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A Numerical Study of Detonation and Plume Dynamics in a Pulsed Detonation Engine

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Abstract

The Pulse Detonation Engine (PDE) is considered to be the propulsion system of future air vehicles. The objective of the present study is to understand the variation in the external flow field of a PDE during take-off and cruise conditions. To do this, the underlying concept of a PDE, namely, detonation is simulated using finite-rate chemistry. Performance of four chemical mechanisms in predicting detonation quantities is evaluated. The global mechanisms predict the detonation quantities with the least error, and are used for simulating detonation in a PDE. Comparative analysis of the plume dynamics for different equivalence ratios reveals a similar trend in the temperature distribution for both mixtures, but not in the pressure distribution. A sub-atmospheric zone is identified, which is largely responsible for the blowdown process. The analysis of the external flow field provides guidelines for the optimum placement of the turbine in the case of a Hybrid PDE.
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Nomenclature

ρ – Density
E – Energy
q – Heat from reaction
P – Pressure
u – Velocity in x-direction
v – Velocity in y-direction
h - Enthalpy
t – Time
Y – Mass fraction
R – Rate of reaction
S - Entropy
A – Pre-exponential factor
E_A – Activation energy
T – Static Temperature
n – Temperature exponent
R – Universal Gas Constant
γ – Specific heat ratio
Δx – Grid density in the axial direction
ϕ – Equivalence Ratio
M – Mach Number
**Subscripts**

i – No. of species

cj – CJ conditions

u – upstream of shock

d – downstream of shock

S – Stoichiometric Mixture

L – Lean Mixture
Chapter 1

Introduction

The need for faster flight, coupled with the desire to conserve resources, has propelled man’s inventive thinking into realms beyond imagination. Since the days of the Wright brothers, aircraft propulsion has come a long way. The invention of the gas turbine, and decades of research on it, has made the gas turbine a very effective source of power, with very high fuel efficiency. The introduction of ramjet engines propelled airplanes to break the sound barrier with ease. The latest in propulsion is the scramjet engine, where the design of a ramjet was improved to reduce losses from the shock waves resulting from the supersonic inlet of air. This improved design led to the historic X-43A hypersonic flight in March 2004. Both these propulsion systems require auxiliary systems for take-off as they require a supersonic inlet of air.

An advanced propulsion system that is being researched is the Pulse Detonation Engine. This system has the ability to take-off without any auxiliary propulsion system and to cross the hypersonic barrier using less fuel. Because many such advantages, which are discussed later, the Pulse Detonation Engine is a very attractive option for aircraft propulsion. Although the concept has been around for more than half a century, its feasibility to perform like the present conventional propulsion system is limited by many factors such as acoustics, vibrations and material properties. These factors are still being investigated to make the Pulse Detonation Engine a viable option as a conventional propulsion system. So, what motivated the present study?
1.1 Motivation for the Present Study

The Pulse Detonation Engine (PDE) is being studied by many researchers worldwide as it is highly scalable, and produces thrust based on the concept of a detonation wave propagating inside a tube and exiting out of it. The PDE can either be used in the stand-alone mode or in the hybrid mode, where it is integrated with a compressor and a turbine. In the later arrangement, the PDE offers advantages such as providing work for pressurizing the fuel and generating electricity for aircraft components. Numerical simulations complement experiments, and are a very useful tool in the validation of any conceptual design. Information on the external flow field is important for design of better stand-alone and hybrid PDE systems. The complete flow process cannot be quantified by experiments due to limitations of the measurement devices. To overcome this and to provide in-depth understanding of the underlying physics of the combustion process and external flow field of a PDE, accurate numerical simulations are necessary. In order to perform these simulations, we first need to understand the operation of the PDE, Hybrid PDE and their underlying concept, namely, detonation.

1.2 Pulse Detonation Engine (PDE)

The basic operating principle of a PDE, its underlying concept, advantages and limitations are described in Sections 1.2.1 and 1.2.2. Section 1.3 discusses the integration of a PDE with a turbine, and describes the advantages of such integration.
1.2.1 Operating Cycle of a PDE

A single cycle of operation of a Pulse Detonation Engine is shown in Fig. 1.1. The PDE is a simple tube, closed at one end with a rotary valve and open to the atmosphere at the other end. This high-thrust air-breathing engine works on the concept of a detonation wave propagating from the closed end to the open end and exiting out of the detonation tube. The sequence of events has been discussed in detail by Bussing and Papas (1994), Lynch and Edelman (1994), and He and Karagozian (2003), and is outlined in Fig 1.1.

The events in each step are described below:

i. The rotary valve or the hydrodynamic valve (dashed line) is opened.

Figure 1.1 Generic PDE Cycle
ii. The tube is filled with fuel and oxidizer mixture.

iii. The valve is closed (solid line), forming a one-end closed tube.

iv. The premixed mixture of fuel and oxidizer (solid color) is ignited at the closed end with a spark ignition system (dark color).

v. Combustion occurs, and the temperature and pressure start to increase, resulting in a detonation wave. The detonation wave transforms to a self-sustained detonation wave followed by rarefaction waves.

vi. The wave exits out of the tube and expands into the atmosphere as a plume. An expansion wave is reflected from the open end towards the closed end and creates a low pressure in its downstream, causing the products of combustion to be expelled out. This process is called ‘blowdown’ process of the PDE cycle.

vii. The expansion pressure wave is reflected from the closed end, and this causes further lowering of pressure, which helps in re-filling of the tube with the fuel and oxidizer mixture.

Hence we can summarize the PDE cycle into four stages, namely,

- Fuel filling
- Spark ignition
- Detonation propagation
- Blowdown

Now that we understand the operation of a PDE, it is easy to identify its advantages and limitations.
1.2.2 Advantages and Limitations of a PDE

The description outlined in the previous section shows that the working of a PDE is very simple, and does not involve any moving parts except for the valve.

The second advantage stems from the fact that the PDE uses supersonic combustion (detonation) instead of sub-sonic combustion (deflagration). Deflagration, the most widely used form of combustion for production of thrust, is a constant pressure heat addition process; on the other hand, owing to its short time of heat addition, detonation is approximated to be the most efficient constant volume process. Production of thrust by detonation is more efficient than deflagration in air-breathing engines. This has been shown by the earlier studies of Eidelman and Yang (1998), Heiser and Pratt (2002) and Wu et al. (2003).

The third advantage of the PDE system is that it is highly scalable, which means that, more the number of PDE tubes, more the thrust produced. Also, thrust is found to increase linearly with the frequency of operation as shown by Mawid et al. (2002).

Although the PDE offers many advantages there are certain limitations at present which do not allow its use as a conventional propulsion system. The acoustics from the detonation process is considered to be a major issue in a PDE for practical applications, as the sound level is about 190 decibels, shown by Allgood (2004), which is much higher than the limits of human audible comfortness. Integration of the PDE arrangement with an airframe is also being researched due to the amplitude and frequency of vibration produced. The open end is prone to thermal cracking, as shown by Schauer et al. (2001) after a sufficiently long period of operation, due to thermal fatigue.
The Hybrid PDE offers many more advantages as compared to the stand-alone operation of a PDE and they are described next.

1.3 Hybrid PDE

An alternative to using the PDE chambers in a stand-alone mode (pure PDEs) for production of thrust is to integrate it with the conventional gas turbine engine (Hybrid PDEs). This concept is of recent interest. The PDE can be integrated with the turbine in two ways. In the first method, as shown in Fig. 1.2a, the PDE is arranged concentrically with the combustor. In the second method, as shown in Fig. 1.2b, the combustor, high pressure compressor and high pressure turbine is replaced with the PDE tubes in an annular arrangement. Studies by Rasheed et al. (2004) and Schauer (2003) have shown that it is possible to extract work by placing a turbine downstream of a PDE. However, when a turbine blade is exposed to a strong shock wave from the PDE, issues such as back pressure affect the blowdown time, and subsequently, the frequency of operation of the PDE.

a) PDE in addition to Gas Turbine Combustor
To study about PDEs and Hybrid PDEs, it is important to understand the concept of detonation. Hence the next section deals with the introduction of detonation and Section 1.5 deals with the analysis of detonation waves.

1.4 Fundamental Concept of a PDE - Detonation

To understand the operation of a PDE, it is essential to understand its fundamental concept, namely, detonation. Detonation is defined as a shock wave propagating at supersonic velocities; the detonation front propagates into unburned gas at a velocity higher than the speed of sound, and is sustained by the energy released by the combustion process. As the traveling detonation wave is supersonic, the gas ahead of the detonation remains undisturbed. The chemical process releases energy and triggers a volumetric expansion of the burned gases which drives the shock wave. Thus, detonation is due to the confluence of hydrodynamic and thermo-chemical processes. A detonation wave in which there is a strong interaction between these processes is said to be self-sustaining or
self-supporting. Although the actual detonation wave is complex, it can confirm to simplified analysis which are presented in the next section.

### 1.5 Analysis of Detonation Waves

Although the actual structure of a detonation wave is highly three-dimensional with convex segments and resulting transverse wave structures as shown in Fig. 1.3, because of its high gradient in the propagating direction, simplified analysis can be performed to study the detonation wave.

![Figure 1.3 Actual Detonation Structure (Wintenberger, 2004)](image)

Two such analyses are the Chapman-Jouguet (CJ) theory, which is a thermodynamic analysis presented by Chapman (1899) and Jouguet (1905), and the ZND theory proposed independently by Zeldovich (1940), von Neumann (1942) and Doering (1943).
1.5.1 Thermodynamic Analysis of the Detonation Wave – CJ Theory

The Chapman-Jouguet (CJ) theory is a thermodynamic analysis relating the flow properties upstream of the combustion wave to those downstream of it. Deflagration and detonation waves are treated as discontinuities where heat addition occurs. To explain the CJ theory, the Rayleigh line and the Hugoniot curve, along with regions in the Rankine-Hugoniot curve are described. These relations are discussed in detail in order to explain the various burning regimes. If there are no temperature or species concentration gradients at the upstream and downstream points, the following assumptions help in making a thorough thermodynamic analysis,

- Steady and one-dimensional flow
- Constant area
- Ideal-gas behavior
- Constant and equal specific heats
- Negligible body forces
- Adiabatic conditions

With the above mentioned assumptions, the conservation of mass, momentum, and energy equations are applied to the control volume shown in Fig. 1.3.

These equations are written as

$$\rho_u V_u = \rho_d V_d$$

(1.1)
The sequence of states at the downstream with fixed upstream parameters, for which Eqns. 1.1 and 1.2 are satisfied, is referred to as the Rayleigh line. The Rayleigh relationship can be obtained from simultaneous solution of the continuity and momentum equations. The Rayleigh line, which relates the initial to the final states, is given by

\[ p_d - p_u = -m^2 \left( \frac{1}{\rho_d} - \frac{1}{\rho_u} \right), \]  \hspace{2cm} (1.4)

\[ p_d - p_u = -\left( \rho_u v_u \right)^2 \left( \frac{1}{\rho_d} - \frac{1}{\rho_u} \right). \]  \hspace{2cm} (1.5)

When the conservation of energy has to be satisfied in addition to the conservation of mass and momentum, we obtain the Rankine-Hugoniot relationship which is,

\[ h_d - h_u = -\frac{1}{2} \left( \frac{1}{\rho_d} - \frac{1}{\rho_u} \right)(p_d - p_u) \]  \hspace{2cm} (1.5)

On Simplification, we get

\[ \frac{\gamma}{\gamma - 1} \left( p_d v_d - p_u v_u \right) - \frac{1}{2} (p_d - p_u)(v_d - v_u) - q = 0. \]  \hspace{2cm} (1.6)

This equation relates the thermodynamic properties across a discontinuity. The Hugoniot equation determines the locus of the possible solutions for downstream properties for a given upstream condition and energy release.
It is customary to plot the Hugoniot on a pressure-specific volume diagram. Figure 1.4 shows the Hugoniot curve with and without energy release for a fixed value of pressure and specific volume (represented by 1), which is the condition at the upstream.

The points where the Hugoniot curve and Rayleigh line are tangential to each other are called the Chapman-Jouguet (CJ) points. There are two CJ points on the Hugoniot curve, the upper CJ point (CJ_U) and the lower CJ point (CJ_L), located respectively where the Raleigh line is tangential to the Hugoniot curve on the detonation and deflagration branches. These points divide the Hugoniot into five regions as shown in

<table>
<thead>
<tr>
<th>Segment of Hugoniot Curve</th>
<th>Characteristics</th>
<th>Burned Gas Velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Region A</td>
<td>Strong Detonation</td>
<td>Subsonic</td>
</tr>
<tr>
<td>Region B</td>
<td>Weak Detonation</td>
<td>Supersonic</td>
</tr>
<tr>
<td>Region C</td>
<td>Does not satisfy Rayleigh and Hugoniot relations</td>
<td></td>
</tr>
<tr>
<td>Region D</td>
<td>Weak Deflagration</td>
<td>Subsonic</td>
</tr>
<tr>
<td>Region E</td>
<td>Strong Deflagration</td>
<td>Supersonic</td>
</tr>
</tbody>
</table>

Table 1.1 Physical Phenomena Associated with Various Segments of the Hugoniot curve
Let us start with Region C. Since any real process going from upstream to downstream conditions should satisfy the Rayleigh and Hugoniot relations (Eqs 1.5 and 1.6), Region C does not represent real solutions, as it does not satisfy both relations. Between the points B and D, no valid Rayleigh line can be drawn.

