Winter 2002

Supersonic Combustion and Mixing Characteristics of Hydrocarbon Fuels in Screamjet Engines

Ahmed A. Taha
Old Dominion University

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SUPERSONIC COMBUSTION AND MIXING CHARACTERISTICS
OF HYDROCARBON FUELS IN SCRAMJET ENGINES

by

Ahmed A. Taha
B.S. July 1988, Cairo University, Egypt
M.S. June 1994, Cairo University, Egypt

A Dissertation Submitted to the Faculty of
Old Dominion University in Partial Fulfillment of the
Requirement for the Degree of

DOCTOR OF PHILOSOPHY
MECHANICAL ENGINEERING
OLD DOMINION UNIVERSITY
December 2002

Approved by:

Dr. Surendra N. Tiwari (Director)

Dr. Taj O. Mohieldin (Co-Director)

Dr. Sushil Chaturvedi (Member)

Dr. Sidney Roberts Jr. (Member)

Dr. Arthur C. Taylor III (Member)
ABSTRACT

SUPERSONIC COMBUSTION AND MIXING CHARACTERISTICS OF HYDROCARBON FUELS IN SCRAMJET ENGINES

Ahmed A. Taha
Old Dominion University
Director: Dr. Surendra N. Tiwari
Co-Director: Dr. Taj O. Mohieldin

A numerical study has been conducted to investigate the combustion and mixing characteristics of hydrocarbon fuels in scramjet engines. The three-dimensional Reynolds Average Navier-Stokes equations have been used to numerically investigate the supersonic combustion of ethylene and propane using different combustor configurations and fuel injection schemes.

Four physical models are used in the current study: the unswept generic rearward-facing step, the side swept rearward-facing step, the wedge with no pilot injection, and the wedge with pilot injection configurations.

The combustion characteristics of gaseous propane in supersonic airflow using the rearward-facing step that is swept inward from both end sides is studied. The effect of sweeping the step on the flow field features of propane combustion is investigated.

The study of the supersonic combustion of ethylene is carried out using different combustor configurations, different main fuel equivalence ratios, and different pilot fuel equivalence ratios. The effect of the combustor configuration on the temperature flow field and the flow structure is investigated by simulating two different combustor configurations, the rearward-facing step and the cavity. Then, the effect of the equivalence ratio of the main fuel injection on the general flow field features and energy field characteristics is studied. Two normal fuel equivalence ratios are used, 0.45 and 0.60. Lastly, the effect of the pilot fuel equivalence ratio on the flame holding mechanism and the combustion and flow field qualities concludes the study. Six pilot injection equivalence ratios are studied: 0.0, 0.02, 0.03, 0.045, 0.06, and 0.08.

The swept step shows the ability to hold the propane flame in the supersonic airstream without extinction. It was found that the side sweeping of the combustor exhibits the high temperature and combustion products concentration in the far field domain while
the area downstream of the normal injection location characterizes lower temperature and products concentration. It is recommended to optimize the combustor length to ensure the complete combustion and consequently the full liberation of the chemical energy stored in the fuel before the fuel exits the combustor.

The main findings from the ethylene study can be summarized in the following points. The step configuration with no pilot injection can afford the flame holding mechanism in the supersonic air stream by creating the flow recirculations in the step base area and featuring permanent high temperature regions surrounding the normal fuel injection. The step configuration showed good mixing capabilities in the far field domain. The wedge configuration proved superiority over the generic rearward-facing step configuration in holding the ethylene flame in the supersonic airstreams, producing overall higher temperature medium throughout the combustor, and exhibiting lower flow losses and higher combustor efficiency. The increase in the equivalence ratio of the ethylene normal fuel injection enhances the general flow field features and energy field characteristics in the combustor except in the step base area where the lower equivalence ratio features better temperature distribution and higher combustion efficiency.

Although the wedge with no pilot injection configuration presents the highest level of temperature distribution in the cavity and downstream regions, the 0.02-pilot equivalence ratio increases the temperature of the upstream face of the normal injection and enhances the flame holding mechanism. The 0.02-pilot equivalence ratio presented the optimum pilot injection case that can promote the flame holding mechanism and keep good combustion and flow field qualities. While further increase of the pilot injection equivalence ratio quenches the high temperature gases in the cavity region, which leads to the deficiency in the flame holding mechanism, the excessive pilot fuel injection shows its positive effect by increasing the average flow field static temperature and absolute pressure in the far field domain.
ACKNOWLEDGMENTS

I would like to express my sincere thanks and deepest appreciation to my advisor, Professor Surendra N. Tiwari, for his continuous and everlasting support, encouragement, and patience and for the constructive and fully-informative graduate courses he taught me during my program. The affectionate parental care he used to offer his students is not less than, by any way, the great academic and professional guidance he is sincerely providing. I gratefully acknowledge the financial support of the Old Dominion University’s Institute for Scientific and Educational Technology (ISET) through NASA Langley Research Center, Cooperative Agreement NCC1-349 under the supervision of Prof. Tiwari.

