in which waves can be propagated in the form of a chemical reaction in an explosive gas mixture. Following Bussing et al. (1994) and Kim (1999), deflagration is a combustion wave that propagates at a subsonic speed. In this mode of combustion process, the chemical reaction propagates at relatively low flame speed of the order of one meter per second. Due to a small decrease in pressure in this mode of combustion, the process can be modeled as a constant pressure process. The laminar or turbulent molecular diffusion of the gas mixture has a significant role in governing the propagation of the detonation wave. This type of combustion process leads to a net decrease of pressure and fluid density.

Detonation is a combustion wave propagating at a supersonic speed. This is a very energetic and violent phenomenon and results in extremely large increases in pressure and temperature. Following Zeldovich (1960) and Bussing et al. (1994), a detonative combustion process can be characterized by a very rapid propagation of explosive chemical reactions. Due to the high speed, this mode of combustion can be modeled as a constant volume process. Unlike the deflagration process, heat conduction and molecular diffusion have a negligible contribution to a detonation process. Energy transfer is mainly governed by the mass flow in a strong compression wave. A detonative combustion process results in an increase in both the pressure and the fluid density.

A detonation wave can be approximated as a strong shock. It can be considered as a discontinuity in the gas flow where heat addition occurs. When the detonation front propagates into the unburned gas mixture in the form of a strong shock at a supersonic speed, there is an enormous rise of pressure and temperature in the gas mixture. The temperature is increased by the compression due to the strong shock. This very high pressure and temperature initiate chemical reactions which proceed violently and give off heat at an explosive rate. The moving shock gets energized by the energy released in the chemical reactions. Eventually a self-sustaining detonation wave is formed. The analysis of a detonation process is based on the equations of conservation of mass, momentum and energy, the equation of state, and chemical kinetics of combustion. [Zeldovich (1960), Kim (1999)].

Basic Engine Operation

The Pulse Detonation Engine is an unsteady propulsion device, which operates in a cyclic manner. The PDE cycle can be described according to the fundamental processes that occur during a cycle. Following Eidelamn et al. (1991) and Bussing et al. (1994), one complete detonation cycle consists of the following processes:

1. Filling of the PDE tube with propellant mixture
2. Detonation initiation
3. Detonation propagation along the tube

4. Exhaust of the detonation products to the atmosphere

These processes are interdependent, and the engine efficiency depends on the timing and interactions between these interdependent processes. The total time required to complete all the processes of a detonation cycle is called the cycle time, and the inverse of the cycle time is called the cyclic frequency.

The PDE tube, closed at the left end and open at the right end, is initially filled with a combustible gas mixture. To start the detonation process a detonation initiation zone is set adjacent to the closed end of the PDE tube. Pressure and temperature in that small zone are set sufficiently high to initiate the detonation. After being initiated at the closed end, the detonation wave propagates through the PDE tube. The strong shock from the detonation propagates at a few thousands meters per second relative to the unburned propulsion mixture. Very high pressure and temperature are developed due to the compression by the shock wave; this triggers the combustion process. Energy released from the combustion supports the detonation wave to travel and eventually a self-sustained detonation wave is formed.

When the detonation wave leaves the PDE tube, rarefaction waves are generated at the open end due to the pressure difference at the tube-exit. The rarefaction waves proceed towards the closed end of the combustor and expel the combustion products, thereby, thrust is produced. Intake of fresh combustible mixture begins after chamber pressure falls up to refill level.