The solutions located in Regions A and B correspond to supersonic waves (detonations). For detonations, gas dynamic considerations are sufficient to determine the propagation speed, independent of the actual structure of the wave. These considerations were independently made by Chapman (1899) and Jouguet (1905), who proposed that detonations travel at one particular velocity, which is the minimum velocity for all the solutions on the detonation branch. Chapman (1899) postulated that at such a solution point, the Hugoniot curve and the Rayleigh line were tangential.

Region A corresponds to strong detonations (supersonic flow to subsonic) but these are observed only in the transient state or if there is an effective piston created by the flow following the wave. In this case the burned gas is sub-sonic from the frame of reference of the wave. They are unstable because rarefaction waves that are formed due to friction, heat loss, turbulence etc. propagating behind the detonation wave will catch up with the detonation front and move the solution point towards CJ\textsubscript{U}. At the upper CJ point the burned gases are sonic relative to the wave and the detonation wave travels at a constant velocity. Thus, for supersonic waves (Region A), there is one special solution, CJ\textsubscript{U}, that is singled out from a thermodynamic point of view. Region B corresponds to weak detonations, as the burned gases travel at supersonic speeds, which tend to overtake the detonation wave.
Solutions of the Hugoniot curve located in Regions D and E correspond to subsonic waves (deflagrations). For deflagrations, the actual propagation speed is determined from the structure of the combustion wave and turbulent and diffusive transport processes. Region D corresponds to weak deflagrations (subsonic) and encompasses the laminar flame solutions. Region E corresponds to strong deflagrations (subsonic to supersonic flows). However, in a constant-area duct, it is not possible to have heat addition and to proceed past the sonic condition. Thus, Region E is not a physically possible region of steady solution and is ruled out.

An analysis of the entropy at the upper and lower CJ points show that minimum entropy exists at the upper CJ point and maximum entropy exists at the lower CJ point (Fickett and Davis, 1979). This shows that the detonation process has higher thermodynamic efficiency than deflagration.

One of the important outcomes of the CJ theory is the definition of detonation velocity. With the assumption that pressure of burned gases is much greater than that of unburned mixture, the detonation velocity \( v_D \) is defined as the velocity at which the unburned mixture enters the detonation wave for an observer riding with the detonation (Fickett and Davis, 1979). One of the main outcomes of the CJ theory is the calculation of the velocity of the propagating detonation wave \( U_{CJ} \). Experimentally measured detonation velocities are typically found to be within 2% of the theoretical CJ velocity (Wintenberger, 2004).

For a CJ detonation in a perfect gas, analytic solutions for the CJ\textsubscript{upper} point may be obtained assuming different values of the specific heat ratio and the perfect gas constant in the reactants and products. The downstream temperature is related to the upstream
temperature by the relation obtained from solving the governing equation for energy with
the use of conservation of mass and the definition of velocity of sound.

\[
T_d = \frac{2\gamma_d}{\gamma_d + 1}\left(\frac{c_{p,u}T_u + q}{c_{p,d}}\right)
\]

(1.7)

The detonation velocity, \(v_D\), is defined in this case as:

\[
v_D = \sqrt{2(\gamma_d + 1)\gamma_d R_d\left(\frac{c_{p,u}T_u + q}{c_{p,d}}\right)}
\]

(1.8)

An even more approximate method of obtaining the detonation velocity is to use constant
specific heat assumptions for both upstream and downstream conditions. In this case the
obtained detonation velocity is given by:

\[
v_D = \sqrt{2(\gamma + 1)\gamma R_d\left(T_u + \frac{q}{c_p}\right)}
\]

(1.9)

When the downstream properties are those of CJ conditions, Eq. 1.8 can be re-written as

\[
U_{CJ} = \frac{\rho_{CJ}}{\rho_u} \sqrt{\gamma_{CJ} R_{CJ} T_{CJ}}
\]

(1.10)

### 1.5.2 One-Dimensional Analysis of the Detonation Wave – ZND Theory

The CJ theory provides a thermodynamic analysis of the detonation wave and
does not account for the chemical reactions that occur behind the shock wave in a
detonation or the structure of a detonation wave. Zel'dovich (1940), von Neumann
(1942), and Doering (1943) independently arrived at a theory for the structure of a one-
dimensional detonation wave. They proposed that the detonation wave can be modeled
as a shock wave coupled with a reaction zone. Their proposed structure is shown in Fig.
1.5. As reactive collisions cannot occur in the region of the shock, the reactions take
place in the region behind the shock. Although the structure of a detonation wave is highly three-dimensional with convex segments and resulting transverse wave structures as shown in Fig. 1.3, the ZND model’s idea of a shockwave followed by a reaction zone is useful.

Chemical reactions are initiated at the von Neumann State, a state corresponding to the maximum pressure and temperature. There exists an induction zone, a region just after the shock which is characterized by the generation of radicals in chain-branching reactions and is usually thermally neutral. After the induction period, the temperature rises due to the energy release caused by the reaction, while the pressure and density decrease due to the expansion of the hot products. This expansion maintains the strength of the leading shock front. The reaction zone, which encompasses the induction and energy release zones, terminates at the Chapman-Jouguet plane, where chemical equilibrium is reached and the flow velocity is sonic relative to the shock wave (Williams, 1985). The ZND model accounts for the finite-rate chemical kinetics behind the shockwave. Detailed chemical mechanisms or simplified mechanisms can be used to capture the chemistry occurring in the reaction zone.

Figure 1.6 ZND Model of a Detonation Wave (Hsu et al. 2000)
1.6 Organization of the Thesis

The present work is broadly organized into four other chapters. Chapter 2 describes the past research available in the literature, and establishes the need for the present study. Chapter 3 defines the numerical methodology employed. Chapter 4 provides information on the chemical kinetics, and the chemistry of hydrogen-air combustion. Chapter 5 presents the results and discussion. Chapter 6 concludes the thesis by summarizing the contribution of the current study, and provides direction for future work.
Chapter 2

Literature Survey

This section highlights some of the past research on the modeling of detonation and simulation of flow process internal and external to a Pulse Detonation Engine. Section 2.1 provides information on one-dimensional detonation simulations and validation of reaction mechanisms for simulation of detonation. Section 2.2 through 2.5 reviews various experimental and numerical studies performed to study flow process in PDEs and Hybrid PDEs. This literature survey is intended to provide the necessary background information and also establish the specific objectives of the present study.

2.1 Modeling of Detonation

Numerical modeling of the time-dependent one-dimensional detonation wave has been performed by many researchers in the past. One of the earliest studies is of Fickett and Wood (1966), who investigated the stability of the steady-state solution of a detonation wave. They found the shock-pressure to oscillate about the steady-state solution with a peak pressure nearly 50 % higher. They found good agreement with the linearized stability analysis of the steady detonation of Erpenbeck (1964).

Saint-Cloud et al. (1972) observed pulsating detonation waves in tubes with a square-wave cross-section. When the induction zone was resolved, the detonation wave
was found to fail and decompose into a shock and a flame. The detonation was re-ignited again after resolving the induction zone and it failed once again.

Sharpe and Falle (1999) used a uniform grid until the qualitative nature of the solutions had converged. They concluded that even to obtain qualitatively correct solution, the resolution had to be increased drastically. Under resolving the reaction zone was found to give spurious solutions. Sharpe and Falle (2000) used an adaptive grid to facilitate study of the detonation for a longer time. They observed that the numerical perturbation in the induction zone is determined by the grid size. They found when this induction zone is not resolved properly; they found an almost reactionless induction zone followed by a thin fire. Because of this they stressed that the induction zone must remain fully refined.

Hwang et al. (2000) simulated the pulsating overdriven detonation wave with single step reaction kinetics. They studied systematically the effect of computational domain size, reaction zone resolution, initial condition and numerical methodology on the detonation wave. They identified that the reaction zone has to be resolved by at least 40 points per reaction zone length.

Yungster and Radhakrishnan (2004) simulated one dimensional detonation using a detailed finite rate chemistry model. They analyzed an over-driven detonation for an equivalence ratio of 0.4 to 2.0 and initial pressure from 0.2 to 0.8 atm. They found qualitative agreement with the numerical simulation of McVey and Tong, but the frequencies obtained from their theory are much higher especially for near stoichiometric mixtures at high pressures. They found better agreement when they modified the original theory to include the effects of a more realistic chemistry.
Some of the other researchers who have used a single, irreversible reaction with an Arrhenius form of reaction rate to study one dimensional detonation are Abousief and Toong (1982) and He and Lee (1995).

Cuttler et al. (1998) carried out a comparative study of different finite-rate reaction mechanisms of hydrogen-air in the temperature range of 700 to 1200 K and a pressure range of 0.5 to 2 atm, to simulate shock-induced combustion and the resulting flow-field over a blunt projectile. They studied eight different complex chemical mechanisms including the 32-step model of Jachimowski (1988), 7-step model of Shang et al. (1995) and 8-step model of Moretti (1965). They found that the final temperature predicted by all the models were the same. In their study, they found the 7-step model to predict the exact heat release and the best interaction between the pressure and reaction rates, and thus produce the best match to experimental results. They state that the accuracy of computation in high-speed reacting flows is affected by the ability of the kinetic model to duplicate the chain branching and terminating reactions. They also found that the 32-step model had a shorter reaction time because of the sudden increase in the induction time due to the modeling of the second explosion limit. They also observed that viscous effects had insignificant impact on the prediction of the shock and reaction front.

Law et al. (2002) reviewed the state of the reaction mechanism development in the simulation of combustion phenomena. They demonstrated the inadequacy of the 1-step global reaction and stressed the need for comprehensive kinetic mechanisms. They defined a comprehensive kinetic mechanism as that mechanism which can describe all classes of combustion phenomena and over all possible ranges of thermodynamic and
system configurations. They explained in detail, the hydrogen-air explosive
ccharacteristics. They stressed that eliminating Nitrogen chemistry will suppress the
catalyzing effect of NO on ignition. They also emphasized in defining the relation of the
transport properties to the diffusion of the free radicals in accurate simulation of the
combustion phenomena.

Yu et al. (1998) presented a theoretical model of the governing equations for
reactive flows. Their emphasized that any special treatment to the stiff source terms in
the species equations without fully resolving the space and time scales of the source
terms will provide numerically stable solutions to show the general trend but will not
show the detailed flame structure.

Jachimowski (1988) presented the optimized 33-step kinetic mechanism for the
combustion of hydrogen-air mixture. The mechanism was assembled by observing the
behavior of the reactive species from shock tube data and flame studies. This mechanism
was found to be capable of satisfactorily reproducing experimental data for different
Mach numbers (M =8, 16 and 25). At different Mach numbers, it was found that
different parts of the reaction controlled the combustion process.

Hsu and Jemcov (2000) conducted a numerical investigation of global, reduced
and complex chemical mechanism in the simulation of a self-sustained detonation. They
analysed the global reaction mechanism of Varma et al.(1986), 7-step model of Shang et
al. (1995), 38-step model of Vajda et al. (1990). They modified the Arrhenius parameters
of the 2-step mechanism, originally proposed by Rogers and Chinitz (1983) to make the
model numerically less stiff for use in the numerical code. They studied a hydrogen-air
mixture at an equivalence ratio of 0.44 to test the induction time captured by the different
mechanisms. They found a good agreement in the computed detonation velocity to the experimental results of Kistiakowsky and Kydd (1956).

Sekar et al. (1998) used a commercial code CFD++ to study 1D, 2D, axisymmetric simulations in terms of detonation wave speed, von-Neumann spike, aspiration, pressure-time history and sequence of cycle events. They emphasized careful treatment of the source term by considering the minimum temperature in the neighbourhood of each computational grid point. This helps in predicting the correct wave speed as well as resolving the von-Neumann pressure spike. When the back pressure to be imposed was smaller than the pressure at local sonic condition, then that value of pressure was used as the back pressure. They used a finite-rate chemistry method with 1-step mechanism of hydrogen-air and ethylene-air mixture in their studies for evaluating the chemical source terms.

2.2 Research on PDE

Bussing and Papas (1994) elucidated the detailed working of a PDE. They performed a 1D simulation of hydrogen-air mixture using a 7-species, 18-step mechanism which neglected the effect of intermediates. They also studied the PDE in the rocket mode of operation by reducing the ambient pressure to 0.04 atm. They observed that the rocket mode operation results in higher post-detonation pressure in the chamber than in the air-breathing mode.