My deep thanks and faithful respect are due to my co-advisor, Professor Taj. O. Mohieldin, for the valuable scientific knowledge I gained from the graduate courses he taught me and the priceless discussions and guidance he offered me during the course of my research. I sincerely appreciate the great help and support my advisors offered me to overcome the health problem I suffered during my program.

My best words of thanks are due to the faculty and staff of the Mechanical Engineering Department, Old Dominion University, and especially to Professor Sushil Chaturvedi, the Department Chair and my committee member, for the wonderful and persistent effort that he does not spare to facilitate and promote the research environment in the Department. My appreciation extends also to my committee members Profs. A. S. Roberts Jr. and A. C. Taylor III for their time and help.

I would like to thanks all my colleagues and fellows at Old Dominion University, my friends who offered me the help and support and among whom I felt the comforting spirit of the one family.

I extend my thanks and gratitude to my former advisors and Professors, M.M. Elkotb and O. M. F. Elbahar, Cairo University, Egypt, who helped me build up my scientific background and research skills.

Last, but not least, special thanks, acknowledgment, and appreciation are due to my dedicated parents, my persistent wife, and my children for their everlasting love, encouragement, and patience. Without their support, this work would have not been possible.
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Chapter I

INTRODUCTION AND CHALLENGES

1.1 Introduction

Supersonic Combustion Ramjet (Scramjet) engines are attractive for both cruise and boost missions in the hypersonic portion of the flight corridor [1]. The flow speed is high in scramjet engines and the mixing and reaction times are limited in the engine combustor. Therefore, combustion is a critical factor in the design of scramjet engines [2].

Sustained airbreathing hypersonic flight shows potential advantages for military applications. Furthermore, airbreathing propulsion could be of particular interest for future reusable launchers in connection with rocket engines. High-speed ramjets (scramjet and dual mode ramjet) are a key technology for these two kinds of military and commercial applications [3]. Missile applications exist that require the performance benefits offered by the supersonic combustion ramjet (Scramjet) propulsion system [4].

The scramjet engine is expected to be the most effective propulsion system, but there are severe conditions for ignition such as low pressure, low temperature, and high airflow speed due to the supersonic incoming air [5]. Constraints on system size and weight have led to the need to improve technology for analyzing and designing such system. Considerable fundamental research has been conducted in response to the increased interest in the development of scramjet propulsion systems. Many experimental and numerical studies of various aspects of fuel injection in the combustor are discussed in [6].

The development of hypersonic airbreathing plane capable of horizontal takeoff and landing and acceleration to low earth orbit has attracted significant interest in the aerospace community for some time. It has a significant weight advantage over presently used rocket propulsion systems by eliminating the need to carry onboard oxygen tanks. One of the major challenges in developing such a plane is the design of a suitable

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propulsion system. Current airbreathing engine designs, which utilize subsonic internal flow velocities, such as turbojet or even ramjet engines, would be inappropriate because of the extreme conditions seen in hypersonic flight. Temperature recovery from the hypersonic free stream would be in the order of 2000K or more, leading to engine materials difficulties and loss of usable energy due to dissociation of air molecules. The induced drag on the vehicle due to strong shocks at the engine inlets is a strong function of the flight Mach number so that it rapidly becomes impractical to use subsonic engines at high speeds. A supersonic combustion RAMJET or SCRAMJET has long been considered to be a feasible engine concept for hypersonic vehicles [7].

Although hydrogen is generally a more energetic fuel than hydrocarbon fuels (i.e., the hydrogen has a greater energy density), some hydrocarbons offer the advantage that they can be liquefied without the use of cryogenic cooling and can also be contained within a smaller volume. The potential for the combustion of storable liquid fuels in supersonic airstreams for efficient propulsion engines at hypersonic speeds has been recognized since the late 1950s [8,9]. The need to increase the fuel energy density for hypersonic flight has long been recognized [10,11]. Liquid hydrocarbons are attractive solutions for the low end of the hypersonic flight regime because of their higher volumetric energy content and the relative simplicity of operational logistics [10,12].