Kailasanath (2000) had reviewed the varied applications of detonation in the field of propulsion. In this work, he discusses the different types of detonation such as standing normal detonations, intermittent or pulsed detonations, rotating detonations and
oblique shock induced detonations. He also compared the efficiencies of the detonation cycle with constant pressure and constant volume cycles. He found that the detonation cycle had an efficiency of 49% whereas the constant pressure and constant volume cycles had efficiencies of 27% and 47% respectively. In his review he observes that the theoretical and computational studies have been “far more encouraging” than experimental studies. He has also presented a concise report on some of the experimental and numerical developments related to ram accelerators and PDE. He had observed that nozzles increase the efficiency of PDEs and effect of nozzle on detonation transmission and detailed dynamics of the flow have not yet been analyzed in detail. He also discusses the research on using PDEs for rocket propulsion.

Kailasanth et al. (1999) produced a status report that analyzed the numerical methodology of previous computational studies in terms of the grid resolution, initial and boundary conditions. They discussed in detail the merits and demerits of open end initiation vs. closed end initiation. It was seen that even though open end initiation produced higher thrust due to reflection of the detonation wave, it gave slightly lower specific impulse and cycling frequency. They discussed the problems in defining the outflow boundary condition considering that the flow could be sonic, subsonic or supersonic. They introduced the pressure relaxation boundary condition imposed at the outflow, which made the pressure to gradually decrease to ambient conditions from the exit of the PDE chamber to the outflow of the domain. They observed variation in the impulse computed with different pressure relaxation lengths. Higher impulse for higher relaxation lengths was observed. They also stressed the importance of resolving the induction distance and induction zone where the OH-radical build-up occurred.
The next two sections deal with performance studies and research involving the external flow process and hybrid PDEs.

### 2.2.1 Performance Analysis

Allgood et al. (2002) studied the effect of exit geometry on the performance of a PDE. They observed that the sensitivity of the PDE with an ejector system to the fill fraction with different diameter ratios was the same as a PDE without an ejector system. Numerical simulations from Allgood et al. (2003) also were in good agreement with their experimental visualizations. Their most recent experimental work, Allgood et al. (2005) related the effect of fill fraction and the addition of nozzle to the PDE geometry. It was found that the optimum nozzle ratio was found to be a function of the PDE fill fraction. For fill fractions equal to or less than 0.5, they found the optimum configuration one without using an exhaust nozzle and for fill fractions close to or more than 1, thrust was enhanced with a converging nozzle.

Schauer et al. (2001) experimentally investigated the individual effects of fuel fill fraction and equivalence ratio on thrust and fuel-specific impulse. The study was conducted using hydrogen-air fuel. They found the thrust to increase with increasing fill fraction and asymptoting for fill-fractions more than one. Thrust was maximum close to stoichiometric conditions. Fuel specific impulse was found to decrease with increasing tube fill-fraction and increasing equivalence ratio.

Li et al (2003) studied the pressure distribution, an indicative of the propulsive efficiency, with various amounts of fuel fill in the PDE chamber. They found that the impulse increases with length of the non-reactive section, eventually approaching an asymptotic value. Fuel-based specific impulse increases but total mixture-based specific
impulse reduces when the fill fraction is less than one, as less chemical energy is released per unit volume. Therefore the total engine output from a partially filled PDE is better compared to one full with fuel-oxidizer mixture.

Mawid et al. (2002) used a commercial flow solver STAR-CD to study the thrust augmentation achieved by integrating a pulse detonation engine to a turbofan engine along with a nozzle. They performed a 3D numerical simulation with a 5-step model for JP-8 fuel. They used a global model for hydrogen-air fuel for purpose of a base line PDE simulation and code validation. They connected the PDE to a dump tank that was three times the diameter in the axis-perpendicular direction and three times the length in the PDE in the downstream direction. Since they were using a nozzle they did not accommodate for the computational domain above the PDE tube. They did not perform any temperature averaging across the shock wave, yet they found a good agreement in the computed thrust and other performance parameters.

He and Karagozian (2003) numerically simulated the reactive compressible flow process in the PDE. They used a one-step reaction for hydrogen-air and methane-air mixtures. They showed results with and without the pressure relaxation type of outflow boundary condition, as suggested by Kailasanath et al. (1999). In the case of no pressure relaxation, they extended the 2D domain about one and half tube lengths downstream and two tube diameters perpendicular to the axial direction. They used the Weighted Essentially Non-Oscillatory (WENO) scheme. It is a higher-order (third order) accurate solver and captures steep gradients without introducing oscillations. Usage of this scheme allowed them to use relatively coarse grids. They showed in their results that the computed impulse is independent of the geometry. They also presented noise data such
as sound levels in decibels by measuring the pressure history of various locations inside and outside the tube.

### 2.2.2 Flow Analysis and Hybrid PDE

Li et al. (2000) studied in extensive detail the flow field evolution inside and external to a PDE. They used the two-step induction parameter model where the radical formation is modeled using the induction parameter and the second step governs the energy release. They employed a very fine grid in the radial direction inside the chamber that they were able to see the fine structures of the triple shock interactions. They used a very large computational domain, about 160 times the diameter in the axis-perpendicular direction and 34 times the length downstream of the exit. They also conducted a study with various fill-fractions. With different fill-fractions, though they observed a decrease in the impulse, the specific impulse based on fuel showed marked increase. This was attributed to the low amount of fuel used per cycle and the inefficiency of the expansion waves to travel fast towards the head end, reducing blowdown time.

Zhang et al. (2001) reported the numerical results of a study on the external flow field of a PDE. Their study used the space time Conservation Element/Solution Element (CE/SE) method, which is a novel shock capturing method that does not use the Riemann Solver. They used a single step chemical reaction of hydrogen-air along with 2-D Eulerian equations and a constant pressure boundary condition. They explained in detail the complex shock-vortex interactions and plume dynamics that take place outside a single PDE tube. They extended the study to analyze the flow field for three PDE tubes.

Schauer et al. (2002) experimentally studied a coupled PDE turbocharger to demonstrate shaft power extraction and self-aspiration. An update on that study with
additional instrumentation and flow configuration was studied in Schauer et al. (2003). They observed a reduction in the wave speed at the exit of the turbine. They also observed a drastic increase in blowdown time when a turbine was integrated to a PDE. The longer blowdown time caused the back pressure to rise and affected the fuel-fill part of the cycle for the successive cycles. The poor performance of the turbine is attribute to the type of turbine (centrifugal compressor) that was used (Garrett T3), which was never meant to operate under a close-to-hypersonic inlet. Apart from this fact, they observed that even after 50,000 detonations the turbine was not affected structurally.

Rasheed et al. (2004) performed both experimental and numerical studies on a PDE with a square duct and placed upstream to a four equally spaced turbine blade passage. They performed single cycle and multi-cycle (7 cycle) CFD and experimental studies. Significant difference was found in the results from the two conditions. A periodic state was reached only after 5-6 cycles. They provided qualitative high speed shadowgraph visualizations. They used a commercial code, CFD++, for the numerical simulations. The fuel inlet was modeled as a timed volumetric source model. They studied the pressure, temperature and mass flow rate at three locations: PDE exit plane, turbine inlet plane and turbine exit plane. No quantitative data was compared to the experimental results. From the CFD simulations and schlieren visualization, they were able to observe that near the turbine inlet plane, the reaction zone was decoupled from the curved shock wave. They were also able to see the under-expanded jets downstream of the turbine blade characterized by the Mach diamond structures. Similar to the studies of Schauer et al. (2002), they observed the shock waves reflecting back upstream from the
turbine blades. They also emphasized that multi-cycle effects need to be studied when investigating PDE interaction studies.

2.3 Specific Objectives of Present Study

From Section 2.1, we see that little work exists in the literature where different mechanisms have been used in the study of a self-sustaining detonation wave. It is also seen that mechanisms that provide results in the shock-induced combustion problem need not successfully simulate the self-sustaining detonation wave. Modification of the source term, as mentioned by Yu et al. (1988), results in spatial and temporal inaccuracy, thus not resolving the detailed flame structure. That rules out the use of simplified algebraic combustion models. So, our first objective is to simulate a one-dimensional detonation using different reaction mechanisms, and validate them for simulation of a self-sustaining detonation wave.

From Section 2.2, we note though there are many experimental and numerical studies relating to the different issues of the PDE and its performance. The external flow field has been studied in order to explain the complete cycle process and the flow features inside the chamber. We find there is scope for a more detailed study on the external plume dynamics of a PDE, as most of the studies have been of qualitative nature. When considering the integration of PDE with other systems, an in-depth understanding of the external flow-field is essential. Therefore, our second objective is to simulate the PDE, using the most optimum mechanism chosen from the first part of this study, and study quantitatively, its external flow field.

The PDE can be operated under stoichiometric conditions during take-off and fuel-lean conditions when cruising. Thus, the third objective is to study the changes in the
flow field resulting from use of different fuel-air mixture composition. This will also provide an understanding and guideline regarding the placement of turbines in a Hybrid Pulse Detonation Engine.
Chapter 3

Hydrogen–Air Detonation and Chemical Mechanisms

The term "detonation" is used to describe an explosive phenomenon whereby the decomposition is propagated by the explosive shockwave penetrating the explosive material (Wikipedia). In Section 3.1, we discuss the chemistry behind the explosive nature of a hydrogen-air mixture. The chemical mechanisms that are employed in the present study are introduced in Section 3.2.

3.1 Hydrogen-Air Detonation Chemistry

The chemistry behind the combustion of hydrogen-air mixtures has been studied in detail by Westbrook and Dryer (1984), and Yetter et al. (1991). The combustion process consists of three steps, namely, initiation, branching or propagation, and termination processes. For a hydrogen-air mixture, the chemical process is explained in the following sections.

3.1.1 Initiation

Initiation is the first step in the chemical process, where the individual molecules of H₂ and O₂ form the free radicals (O, H and OH) due to the initial high energy supplied.

\[ \text{H}_2 + \text{M} \rightarrow \text{H} + \text{H} + \text{M} \]  

(R 3.1)
Here, ‘M’ is the third body that takes away the excess energy released from these reactions. For hydrogen-air detonation, the intermediates (HO$_2$ and H$_2$O$_2$) or the molecules (H$_2$, O$_2$ and N$_2$) serve as third bodies. Among these, some will be more efficient than others in transporting the excess energy. It is important to include these efficiencies in the chemical model for accurate simulation of the detonation process.

### 3.1.2 Branching

Branching steps are those where the free radicals are formed and continuously produced. There are two types of chain branching: strong and weak branching. Strong branching is characterized by the formation of O, H and OH, and weak chain branching is characterized by the formation of the intermediates HO$_2$ and H$_2$O$_2$. Following are some examples of branching steps in the hydrogen-air reaction mechanism.

\[
H + O_2 \rightarrow O + OH \quad (R \ 3.3)
\]
\[
O + H_2 \rightarrow H + OH \quad (R \ 3.4)
\]
\[
H_2 + OH \rightarrow H_2O + H \quad (R \ 3.5)
\]
\[
O + H_2O \rightarrow OH + OH \quad (R \ 3.6)
\]

### 3.1.3 Termination

Terminating reactions are those in which radicals recombine to form molecules or intermediates, which are not as reactive as the free radicals. This step is highly exothermic, due to the large amount of energy release associated with it. Some examples of terminating reaction steps are shown below:
3.1.4 Explosive Characteristics of Hydrogen-Air

The explosive nature of hydrogen-air is best explained with the Pressure-Temperature plot depicting the explosion limits as shown in Fig. 3.1.

![Diagram of explosive limits for hydrogen-oxygen combustion](image)

**Figure 3.1 Explosive Limits for Hydrogen-Oxygen Combustion (Law et al., 2002)**

Each limit corresponds to a particular value of P and T, which governs whether the gas explodes or not. The first limit is the threshold for the gas to explode. Up to this limit, the radicals (O, H and OH) that are formed, are consumed either due to the reactions at the wall or due to the domination of chain terminating steps. Only when the ratio of radicals produced to radicals destructed is high, explosion occurs. The second
limit corresponds to the formation and destruction of the intermediate HO\textsubscript{2}. Temperatures and pressures higher than the second limit make the intermediates reactive. Again, as in the first case, the concentration of HO\textsubscript{2} has to be high enough for the chain to propagate into the third limit. At the third limit, H\textsubscript{2}O\textsubscript{2} is formed and is simultaneously consumed. As concentration of H\textsubscript{2}O\textsubscript{2} increases, the third limit is reached above which explosion occurs again. This is because, once H\textsubscript{2}O\textsubscript{2} becomes reactive, it continues to dissociate into hydroxyl radicals resulting in build up of the reactive OH concentration, and release of energy.

3.2 Chemical Mechanisms

As stated earlier in Section 2.3, the goal of the present study is to identify the effect of modeling various classes of mechanisms on the detonation parameters. This study allows us to evaluate the chemical mechanisms to be used in simulating the detonation phenomenon, and to study the resulting detonation structure. For this purpose, three classes of mechanisms are chosen. They are:

i. Global Mechanisms - 1-step and 2-step mechanisms

ii. Reduced Elementary Mechanisms – 8-step mechanism


3.2.1 Global Mechanisms

Even though global mechanisms represent a “black-box” approach, they provide a good approximation to the actual combustion process. The reaction mechanism and the Arrhenius parameters of the 1-step global mechanism for hydrogen-air proposed by
Varma et al. (1986) are employed. These parameters, shown for reaction R 3.11, correspond to an equivalence ratio of 0.44 (lean mixture).

\[
H_2 + O_2 \rightarrow H_2O \quad (R \ 3.11)
\]

\[A = 9.87E+08\]

\[E_A = 3.10E+07\]

\[N = 0\]

The Arrhenius parameters used for stoichiometric conditions, shown for reaction R 3.12, are those used by Mawid et al. (2002)

\[
H_2 + O_2 \rightarrow H_2O \quad (R \ 3.12)
\]

\[A = 5.00E +09\]

\[E_A = 5.50E+09\]

\[N = 0\]

A 2-step global mechanism proposed by Roger and Chinitz (1983) is employed as it captures the production of OH in two steps. This mechanism is too stiff for integration in the code, and hence, a modified version of it, by Hsu and Jemcov (2000) is used. Even after modification, it can be seen that the pre-exponential terms are very large, and thus, this 2-step mechanism requires a very low time step compared to the other reaction mechanisms.

\[
H_2 + O_2 = 2OH \quad (R \ 3.13)
\]

\[A = 2.50E +23\]

\[E_A = 1.00E+08\]

\[N = -3\]

\[2OH + H_2 = 2 H_2O \quad (R \ 3.14)\]
\[ A = 8.10 \times 10^{29} \]
\[ E_A = 7.87 \times 10^7 \]
\[ N = -5 \]

### 3.2.2 Reduced Elementary Mechanisms

The 8-step mechanism of Moretti et al. (1965) comes in this category. This mechanism was used by Cuttler et al. (1998) to simulate shock-induced combustion over a blunt projectile fired into a supersonic flow. Since mechanisms used for shock-induced combustion are expected to simulate the self-sustaining detonation process, this mechanism is selected. The formation and destruction of the OH radical is branched out in many reactions, and hence this mechanism is less stiff compared to the 2-step mechanism and allows use of a larger time step than that used for the 2-step mechanism. The performance of this mechanism is not known for the self-sustaining problem, and therefore, it does not substitute the usage of the 2-step mechanism. Table 3.1 shows the 8-step mechanism. The third-body efficiency is taken as 1 for all species in these reaction mechanisms. It should be noted that this mechanism does not model the formation and destruction of the intermediates HO\(_2\) and H\(_2\)O\(_2\).

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>N</th>
<th>A</th>
<th>(E_A)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(H + O_2 \rightarrow OH + O)</td>
<td>0</td>
<td>(3 \times 10^{11})</td>
<td>73249864</td>
</tr>
<tr>
<td>2</td>
<td>(O + H_2 \rightarrow OH + H)</td>
<td>0</td>
<td>(3 \times 10^{11})</td>
<td>33507032</td>
</tr>
<tr>
<td>3</td>
<td>(H_2 + OH \rightarrow H + H_2O)</td>
<td>0</td>
<td>(3 \times 10^{11})</td>
<td>25109488</td>
</tr>
<tr>
<td>4</td>
<td>(2OH \rightarrow O + H_2O)</td>
<td>0</td>
<td>(3 \times 10^{11})</td>
<td>25109488</td>
</tr>
<tr>
<td>5</td>
<td>(H_2 + M \rightarrow 2H + M)</td>
<td>-1</td>
<td>(1.85 \times 10^{11})</td>
<td>448977600</td>
</tr>
<tr>
<td>6</td>
<td>(H_2O + M \rightarrow OH + H + M)</td>
<td>-1</td>
<td>(9.66 \times 10^{12})</td>
<td>517155680</td>
</tr>
<tr>
<td>7</td>
<td>(OH + M \rightarrow O + H + M)</td>
<td>-1</td>
<td>(8.00 \times 10^{10})</td>
<td>434011680</td>
</tr>
<tr>
<td>8</td>
<td>(O_2 + M \rightarrow 2O)</td>
<td>-1</td>
<td>(5.80 \times 10^{10})</td>
<td>503852640</td>
</tr>
</tbody>
</table>

Table 3.1 8-step Mechanism of Moretti et al. (1965)
### 3.2.3 Detailed Elementary Mechanisms

This class of mechanisms attempt at modeling all the relevant physics of the problem, and they account for the formation and destruction of all radicals and intermediates. Two mechanisms of this type are studied; the first mechanism is the 19-step mechanism of Jachimowski (1988), shown in Table 3.2, which was modified by Yungster et al. (2004) to simulate detonation. All the reactions in this mechanism are reversible. The second mechanism is the 38-step mechanism of Vajda et al (1990), shown in Table 3.3. This mechanism provides different rate constants for all the reverse reactions, and therefore, all reactions are forward in nature. This mechanism was used by Hsu and Jemcov (2000), and it provided the best results for the self-sustaining detonation wave and is used here for purposes of comparison.

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>N</th>
<th>A</th>
<th>$E_A$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$H_2 + O_2 = HO_2 + H$</td>
<td>0.0</td>
<td>1.0000E+11</td>
<td>234444296.3</td>
</tr>
<tr>
<td>2</td>
<td>$H + O_2 = OH + O$</td>
<td>0.0</td>
<td>2.6000E+11</td>
<td>7033255.62</td>
</tr>
<tr>
<td>3</td>
<td>$H_2 + O = OH + H$</td>
<td>1.0</td>
<td>1.8000E+07</td>
<td>37259902.73</td>
</tr>
<tr>
<td>4</td>
<td>$H_2 + OH = H + H_2O$</td>
<td>0.0</td>
<td>2.2000E+10</td>
<td>21560486.36</td>
</tr>
<tr>
<td>5</td>
<td>$OH + OH = H + H_2O$</td>
<td>0.0</td>
<td>6.3000E+09</td>
<td>4563275.296</td>
</tr>
<tr>
<td>6\textsuperscript{b}</td>
<td>$H + OH + M = H_2O + M$</td>
<td>-2.0</td>
<td>2.2000E+16</td>
<td>0</td>
</tr>
<tr>
<td>7\textsuperscript{b}</td>
<td>$H + H + M = H_2 + M$</td>
<td>-1.0</td>
<td>6.4000E+11</td>
<td>0</td>
</tr>
<tr>
<td>8\textsuperscript{b}</td>
<td>$H + O + M = OH + M$</td>
<td>0.6</td>
<td>6.0000E+10</td>
<td>0</td>
</tr>
<tr>
<td>9\textsuperscript{b}</td>
<td>$H + O_2 + M = HO_2 + M$</td>
<td>0.0</td>
<td>2.1000E+09</td>
<td>-4186466.688</td>
</tr>
<tr>
<td>10</td>
<td>$O + O + M = O_2 + M$</td>
<td>0.0</td>
<td>6.0000E+07</td>
<td>-7535673.296</td>
</tr>
<tr>
<td>11</td>
<td>$HO_2 + H = H_2O + O$</td>
<td>0.0</td>
<td>1.4000E+11</td>
<td>4521453.864</td>
</tr>
<tr>
<td>12</td>
<td>$HO_2 + H = H_2O + O$</td>
<td>0.0</td>
<td>1.0000E+10</td>
<td>4521453.864</td>
</tr>
<tr>
<td>13</td>
<td>$HO_2 + O = O_2 + OH$</td>
<td>0.0</td>
<td>1.5000E+10</td>
<td>3977193.24</td>
</tr>
<tr>
<td>14</td>
<td>$HO_2 + OH = H_2O + O_2$</td>
<td>0.0</td>
<td>8.0000E+09</td>
<td>0</td>
</tr>
<tr>
<td>15</td>
<td>$HO_2 + OH = H_2O_2 + O_2$</td>
<td>0.0</td>
<td>2.0000E+09</td>
<td>0</td>
</tr>
<tr>
<td>16</td>
<td>$H + H_2O_2 = H_2 + HO_2$</td>
<td>0.0</td>
<td>1.4000E+09</td>
<td>15071429.74</td>
</tr>
<tr>
<td>17</td>
<td>$O + H_2O_2 = OH + HO_2$</td>
<td>0.0</td>
<td>1.4000E+10</td>
<td>26793652.86</td>
</tr>
<tr>
<td>18</td>
<td>$OH + H_2O_2 = H_2O + HO_2$</td>
<td>0.0</td>
<td>6.1000E+09</td>
<td>5986700.576</td>
</tr>
<tr>
<td>19\textsuperscript{b}</td>
<td>$H_2O_2 + M = OH + OH + M$</td>
<td>0.0</td>
<td>1.2000E+11</td>
<td>190485980.3</td>
</tr>
</tbody>
</table>

Third-body efficiencies: 6: $H_2O = 6.0$; reaction 7: $H_2O = 6.0$; reaction 8: $H_2O = 5.0$; reaction 9: $H_2O = 16.0, H_2 = 2.0$; reaction 19: $H_2O = 5.0$

Table 3.2 19-step Mechanism of Jachimowski et al. (1988)
<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>N</th>
<th>A</th>
<th>E&lt;sub&gt;A&lt;/sub&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H + O → O+ OH</td>
<td>0.0</td>
<td>1.640E+11</td>
<td>6.473E+07</td>
</tr>
<tr>
<td>2</td>
<td>O + OH → H + O₂</td>
<td>0.387</td>
<td>8.900E+07</td>
<td>-7.067E+06</td>
</tr>
<tr>
<td>3</td>
<td>O + H₂ → H + OH</td>
<td>2.67</td>
<td>5.080E+01</td>
<td>2.633E+07</td>
</tr>
<tr>
<td>4</td>
<td>H + OH → O + H₂</td>
<td>2.64</td>
<td>2.880E+01</td>
<td>1.872E+07</td>
</tr>
<tr>
<td>5</td>
<td>H₂ + OH → H₂O + H</td>
<td>2.00</td>
<td>6.300E+03</td>
<td>1.239E+07</td>
</tr>
<tr>
<td>6</td>
<td>H₂O + H → H₂ + OH</td>
<td>1.89</td>
<td>6.770E+04</td>
<td>7.653E+07</td>
</tr>
<tr>
<td>7</td>
<td>O + H₂O → OH + OH</td>
<td>1.32</td>
<td>3.980E+06</td>
<td>7.009E+07</td>
</tr>
<tr>
<td>8</td>
<td>OH + OH → O + H₂O</td>
<td>1.40</td>
<td>2.100E+05</td>
<td>-1.663E+06</td>
</tr>
<tr>
<td>9</td>
<td>H + H + M → H₂ + M</td>
<td>-1.67</td>
<td>1.080E+14</td>
<td>3.442E+06</td>
</tr>
<tr>
<td>10</td>
<td>H₂ + M → H + H + M</td>
<td>-1.4</td>
<td>4.580E+13</td>
<td>4.368E+08</td>
</tr>
<tr>
<td>11</td>
<td>O + O + M → O₂ + M</td>
<td>-0.5</td>
<td>6.170E+09</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>12</td>
<td>O₂ + M → O + O + M</td>
<td>-0.65</td>
<td>4.940E+11</td>
<td>4.975E+08</td>
</tr>
<tr>
<td>13</td>
<td>O + H + M → OH + M</td>
<td>-1.0</td>
<td>4.720E+12</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>14</td>
<td>OH + M → O + H + M</td>
<td>-0.76</td>
<td>1.130E+12</td>
<td>4.257E+08</td>
</tr>
<tr>
<td>15</td>
<td>H + OH + M → H₂O + M</td>
<td>-2.0</td>
<td>2.250E+16</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>16</td>
<td>H₂O + M → H₂O + M</td>
<td>-1.84</td>
<td>1.020E+17</td>
<td>4.975E+08</td>
</tr>
<tr>
<td>17</td>
<td>H₂ + O₂ + M → H₂O₂ + M</td>
<td>0.0</td>
<td>2.000E+09</td>
<td>-4.184E+06</td>
</tr>
<tr>
<td>18</td>
<td>HO₂ + M → H + O₂ + M</td>
<td>-0.074</td>
<td>4.470E+09</td>
<td>2.108E+08</td>
</tr>
<tr>
<td>19</td>
<td>H + HO₂ → H₂ + O₂</td>
<td>0.0</td>
<td>6.630E+10</td>
<td>8.895E+06</td>
</tr>
<tr>
<td>20</td>
<td>H₂ + O₂ → H + HO₂</td>
<td>0.35</td>
<td>1.250E+10</td>
<td>2.272E+08</td>
</tr>
<tr>
<td>21</td>
<td>H + HO₂ → HO + OH</td>
<td>0.0</td>
<td>1.690E+11</td>
<td>3.657E+06</td>
</tr>
<tr>
<td>22</td>
<td>OH + OH → H + HO₂</td>
<td>0.71</td>
<td>5.390E+07</td>
<td>1.426E+08</td>
</tr>
<tr>
<td>23</td>
<td>HO₂ + OH → H₂O + O₂</td>
<td>-1.0</td>
<td>1.450E+13</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>24</td>
<td>H₂O + O₂ → HO₂ + OH</td>
<td>-0.76</td>
<td>2.940E+13</td>
<td>2.825E+08</td>
</tr>
<tr>
<td>25</td>
<td>HO₂ + O → O₂ + OH</td>
<td>0.0</td>
<td>1.810E+10</td>
<td>-1.661E+06</td>
</tr>
<tr>
<td>26</td>
<td>O₂ + OH → HO₂ + O</td>
<td>0.32</td>
<td>1.930E+09</td>
<td>2.091E+08</td>
</tr>
<tr>
<td>27</td>
<td>HO₂ + HO₂ → H₂O₂ + O₂</td>
<td>0.0</td>
<td>1.000E+10</td>
<td>4.184E+06</td>
</tr>
<tr>
<td>28</td>
<td>H₂O₂ + O₂ → HO₂ + HO₂</td>
<td>-0.36</td>
<td>1.220E+12</td>
<td>1.453E+08</td>
</tr>
<tr>
<td>29</td>
<td>H₂O₂ + OH → H₂O + H₂O</td>
<td>0.0</td>
<td>7.000E+09</td>
<td>5.983E+06</td>
</tr>
<tr>
<td>30</td>
<td>H₂O + HO₂ → H₂O₂ + OH</td>
<td>0.6</td>
<td>1.160E+08</td>
<td>1.474E+08</td>
</tr>
<tr>
<td>31</td>
<td>H₂O₂ + H → H₂O + OH</td>
<td>0.0</td>
<td>1.000E+10</td>
<td>1.502E+07</td>
</tr>
<tr>
<td>32</td>
<td>H₂O + OH → H₂O₂ + H</td>
<td>1.31</td>
<td>5.300E+04</td>
<td>2.953E+08</td>
</tr>
<tr>
<td>33</td>
<td>H₂O₂ + H → HO₂ + OH</td>
<td>0.0</td>
<td>4.820E+10</td>
<td>3.325E+07</td>
</tr>
<tr>
<td>34</td>
<td>HO₂ + H₂ → H₂O₂ + H</td>
<td>0.71</td>
<td>7.450E+07</td>
<td>1.105E+08</td>
</tr>
<tr>
<td>35</td>
<td>H₂O₂ + M → OH + OH + M</td>
<td>0.0</td>
<td>1.200E+11</td>
<td>1.904E+08</td>
</tr>
<tr>
<td>36</td>
<td>OH + OH + M → H₂O₂ + M</td>
<td>1.15</td>
<td>1.400E+05</td>
<td>-2.679E+07</td>
</tr>
<tr>
<td>37</td>
<td>O + OH + M → HO₂ + M</td>
<td>0.0</td>
<td>1.000E+11</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>38</td>
<td>HO₂ + M → O + OH + M</td>
<td>-0.47</td>
<td>7.490E+13</td>
<td>2.868E+08</td>
</tr>
</tbody>
</table>

Third-Body Efficiency: H₂O = 16 and H₂ = 2.5 for all reactions

Table 3.3 38-step Mechanism of Vajda et al. (1990)
Chapter 4

Numerical Methodology

This chapter describes the numerical methodology followed to simulate the flow processes of the Pulse Detonation Engine. As shown in Fig 4.1a, the flow inside the PDE tube is modeled as 1-dimensional, and when it exits the tube (Fig 4.1b) it becomes two dimensional in nature.

(a) One-Dimensional Flow inside the PDE Tube

(b) Two-Dimensional Flow outside the PDE Tube

Figure 4.1 Flow Processes in a Pulse Detonation Engine

The 1-D flow is modeled first, and then the solution with the wave at almost the exit is used as the initial condition for the 2-D simulation. Before modeling the 1-D flow for the PDE, it is used to study the performance of reaction mechanisms mentioned in Section 3.2. The geometry, governing equations, boundary and initial conditions are first described for the 1-D study. The same is then provided for the 2-D simulation of the external flow-field. The last part of this Chapter describes the flow solver used in the present study.
4.1 Numerical Methodology for Simulation of Internal Flow of the PDE

The internal flow of the PDE is the supersonic combustion of fuel and air, namely detonation. The numerical methodology implemented to study the performance of reaction mechanisms in simulating detonation is described in Sections 4.1.1 through 4.1.6.

4.1.1 Geometry for 1-D Simulation of Detonation

The geometry used for 1-D simulation of detonation is a tube with its upstream end closed. Since the flow inside the tube is supersonic, the downstream boundary does not affect the internal flow, and therefore, any boundary can be used. In this case, a wall boundary is used, which makes the geometry a tube closed at both ends. The length of the tube is decided based on the distance from the upstream end at which a self-sustained detonation wave is formed. This distance is dependent on the richness of the fuel-oxidizer mixture and is shorter for a stoichiometric mixture than for a lean mixture. Therefore, the length of the tube is finally decided from the distance at which the self-sustained detonation is formed in the lean mixture.
4.1.2 Grid for 1-D Simulation of Detonation

Performing a 1-D simulation with a 2-D solver requires discretization only in the
direction of the flow (axial direction), and no interior points are required in the second
direction. Figure 4.3 shows the grid used in the simulation of 1-D detonation. The length
of the tube is varied based on the equivalence ratio, as the distance at which a self-
sustaining detonation wave is formed is dependent on the richness of the mixture. The
value of $\Delta x$ is chosen based on the size of the reaction zone, which is also dependent on
the richness of the mixture.

![Figure 4.3 One-Dimensional Grid for Simulation of Detonation]

4.1.3 Governing Equations for 1-D Simulation of Detonation

The governing equations employed for studying the performance of the chemical
mechanisms are the 1-D Euler equations, along with the required number of species-
continuity equations. The system of equations is shown below:

$$
\frac{\partial}{\partial t} \int_v W dV + \oint F dA = \int_v H dV
$$

(4.1)

where, $W = \begin{bmatrix} \rho \\ \rho u \\ \rho E \\ \rho Y_i \end{bmatrix}$, $F = \begin{bmatrix} \rho u \\ \rho u^2 + P \\ \rho (E + P) u \\ \rho u Y_i \end{bmatrix}$ and $H = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \hat{q} \end{bmatrix}$.

Here, $\hat{q}$ is the rate at which heat is released from the reactions. The reaction source term
is given by
\[
\frac{dY_i}{dt} = -k(T)\left[Y_i\right]^n\left[X_i\right]^m, \quad (4.2)
\]

and the rate constant of the reaction is given by

\[
k(T) = A_i T^n e^{-\frac{E_i}{RT}}, \quad (4.3)
\]

### 4.1.4 Boundary Conditions for 1-D Simulation of Detonation

Figure 4.4 shows the boundary conditions used for the 1-D simulation. The ends are taken to be adiabatic, slip walls. The detonation wave is initiated at the left end, and propagates towards the right. As discussed earlier, since the detonation wave propagates at supersonic conditions, implementing a wall-boundary condition at the right end does not affect the solution till the wave reaches that boundary. This is because the nature of the unsteady supersonic Euler equations is hyperbolic (Tannenhill et al. 1997), and the zone of influence lies behind the traveling shock wave.

**Symmetry**

```
<table>
<thead>
<tr>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;Wall&quot;</td>
</tr>
</tbody>
</table>
```

**Figure 4.4 Schematic Sketch of the Boundary Conditions for 1-D Simulation**

The “Wall” boundary condition is given by

\[
u = 0, \quad \frac{d\nu}{dy} = 0 \text{ and } \frac{dT}{dy} = 0 \quad (4.4)
\]

To perform a 1-D simulation with a 2-D solver, the lateral boundaries have to be defined as symmetry planes. Hence, the symmetry boundary condition, as defined in Eq. 4.5, is implemented on the top and bottom where the gradient of any quantity is zero.
\[
\frac{d\phi}{dv} = 0, \text{ where } \phi \text{ is any quantity}
\] (4.5)

4.1.5 Initial Conditions for 1-D Simulation of Detonation

Initial conditions for mass fraction of reactant species, velocity, pressure, and temperature are provided. In the case of stoichiometric mixture, the mass fraction of hydrogen is 0.0283125, oxygen is 0.2265005, and the rest is nitrogen. For the lean mixture of equivalence ratio 0.44, the mass fraction of hydrogen is 0.01266, oxygen is 0.230243, and the rest is nitrogen. The velocity of the fuel-air mixture is initially zero throughout the tube. It has been shown in previous studies by Morris (2004) and Yungster and Radhakrishnan (2004) that initial conditions of pressure and temperature have a profound effect on the wave propagation characteristics. In the present case, the initial pressure and temperature for all simulations inside the tube are set as 1 atm and 300 K.

In experimental studies, self-sustained detonation is achieved using traditional Deflagration to Detonation Transition (DDT) devices that accelerate the transition of a deflagration wave to a detonation wave (Allgood, 2004). In simulations, a self-sustained detonation can be easily attained using high pressure and temperature as ignition conditions. This technique is known as direct initiation. As we already know, detonation is a process where the shockwave provides energy for the reactions, and the reactions fuel the shock. Therefore, it is logical to start the chemical reactions by supplying flow conditions at the von-Neumann spike, which is the maximum pressure at the wave front at any instant. Therefore, ignition is provided by a high pressure and temperature condition patched to a few cells near the head end as shown in Fig 4.5.
4.2 Numerical Methodology for Simulation of External Flow of the PDE

When the detonation wave exits the PDE tube, the gases expand into the atmosphere. The flow no longer remains one-dimensional. As discussed earlier in Section 2.3, the second and third objectives of the present study are to simulate this external flow and study it for two operating conditions namely, take-off and cruise conditions. Sections 4.2.1 through 4.2.5 provide details of the numerical methodology to study the flow external to the PDE tube.

4.2.1 Geometry for Study of External Flow Field of PDE

The downstream end of the previously described closed tube is now left open as shown in Fig. 4.6. The head-end now depicts a valve, which stays closed once the fuel is filled inside the tube. The PDE tube has a length of 0.2 m and diameter of 0.02 for both fuel mixture compositions studied, as the 1-D simulations showed that a self-sustaining detonation is formed for both mixtures within this length.

![Figure 4.6 Geometry for a PDE](image)
4.2.2 Grid for Study of External Flow Field of PDE

The grid for simulating the external flow field of the PDE requires special consideration due to its nature. The flow external to the PDE has subsonic regions and, hence, the downstream conditions influence the flow. Since atmospheric conditions are given downstream, the boundary has to be placed far away from the exit of the tube. The flow field immediate to the exit of the tube has strong gradients, and the grid size has to be very small. The flow far away from the exit has gradual variations, and the step size can be larger. Since the grid size has to be very small in a region close to the tube exit in both axial and radial directions, a multi-block technique is used. Figure 4.7 shows a schematic of how the computational domain is split into 9 blocks for simulating the PDE’s flow field. The domain extends downstream to about ten times the length of the tube, and the far-field in the y-direction is set at 100 times the diameter. This large a domain allows us to impose boundary conditions that do not interfere with the flow exiting the PDE chamber.

Domain 1 represents the tube, and has a 1-D grid. All the other domains have 2-D grids. Domains 2 and 3 immediately external to the exit of the tube have a grid size of 0.3 mm in both directions as complex flow features exist in these regions. Domains 4, 5, 6, 7, 8 and 9 are far-field to the PDE, and the changes occurring in these regions are very gradual. Therefore, the grids are stretched in this domain at a ratio of 1.025. A total of approximately 220,000 grid points are used for simulating the PDE. To achieve this non-uniform distribution of grid points, non-conformal grids (Fluent 6.1 Manual, 2003) are used. In Fig. 4.7, the dotted lines show the non-conformal boundaries, which are the
interfaces between domains of different grid densities. Figure 4.8 shows the grid near the exit of the tube.

Figure 4.7 Schematic of the Multi-Block Division of the Computational Domain

Figure 4.8 Grid Showing Multi-Block Point Distribution near the Exit of the Tube
4.2.3 Governing Equations for Study of External Flow Field of PDE

The governing equations remain the same as before except now the second dimension is included. These equations for simulating the two-dimensional flow-field external to the PDE, given by Eq. 4.6, are also reactive because some amount of reaction is expected to occur even outside the PDE exit.

$$\frac{\partial}{\partial t} \int_V W dV + \oint F dA + \oint G dA = \int_V H dV$$  \hspace{1cm} (4.6)

where, $W = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho Y_i \end{bmatrix}$, $F = \begin{bmatrix} \rho u \\ \rho u^2 + P \\ \rho u v \\ \rho (E + P) u \\ \rho u Y_i \end{bmatrix}$, $G = \begin{bmatrix} \rho v \\ \rho u v \\ \rho v^2 + P \\ \rho (E + P) v \\ \rho v Y_i \end{bmatrix}$ and $H = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$

4.2.4 Boundary Conditions for Study of External Flow Field of PDE

Figure 4.9 shows the boundary conditions used for the 2-D PDE simulation. Adiabatic, slip-wall boundary conditions are used to define the PDE walls. A reflective wall boundary condition is used on the left wall.

![Diagram of Boundary Conditions for PDE Simulation](image)
This simulates a condition where the PDE is attached to a wall which, in reality, is a possible situation, as it needs to be integrated with the airframe at its head-end. Similar treatment of the left boundary condition can be found in the work of Kailasanath et al. (2000). Constant-pressure boundary condition is used at the top and exit boundaries. Axis boundary condition is implemented at the bottom boundary.

### 4.2.5 Initial Conditions for Study of External Flow Field of PDE

As shown in Fig. 4.10, the computational domain is divided into two zones, namely, ‘tube’ and ‘air’. The ‘tube’ zone is initialized with the 1-D solution of the closed tube, with the wave very close to the exit of the tube. The ‘air’ zone is initialized with mass fraction of oxygen (0.233), and mass fraction of nitrogen (0.667), corresponding to the composition of air. The initial pressure and temperature are set at 1 atm and 300 K, respectively.

![Figure 4.10 Initial Conditions for PDE Simulation](image)

---

This simulates a condition where the PDE is attached to a wall which, in reality, is a possible situation, as it needs to be integrated with the airframe at its head-end. Similar treatment of the left boundary condition can be found in the work of Kailasanath et al. (2000). Constant-pressure boundary condition is used at the top and exit boundaries. Axis boundary condition is implemented at the bottom boundary.

### 4.2.5 Initial Conditions for Study of External Flow Field of PDE

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![Figure 4.10 Initial Conditions for PDE Simulation](image)
4.3 Flow Solver for Simulation of Internal and External Flows of a PDE

To justify the selection of the flow solver, goals of the present study and the requirements of the solver are re-stated.

Goals:

The goals of the present study, as discussed in Section 2.3, are:

1. To evaluate performance of chemical mechanisms in simulating 1-D detonation parameters.
2. To simulate and analyze the internal and external flow of a PDE for two operating conditions.

Requirements of the Solver:

The solver should be able to:

1. Simulate compressible flows.
2. Simulate 1-D and 2-D flows.
3. Model detailed complex chemical mechanisms.
4. Employ variable specific heat capacities.
5. Perform parallel computations.
6. Employ a stable scheme to capture discontinuities.

A variety of software such as GPACT, CFD++, STARCD, and FLUENT met our requirements. These codes have been previously used successfully in simulating detonation by Ebrahimi and Merkle (2002), Sekar et al. (1998), Mawid et al. (2002) and Hsu and Jemcov (2000), respectively. The commercial code, FLUENT 6.1 (2003), met all the above requirements, and was readily available and is used for this study.
FLUENT 6.1 (2003) employs Roe’s upwind scheme for discretization of convective terms, and Runge-Kutta method for time integration. These are commonly used schemes for compressible flow simulations. The code also allows for easy inclusion of complex chemical mechanisms.

For detonation, as convection dominates diffusion, no mass diffusion was used. For compressible flow, it is essential to solve the governing equations of mass, momentum, energy and species continuity in a coupled manner, and hence a coupled flow solver is used. Density is computed using the ideal gas law. The specific heat capacity at constant pressure is defined by the mixing law shown in Eq. 4.7.

\[ c_p = \sum Y_i c_{p_i} \quad (4.7) \]

A two temperature-range (300-1000 K and 1000-5000 K) piecewise polynomial function of temperature dependence is used for computing specific heat capacities for each species for more accurate simulations.

For reactive flow simulations, the Damkohler number, defined as the ratio of convective time to the reaction time, should be kept around unity (Tannenhill et al., 1997). The reaction time is very small, of the order of $10^{-8}$ to $10^{-10}$ seconds, and therefore, the time steps of these orders are employed. This translates to using a CFL number of 0.1 or 0.01 based on the stiffness of the chemical mechanism. Because of such small time steps, an explicit method is used for both temporal and spatial discretization.
Chapter 5

Results and Discussion

The problem and the formulation were discussed so far. In this Chapter, the results obtained are presented along with their analysis. As in the previous Chapter, first part of this Chapter deals with the 1-D flow inside the PDE tube. Prior to performing the PDE simulation, performance of reaction mechanisms in capturing the detonation quantities such as peak pressure, detonation velocity, is studied comparatively. The results and discussion of this study is presented in Sections 5.2 through 5.6. The optimum mechanism is chosen from this study, and is used for simulating the PDE’s internal and external flow. Sections 5.7 through 5.9 provide the results and discussion on the flow features external to the PDE tube, and also presents the comparison for two operating conditions.

5.1 Propagation of a Detonation Wave

Once the ignition conditions of high pressure and high temperature is given a detonation wave is formed. The formation of a self sustaining detonation wave from direct initiation conditions have been shown by Yungster and Radhakrishnan (2004) and Ebrahimi and Merkle (2002). Initially an over-driven detonation wave is formed. The gases behind the shockwave expand causing the detonation wave to decay from an over-driven state. When the combustion products reach an equilibrium state, they travel at
sonic conditions with respect to the leading shock wave, and become self-sustaining in nature.

### 5.2 Computation of Detonation Velocity

Detonation velocity is one of the most important parameters of interest in the present study. It can be computed by two methods. In the first method, the point, shown in Fig. 5.1, corresponding to the location where equilibrium conditions are reached is located after the wave becomes self-sustaining and the flow variables are computed at that point. At this point the detonation velocity is computed using Eq. 1.10.

![Figure 5.1 Plot of Reaction Rate showing the Location of Termination of the Reaction Zone for a Lean Mixture](image)

In the second method, the detonation velocity can be computed by tracking the middle point of the shock wave over an interval of time and the velocity is then computed from the distance traveled. Once a self-sustaining detonation wave is formed, the second method is the reliable way to compute the detonation velocity, as it is difficult to obtain a
single point where equilibrium conditions are achieved. In the present study, both methods were used to verify the computed velocity and the error was found to be within 2% of the value of theoretical CJ velocity.

5.3 Effect of Numerical Resolution on Detonation Simulation

Since CFD simulations employing finite-rate chemical reactions are very sensitive to the numerical resolution, the effect of numerical resolution on the simulation of detonation is studied. It is done for the stoichiometric mixture first, and then for the lean mixture. The goal of this part of the study is to identify the numerical resolution that will best resolve the reaction zone and the detonation structure.

5.3.1 Stoichiometric Mixture

The Detonation Database (1999) shows the length of the reaction zone for a stoichiometric mixture of hydrogen-air is 0.215 mm. The reaction zone was resolved using 2, 4, 10 and 20 points. These values correspond to \( \Delta x \) of 0.1, 0.5, 0.02 and 0.01 mm, respectively. The temperature distribution near the wave front is examined for convergence in addition to detonation velocity, head-end pressure and peak pressure. Simulation of the stoichiometric mixture is done using the global reaction mechanism of Mawid et al. (2002). Table 5.1 shows the convergence in detonation velocity, and head-end pressure, and the error in the computed value of detonation velocity. The coarser grids predict a lower detonation velocity, a behavior that was also observed by Morris (2004). Figure 5.2 shows the variation of temperature with respect to the numerical resolution in the region of the shock wave and the waves corresponding to 10 and 20 points in the reaction zone merge at the wave front. Hence, 10 points inside the reaction
zone were considered sufficient to resolve the detonation wave. In Fig. 5.2, a small difference exists in the region corresponding to the von-Neumann spike. The error in the peak pressure predicted for 10 points is 3.7% from the reference value of 28 atm.

<table>
<thead>
<tr>
<th>Grid Density (mm)</th>
<th>Detonation Velocity</th>
<th>% Error from CJ Value</th>
<th>Head End Pressure (atm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>1947</td>
<td>1.217656012</td>
<td>5.59</td>
</tr>
<tr>
<td>0.05</td>
<td>1954</td>
<td>0.862506342</td>
<td>5.62</td>
</tr>
<tr>
<td>0.02</td>
<td>1961.36</td>
<td>0.489091832</td>
<td>5.64</td>
</tr>
<tr>
<td>0.01</td>
<td>1961.87</td>
<td>0.463216641</td>
<td>5.64</td>
</tr>
</tbody>
</table>

Table 5.1 Convergence of Detonation Velocity and Head-End Pressure for Stoichiometric Mixture

![Figure 5.2](image)

Figure 5.2 Temperature Distribution for Varying Grid Resolution for Stoichiometric Mixture

### 5.3.2 Lean Mixture

The 1-step reaction mechanism of Varma et al. (1986) is used for simulating the detonation in the lean mixture. The reaction zone for the lean mixture of
equivalence ratio 0.44 is of the order of 5 mm. From the results of the stoichiometric mixture, it was felt that 10 points in the reaction zone maybe sufficient to predict detonation velocity and peak pressure within 0.48% and 3.7% error, respectively. Ten points in the reaction zone would correspond to a $\Delta x$ of 0.5 mm. Figure 5.3 shows the pressure distribution at the wave front for a grid resolution corresponding to 10 points. From the figure, we can see that the reaction zone is spread over many cells. The error in the von Neumann pressure is about 25%. Therefore, it can be seen that 10 points in the reaction zone is not sufficient to resolve the detonation wave of a lean mixture. Therefore, it was essential to continue the investigation of the effect of numerical resolution. Since the CFL number is kept constant to resolve the chemical time scales, increasing grid resolution by a factor of 2, results in increasing the computational time by a factor of 4. This necessitated the use of flow-adaptive grids.

![Figure 5.3 Pressure Distribution for 10 Points in the Reaction Zone for a Lean Mixture](image-url)
5.3.3 Effect of Numerical Resolution using Flow-Adaptive Grids

Flow-adaptive grids are used to resolve regions of high gradient by increasing the numerical resolution in that region. In FLUENT 6.1, dynamic grid adaption works by addition and subtraction of cells in the region of the gradient. Addition of cells takes place when the refinement criterion is met, and cells are removed when the coarsening criterion is met. The criterion is based on the normalized value of the gradient of reaction rate. The refinement criterion is 0.01 and the coarsening criterion is 0.001. This range of values resolves the entire reaction zone for the lean mixture. The numerical resolution in the reaction zone is controlled by the refinement level. An increase in refinement level by 1 increases the resolution of the reaction zone by a factor of 2 in both directions.

Detonation being approximated as a one-dimensional problem, resolution in the y-direction is not required. Though resolution in the y-direction does not affect the solution (due to inviscid conditions), it introduces unnecessary grid points. An appropriate form of grid adaption is that due to Ghia et al. (1983), where the grid points are moved with the help of forcing functions near the region of high gradient, and the same number of cells exists at any instant. In the present study, in spite of the addition of excess grid points in the y-direction, the total number of points is small compared to that of a uniform grid with the same resolution. Hence, the usage of dynamically adaptive grids is justified. Since 10 points are not sufficient to resolve the reaction zone, four levels of refinements using adaptive grids are used. Figures 5.4 a-d shows the adapted grid at different levels of refinements. Level 1 refinement corresponds to 20 grid points (Δx = 0.25 mm), level 2 corresponds to 40 grid points (Δx = 0.12 mm), level 3
corresponds to 80 grid points ($\Delta x = 0.062 \text{ mm}$) and level 4 corresponds to 160 grid points ($\Delta x = 0.031 \text{ mm}$) in the reaction zone. Figure 5.5 shows the pressure distribution obtained from different levels of refinement of the flow-adaptive grid in the region of the gradient. It can be seen that the structure of the wave is the same for both level-2 and level-3, except for the peak value. The calculated detonation velocity and the error from the theoretical CJ value are shown in Table 5.2, which shows convergence for the finest grids. The error in detonation velocity is only 0.38 % in the finest grid. The peak pressure from the level-3 grid is about 17.31, which differs from the reference pressure value of 20.1 atm (Detonation Database, 1999) by 13.8 %.
(d) Level 4 Refinement – 160 points

Figure 5.4 Varying Levels of Refinement in the Reaction Zone

<table>
<thead>
<tr>
<th>Level of Refinement</th>
<th>Detonation Velocity (m/s)</th>
<th>% Error from Experimental Value</th>
<th>Peak Pressure</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Refinement</td>
<td>1538</td>
<td>0.90</td>
<td>15.22</td>
<td>24.27</td>
</tr>
<tr>
<td>1</td>
<td>1544</td>
<td>0.51</td>
<td>15.22</td>
<td>24.27</td>
</tr>
<tr>
<td>2</td>
<td>1546</td>
<td>0.38</td>
<td>15.46</td>
<td>23</td>
</tr>
<tr>
<td>3</td>
<td>1546</td>
<td>0.38</td>
<td>17.31</td>
<td>13.8</td>
</tr>
<tr>
<td>4</td>
<td>-NA-</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 5.2 Convergence in Detonation Velocity and Error in Peak Pressure

Figure 5.5 Pressure Distribution for Varying Levels of Refinement for Lean Mixture
5.4 Pulsating Self-Sustaining Detonation

One-dimensional detonation is simulated for a stoichiometric mixture using flow-adaptive grids. Figure 5.6 shows the oscillatory nature of the detonation wave and Fig 5.7 shows the adapted grid at the location of the first wave in Fig. 5.6. Figure 5.8 shows the mechanism proposed by Mcvey and Toong (1971), who explained this oscillating behavior using the concepts of reaction fronts being formed behind the wave. The formation of new reaction fronts send out rarefaction waves in both directions. These rarefaction waves have the effect of dampening the leading shock wave.

![Figure 5.6 Pulsating Detonation Wave seen in a Stoichiometric Mixture](image)
Figure 5.7 Adapted Grid for Stoichiometric Mixture

Figure 5.8 McVey and Toong Wave-Interaction Mechanism
5.5 Detonation Simulations using Multi-Step Chemical Mechanisms

The multi-step chemical mechanisms are used only in the simulation of detonation for the lean mixture with level-1 refinement of the grid. The elementary multi-step reaction mechanisms studied are the 8-Step mechanism of Moretti (1965), 19-step mechanism of Jachimowski (1988) and the 38-Step mechanism of Vajda (1990). The elementary mechanisms are independent of the richness of the mixture (Turns, 2000), and hence their performance is independent of the equivalence ratio. The 2-step mechanism of Roger and Chintz (1983) cannot be directly used for lean mixture as the Arrhenius parameters are too large and they make the equations too stiff for integration in FLUENT 6.1. Hence, the modified version of the 2-step mechanism by Hsu and Jemcov (2000) are used in the present study.

5.5.1 Induction Time

During the ignition process the time history of head-end pressure for all reaction mechanisms is recorded and is shown in Fig. 5.9. Immediately after ignition, combustion occurs at the fuel-mixture interface. This reflects as a pressure build-up at the wall. Hence, the pressure history at the wall is an indication of the ignition delay or induction time predicted by a chemical mechanism. The time history of pressure is plotted till the instant when the pressure starts decreasing at the head. A pressure decrease at the wall indicates that the wave is moving downstream. The 19-step mechanism predicts an induction time that is longer than that for the 38-step mechanism.
The 19-step exhibits a gradual slope, which means that the detonation wave is not formed instantly. The 38-step mechanism predicts this behavior more accurately than the 19-step mechanism, and also maintains the peak pressure for a longer duration as compared to any other reaction mechanism. The 1-step mechanism does not show any induction time, but comes close to the performance of the 38-step mechanism in predicting the peak pressure rise. The 2-step mechanism shows a small induction time, and also initially shows a drop in pressure. The 8-step elementary mechanism does not show the formation of a detonation wave.
5.5.2 Comparison of Flow Variable Distribution for Multi-Step Mechanisms

Here the distribution of flow variables such as pressure, temperature and velocity obtained from the three reaction mechanisms that successfully simulated the self-sustaining detonation wave are compared.

5.5.2.1 Pressure Distribution

Figure 5.10 shows the normalized pressure distribution predicted by the three reaction mechanisms. Pressure is normalized with the downstream condition of 1 atm.

![Figure 5.10 Comparison of Normalized Pressure Distribution of Multi-Step Mechanisms near the Shock Front](image-url)
The waves are linearly aligned at almost the same time instant for the purpose of comparison. The von Neumann spike for a 0.44 equivalence ratio is 20.1 atm, and the theoretical CJ value is 11.03 atm25. Table 5.3 shows the error in the peak pressure, and the pressure predicted at the equilibrium conditions. (Detonation Database, 1999). All the reaction mechanisms show a similar trend at the reaction front. Behind the spike, the initial slope is the same for all reactions. This slope represents the expansion of the products. The 38-step mechanism predicts the conditions behind the pressure spike quite accurately, as compared to other mechanisms. The decrease in slope for the 19-step and 2-step mechanisms is very gradual and, hence the larger error in the value of pressure at the equilibrium conditions.

Table 5.3 Error in Pressure at Peak and Equilibrium Conditions for Multi-Step Mechanisms

<table>
<thead>
<tr>
<th>Mechanism</th>
<th>von Neumann Conditions</th>
<th>Error</th>
<th>Value at Equilibrium Conditions</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-Step</td>
<td>15.87</td>
<td>21 %</td>
<td>11.81</td>
<td>7 %</td>
</tr>
<tr>
<td>19-Step</td>
<td>16.31</td>
<td>19 %</td>
<td>11.52</td>
<td>4 %</td>
</tr>
<tr>
<td>38-Step</td>
<td>16.50</td>
<td>18 %</td>
<td>11.06</td>
<td>0.27 %</td>
</tr>
</tbody>
</table>

5.5.2.2 Temperature Distribution

Figure 5.11 shows the normalized temperature distribution near the wave front. Temperature is normalized with the downstream condition of 300 K. The value of temperature at the equilibrium conditions is 7. As shown in Table 5.4, all the mechanisms capture the temperature rise within 3 %, the error being least in the case of the 38-step mechanism. All the mechanisms predict the peak temperature at a point which is behind the peak pressure. This is in accordance with the ZND structure of the detonation wave where the peak temperature occurs behind the von Neumann spike in
pressure. The 38-step mechanism captures this physics better than the other reaction mechanisms. Table 5.4 shows no temperature value for von Neumann conditions. This is because the actual ZND structure is not captured, and when this zone is resolved, the detonation was found to be failing as discussed later.

![Figure 5.11 Comparison of Temperature Distribution of Multi-Step Mechanisms near the Shock Front](image)

<table>
<thead>
<tr>
<th>Mechanism</th>
<th>Value at Equilibrium Conditions</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-Step</td>
<td>6.78</td>
<td>3 %</td>
</tr>
<tr>
<td>19-Step</td>
<td>6.87</td>
<td>1.85 %</td>
</tr>
<tr>
<td>38-Step</td>
<td>6.91</td>
<td>1.28 %</td>
</tr>
</tbody>
</table>

Table 5.4 Temperature at Equilibrium Conditions Predicted by Multi-Step Mechanisms

73
5.5.2.3 Velocity Distribution

Velocity is normalized by the speed of sound, and the Mach number distribution is shown in Fig 5.12. The detonation velocities predicted by the reactions are shown in Table 5.5. Kistiakowsky and Kydd (1956) found the experimental detonation velocity to be 1552 m/s. All reaction mechanisms predict a detonation velocity with an error of less than 2%, confirming the observation of Wintenberger (2004). Figure 5.12 shows that the Mach number distribution of the burned gas is more accurately predicted by the 38-step mechanism than by the other mechanisms. At the CJ plane, the velocity of the burned gases must be sonic but, as seen from Fig 5.12 that the Mach number is found to be lower than 1. In spite of this, the detonation velocity predicted by all the mechanisms is within 2% of the experimental value.

![Figure 5.12](image.png)

**Figure 5.12** Comparison of Mach Number Distribution of Multi-Step Mechanisms near the Shock Front
<table>
<thead>
<tr>
<th>Mechanism</th>
<th>Detonation Velocity</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-Step</td>
<td>1534</td>
<td>1.15 %</td>
</tr>
<tr>
<td>19-Step</td>
<td>1536</td>
<td>1.03 %</td>
</tr>
<tr>
<td>38-Step</td>
<td>1541</td>
<td>0.71 %</td>
</tr>
</tbody>
</table>

Table 5.5  Computed Detonation Velocities from Multi-Step Chemical Mechanisms

The detonation velocities predicted by the 2-step and 19-step mechanism are lower because these mechanisms predict a higher velocity for the burned gases, shown in Fig. 5.12. It can also be seen in the figure that the velocity of the burned gas is over-predicted by the 2-step mechanism, and hence it predicts the lowest detonation velocity.

5.5.3 Failure to Predict Self-Sustaining Detonation

In the present study, failure to predict a self-sustaining detonation was observed under three conditions, and they are discussed here.

5.5.3.1 Global Reaction Mechanism

The ability to predict a self-sustaining detonation failed with the usage of the global reaction mechanism of the lean mixture with a level-4 refinement grid with 160 points \((\Delta x = 0.03 \text{ mm})\) in the reaction zone. This is because, at such a fine grid, the oscillations at the reaction front are partially resolved, and they need to be resolved completely. The occurrences of these oscillations at the reaction front are explained by the McVey and Toong (1971) mechanism. These oscillations are responsible for the pulsating nature of the detonation wave, and also, for the instability of detonation waves.
5.5.3.2 Detailed Reaction Mechanism

Earlier, in the simulation of detonation using the global reaction mechanism, it was seen that level-2 refinement ($\Delta x = 0.12$ mm) resolves the reaction zone and the wave structure. When the same level of refinement was used with the elementary mechanisms, both the 19 and 38-step mechanisms failed to generate a self-sustained detonation wave. The reason the mechanisms failed is due to the fact that the fine grids partially resolved the induction zone as observed by Saint-Cloud et al. (1972).

The length of the induction zone can be computed from Fig. 5.9. Induction time for the 38-step mechanism from the level-1 refinement is about $8.33 \times 10^{-8}$ and the experimental wave velocity is about $1552$ m/s$^{18}$. Thus, the induction zone will be $0.13$ mm, which is in the order of the $\Delta x$ of the level-2 refinement. Thus to investigate this further, a level-3 grid with 80 points in the reaction zone, shown in Fig 5.4c, is used to simulate detonation. This places 2 grid points in the induction zone. The resulting normalized pressure, temperature and density distributions are shown in Figs. 5.13a-f. It can be seen that initially a strong detonation wave is formed and then it decays. But it can also be seen that the detonation fails because it attempts to resolve the detonation structure, which is similar to the ZND structure. The explanation for this behavior is provided by Sharpe and Falle (2000) and Hwang et al. (2000), where they state that at these resolutions, it is important to resolve the induction zone accurately. They also recognized that the difficulty in doing this will be that the order of error in the scheme produces perturbations that are comparable to the order of fluctuations in the reaction front. Because of this limitation, the flow variables are compared between the multi-step reaction mechanisms on only the level-1 of the grid i.e., 20 points in the reaction zone.
Figure 5.13  Failing Detonation showing ZND Detonation Structure for the 38-Step Mechanism
5.5.3.3 Eight-Step Reaction Mechanism

The 8-step elementary mechanism of Moretti (1965) was not able to predict a self-sustaining detonation. Hsu and Jemcov (2000) showed that the 7-step reduced elementary mechanism of Shang et al. (1965) did not produce a self-sustaining detonation wave. Both the 7-step and 8-step mechanisms do not allow modeling of the second explosion limit of hydrogen-air as these mechanisms do not take into account the formation and destruction of the intermediates, HO₂ and H₂O₂. But this cannot be generalized because some earlier studies used a mechanism that did not model the intermediates, and yet they were successful. As shown in Fig. 5.9, the 8-step mechanism shows a very long induction zone, and then failed to predict the formation of a detonation wave.

![Figure 5.14 Failing Detonation of the 8-Step Mechanism of Moretti et al. (1965)](image)

This is further confirmed by the plot of the pressure distribution in Fig. 5.14. In this plot, the initial conditions for all variables were supplied from the 2-step mechanism.
It can be clearly seen that the 8-step mechanism fails to sustain the detonation wave and there is a rapid decrease in the peak pressure over time. The same behavior was also observed in the case of the 7-step mechanism. The shock front loses energy and the resulting expansion waves from the dying shock are sent out towards the head end, further reducing the pressure at the wall.

### 5.5.4 OH Radical Concentration and Detonation Structure

Figure 5.15 shows the OH mole fraction distribution at the wave front. The value of the actual concentration can be commented on only if experimental data is available.

![Figure 5.15 Comparison of Mole Fraction Distribution of OH predicted by Multi-Step Mechanisms](image.png)

Analysis of the concentration of OH plot should be done along with the plot of pressure distribution (Fig. 5.10), temperature distribution (Fig. 5.11) and the plot of OH source term distribution (Fig. 5.16).
It can be seen that the peak concentration of the OH radical is found at the von Neumann spike. It also means that OH is formed until the region of the peak pressure, and then it is consumed. In Fig. 5.16, a positive source term value means production of OH and a negative source term will mean consumption of OH. The consumption can be seen in the OH source distribution curve in Fig. 5.16. The consumption of OH results in heat release, as destruction of OH is a chain terminating step and hence the peak in temperature seen in Fig. 5.11 lies behind the peak in pressure. The 38-step mechanism captures this physics accurately. According to the ZND theory, the induction zone is characterized by the presence of free-radicals such as O, H and OH. The present study supports the ZND theory, and provides evidence to disprove the conclusion of Hsu and Jemcov (2000), that there is no induction zone behind the leading shock of a self-sustaining detonation wave. This is further confirmed by the plot of OH source term in Fig 5.17, taken during the failing stage on the finest grid. Resolving the region before the
pressure spike, resolves the production of OH in the induction zone, but it is not done accurately resulting in the failing detonation.

![Graph showing OH Source Term Distribution on Grid with Level 4 Refinement for 38-Step Mechanism.](image)

**Figure 5.17** OH Source Term Distribution on Grid with Level 4 Refinement for 38-Step Mechanism

### 5.6 Flow Development External to the PDE Tube – Stoichiometric Mixture

In the present study, detonation propagation inside the PDE tube is accounted for by interpolating the solution from the 1-D simulation with the wave positioned close to the exit. Flow development in the external domain is explained in terms of velocity magnitude contours of the stoichiometric case simulation, and is shown in Figs. 5.18 a-f. The pressure contours for both mixtures are presented in Figs. 5.19 a-h. The detonation wave that is propagating in the tube exits out of the open end into ambient atmospheric
conditions, as a non-reactive shock. Due to the high gradient at the exit in all directions, the non-reactive shock remains planar at the axis, and becomes curved near the corners of the tube at the exit, as shown in Fig. 5.18a. The pressure behind this curved spherical part of the shock is lower than that behind the planar part of the shock. The gases in the curved part of the shock expand into the atmosphere, forming expansion waves. These expansion waves cause increase in velocity near the corners of the tube exit, as seen in Fig. 5.18 b. The expansion waves also propagate into the tube.

A very low sub-atmospheric pressure exists outside the tube because of the flow of a high speed jet, and the resulting pressure gradient causes the products of combustion to flow out, thus enhancing the blowdown process. Expansion waves travel upstream into the tube reducing the pressure at the head end. In practice, these conditions strongly support purging and refueling, as a favorable pressure gradient is available for fuel flow. At this time, the flow outside enters the tube, and is two dimensional in nature. Since only 1-D simulation is performed inside the tube, the computations are stopped when this phenomenon occurs. Two counter-rotating strong vortical structures are observed near the exit of the tube as a result of the high speed jet exiting out of the tube. These are observed from the velocity and pressure contours shown in Figs. 5.18c and 5.19c, respectively. The shock is located between these two vortical structures, as seen in Figs. 5.20 d-f and from the velocity magnitude contours in Fig. 5.19 c-f. These counter-rotating vortices keep the flow accelerating and preserve the strength of the shock, as seen in Figs. 5.20 d-g. Subsequently, the pressure gradient changes direction, and the flow reverses direction. This results in increase in pressure behind the shock, as marked by “A” in Figs. 5.21 g and h.
Figure 5.18 Flow Development – Instantaneous Velocity Magnitude Contours
Figure 5.19  Flow Development – Instantaneous Pressure Contours
5.6.1 Comparison of the Plume Dynamics with Experimental Studies

The simulated external flow features of the PDE are compared with those of the experimental shadowgraph visualizations by Glaser et al. (2004) at the University of Cincinnati PDE Research Facility. Shadowgraph images are captured by the bending of light due to density differences. In the experimental setup, an ethylene-oxygen mixture of equivalence ratio 0.49 was used. It is possible to compare the results of the stoichiometric mixture of hydrogen-air to these images, as both mixtures have the same detonation velocity of 1971 m/s. Although the exact assessment would require comparing the second derivative of density from the numerical solutions, a good estimate could be obtained from comparing the pressure and velocity field to these images.

Figures 5.20 a and b show the formation of the curved shock wave, with the shock intensity being maximum at the center and decreasing in the curved portion away from the center. In the shadowgraph image, this behavior is seen as a strong gradient in density at the axis, and decreasing in density gradient in the region of the curved shock. These features are indicated by arrows in Figs 5.20 a and b. Figure 5.20 c and d show the formation of the Mach disk. The Mach disk is a region where the velocity of the exiting under-expanded jet is the highest. The Mach disk, marked by dashed circles, can be clearly seen in the velocity field rather than in the pressure field, and hence, the velocity contours are compared to this shadowgraph image. The structure of the under-expanded jet can be seen in Figs 5.20 d and e. Figures 5.20 e and f show the oblique waves formed due to the decaying of the Mach disk.
Figure 5.20  External Flow Features – Comparison with Shadowgraph Visualizations
5.7 Flow Development External to the PDE Tube – Effect of Mixture Equivalence Ratio

One of the main objectives of the present work is to study the flow field variations for two equivalence ratios. From our 1-D results, we are able to see that the one-step mechanisms of Varma et al. (1986) and Mawid et al. (2002) produced the best results in both the lean and stoichiometric mixture cases, respectively. Hence, the initial detonation wave is interpolated from the results obtained from these mechanisms. The location of the detonation wave is almost at the exit of the tube during the start of the 2-D simulation. Figures 5.21a-f show the pressure distribution and temperature distribution along the axis at different instants of time after the wave exits the tube for both stoichiometric and lean mixtures. Though the length of the computational domain is 10 times the length of the PDE tube, in Figs. 5.21a-c the quantities are shown only for one length of the tube downstream, and in Figs. 5.21d–f, for a length of three times the tube.

5.7.1 Pressure Distribution

Figures 5.21a and b show that the location of the shock is the same for both stoichiometric and lean mixtures, and it remains the same until the formation of the sub-atmospheric pressure zone near the exit of the tube. Before the low pressure zone outside the exit of the tube goes sub-atmospheric, there is a difference in the intensity of the shock for the two mixtures. After the sub-atmospheric region forms, the shock for the stoichiometric mixture travels faster than the lean mixture, seen from Figs. 5.21c–f, and maintains a constant difference.
Pressure Distribution

Temperature Comparison

(a) 1.1298e-05 s

(b) 2.3480e-05 s

(c) 1.4776e-04 s
Figure 5.21 Comparison of Pressure and Temperature Distributions between Lean and Stoichiometric Mixture
Figures 5.21c-f again shows that the low pressure reached by both mixtures remains the same. It is seen that the difference in the velocity of the shocks after the formation of the sub-atmospheric region remains the same. This is because the sub-atmospheric zone produces an adverse pressure gradient causing pressure to build up behind the traveling shock, and hence, slows the shock for the stoichiometric mixture.

Figures 5.21a-c show that the intensity of the shock decreases faster for the stoichiometric mixture than for the lean mixture. To explain this, an analysis of the velocity components at the same time instant is essential. Comparison of the x-velocity for both mixtures is shown at time $t = 5.3697 \times 10^{-4}$ s in Fig. 5.21. Velocities for both mixtures become zero at the point where constant pressure prevails inside the tube as shown in Fig. 5.22a. The difference in slopes shows that the stoichiometric mixture relaxes faster than the lean mixture. Figures 5.23a and b show the comparison of the y-velocity vectors at the exit of the tube for lean and stoichiometric mixture at the same time.

When the velocity components are compared between the two mixtures, it is observed that the velocity is relatively large in the y-direction (about 45 %) than in the x-direction (about 25 %) for the stoichiometric mixture outside the PDE chamber. This shows that the expansion process plays an important role in increasing the y-velocity, thus making the axial velocities of the shocks in the external domain almost comparable. The pressure plots also confirm that the stoichiometric mixture undergoes a faster relaxation than the lean mixture. This can be seen in Figs. 5.21 a –h, and also, by observing the pressure at the head-end over time. This faster relaxation of the stoichiometric mixture allows for smaller cycle times and production of greater thrust.
Figure 5.22 Comparison of X-Velocity Distribution at 5.3697e-06 s for Lean and Stoichiometric Mixture

(a) Lean Mixture 
(b) Stoichiometric Mixture

Figure 5.23 Comparison of Y-Velocity Vectors at 5.3697e-06 s between Lean and Stoichiometric Mixtures
5.7.2 Temperature Distribution

The temperature distribution is presented in the right column of Figs. 5.20a-f. Unlike the pressure distribution, the trend followed by the temperature remains the same throughout. There is a low dip in temperature in the region corresponding to the sub-atmospheric zone. A constant difference exists between the temperatures for the stoichiometric and lean mixtures. It should be noted that the peak in temperature does not fall at the same location as the peak in pressure, but, occurs behind it. This is because the shock has detached itself from the burned gases and is traveling faster than the gases. The distance between the shock and the burned gases is larger in the case of the lean mixture as compared to the stoichiometric case, a phenomenon experimentally observed by Glaser et al. (2004). Figure 5.24 shows the comparison of temperature distribution at 2.4454e-04 sec between the two mixtures. The most detrimental effect of high temperatures occurs near the tube exit, where the tip is prone to cracking as observed by Schauer et al. (2001).

![Comparison of Temperature Contours between Lean and Stoichiometric Mixtures at 2.4454e-04 s](image)
5.8 Comments on Turbine Placement

Figure 5.25 shows the experimental results of Schauer et al. (2001) comparing blowdown time of the PDE with nozzles and a turbine. In their set up, the turbine was attached directly to the exit of the PDE, and the turbine was directly exposed to the detonation waves. Figure 5.25 shows that the blowdown time is drastically increased when compared to Pure PDE and PDE with nozzles.

The extended blowdown time is because the turbine is placed at a location where the sub-atmospheric zone forms. If the turbine is placed at a sufficient distance allowing for the formation of this zone, then the blowdown time would decrease. Let us assume that the turbine is placed at one tube length away from the exit of the PDE. By placing it at this location, the amount of available work decreases. This can be seen by calculating the specific flow exergy, which provides the maximum theoretical work available per unit mass of the burned gas. When the turbine is placed at one tube length, there is a
25% decrease in the available work. This decrease is because the high temperature gases expand into atmospheric conditions in the present study. By housing the PDE exit and turbine arrangement, and with steady state operation, the ambient temperature could be raised, increasing the amount of available work.

Also, from Fig 5.21c, we can see that there is very little difference in the pressure intensities for both rich and lean mixture. This shows that the amount of back pressure would be the same with both operating conditions, resulting in uniform loading of the turbine blades.

The lower equivalence ratio mixture was found to have increased blow down time, confirming the results of Schauer et al (2001) and Allgood (2004). This blowdown time will still increase for the lean mixture in the presence of the turbine.
Chapter 6

Conclusion and Future Work

6.1 Conclusion

The flow field of a Pulse Detonation Engine is simulated and analyzed for two operating conditions: take-off (fuel-rich) and cruise (fuel-lean). First, one-dimensional detonation is simulated for a rich (stoichiometric) and a lean ($\phi = 0.44$) fuel mixture of hydrogen-air. To understand and accurately simulate detonation, multi-step finite-rate chemical mechanisms were employed for the lean mixture. An important observation was that the number of points required for resolving the reaction zone of the stoichiometric mixture (10 grid points) is not adequate for the lean mixture (greater than 80 points). The ability to simulate detonation failed in three situations:

(i) when the global mechanism was used on very fine grids (more than 80 points in the reaction zone) for lean mixture.

(ii) when a detailed reaction such as the 38-step mechanism was used on very fine grids (more than 160 points in the reaction zone) for the lean mixture, which partially resolves the induction zone of the ZND structure.

(iii) when the 8-step mechanism was used.

Although the elementary mechanisms failed for the lean mixture on fine grids, we expect them to perform much better in the stoichiometric case, as the induction zone is very small and will not be seen at all by the simulation. The peak pressure was
accurately captured by the global mechanisms for the lean mixture and the stoichiometric mixture, with less than 14% and 4% error, respectively, and the detonation velocity exhibits less than 0.5% error for both mixtures. On a relatively coarse grid, the 38-step mechanism captured the structure of the detonation structure more accurately than did the 2-step and 19-step mechanisms.

Detonation wave parameters predicted by the global mechanisms were used in simulating the flow field of the PDE. Analysis of the flow-field for the two equivalence ratios was primarily based on the pressure, temperature and velocity distributions over time. The stoichiometric mixture was found to relax faster compared to the lean mixture showing a faster blowdown time. The temperature distribution showed a very large but constant difference and a constant trend, unlike the pressure distribution, over time for the two mixtures. By placing the turbine at one tube length from the sub-atmospheric zone, decrease in blowdown time is possible. But, this also results in decrease of available work. Some of this work loss can be compensated for over multi-cycle operations as the internal energy of the ambient air will be high. At a distance of one tube length, the intensity of the pressure is found to be almost the same for the stoichiometric and lean mixture, indicating uniform load on the turbine for both of these operating conditions.

6.2 Future Work

The analysis of the external flow field was performed considering the flow to be inviscid. Although the approximation holds strong for the present study, diffusion and viscous heating play a major role in the external flow development. By performing
viscous simulations, the vortical structures will also be resolved properly. Hence, viscous effects should be included in future studies.

The adaptive grid that was used in the interior of the tube can be improved to perform adaption in one dimension only. Also, in the present study, adaption was made based on only reaction rate. For use in the external flow field, the flow adaption should be based on more than one variable. Future work should include modifying the present code for generating better flow-adaptive grids.

The present study does not account for the presence of the turbine. Detailed insight into the variation in the flow field can be obtained by simulating the PDE along with the turbine blades.

Another direction for future work will be to conduct detailed thermodynamic analyses to accurately compute the difference in efficiencies of the system when using stoichiometric and lean mixtures. A thermodynamic analysis of the entire PDE-Turbine system should also be performed.
References


Wikipedia, the free encyclopedia (http://en.wikipedia.org/wiki/Explosive)