For a Mach number range of 4-10, hydrocarbon fuels provide sufficient thrust and are also being considered. The high density of hydrocarbon fuels, as well as ease of handling, make them very attractive for volume-constrained systems such as missiles and hypersonic research vehicle (HRV) [13].

Most of the scramjet combustion work, currently being conducted, uses liquid hydrocarbon fuels or hydrogen [14]. The Air Force’s Hypersonic Technology 9-years-Program (HyTech) is developing a technology base for Mach 4-8 liquid-hydrocarbon fueled scramjet propulsion systems. The goal of the HyTech Program is to develop and demonstrate the operability, performance and durability of a Mach 4-8 hydrocarbon scramjet propulsion system [15].

The investigation of the liquid hydrocarbon fuel-based scramjet combustor is one of the major purposes of the hypersonic flight technology program. A primary problem to be solved is the longer ignition delay for hydrocarbon combustion. As an example, under
the typical working conditions in a scramjet combustor, the ignition delay for kerosene is 5~10 ms [16,17], while the typical residence time available for complete mixing and combustion is extremely limited to less than 2 ms in scramjet combustor [18]. Therefore, injection and mixing enhancement play important role in designing scramjet combustor [19].

Because the missile applications impose demanding volume constraints, a strong motivation exists for the development of a hydrocarbon-fueled air-frame-integrated scramjet. Although studies of supersonic combustion of hydrocarbon fuels have been performed intermittently over the past forty years [18,20], they yielded only a limited design database [4].

Although the energy/mass density of liquid hydrocarbon is lower than that of hydrogen, some of the mass increase would be recovered by a small and lighter structure of the vehicle. Liquid hydrocarbon fuels require substantial residence time to achieve vaporization and complete exothermic reactions, and such time is unlikely to be available in reasonable-sized supersonic combustors. The chemical kinetics of hydrocarbons are slow in comparison with gaseous fuels, such as hydrogen. For many realistic operating conditions, exothermic reactions cannot be achieved within the available residence time. Use of a pilot flame with fast kinetics (i.e., gaseous hydrogen) can provide locally, at the liquid injection location, the conditions necessary to accelerate the hydrocarbon reactions rates and reduce the Damkohler number, defined as the ratio between the characteristic fluid residence time in the reaction zone and the chemical reaction time scale, i.e., high temperature and low fluid velocities. For such a system it is necessary to verify: (a) the level of piloted energy required to ignite and maintain stable combustion of the liquid fuel, and (b) the interaction between the pilot flame and the heat sink represented by the injected hydrocarbon [21].

Extensive literature survey that reviews the previous related research work is reported in Chap. 2.

1.2 Challenges in Supersonic Combustion

The high-speed propulsion community has to orient more research activities to address some of the technical issues, which must be resolved to realize the full potential of the scramjets. Among these issues are the fuel-air mixing enhancement, the
structurally-compatible injection systems, the fuel densification to increase the energy/unit volume of the fuel used, and the turbulence modeling that is capable of predicting transition in the inlet, heat transfer, shear and mixing in the combustor, and possible relaminization in the nozzle [22].

Future direction of supersonic combustion research is discussed recently by Tishkoff et al. [6]. There is still serious question as to whether or not stable supersonic combustion is possible over the range of expected operating conditions. The successful development of the supersonic combustion ramjet (scramjet) for use on future hypersonic vehicles is reliant on detailed understanding of the complex flow field present in different regions of the system over a range of operating conditions. To model chemical reaction of fuel and air in an engine, reduced kinetic models must be developed to reduce computational time required for solving the species equations, particularly for hydrocarbon fuels. To support hydrocarbon-based scramjet engine development, a comprehensive data set for C7 – C12 aliphatic fuel components under scramjet conditions should be developed. The aliphatic fuels database should be utilized to derive suitable starting and reduced mechanisms for candidate fuels. Changes in the state of the fuel can affect the reactivity of the fuel and the resulting combustion efficiency significantly. There is a lack of understanding of the physical processes that may contribute to these effects. To understand these phenomena changes in the fuel state must be studied in a realistic simulation of the scramjet preheating and combustion processes.

Fuel-air mixing, flame holding, pressure losses, and thermal loading are among the major issues that need to be resolved for the successful design and implementation of hydrocarbon-fueled supersonic combustion ramjet (scramjet) engines. A successful fuel injection scheme must provide rapid mixing between the fuel and oxidizer streams, minimum total pressure losses, and have no adverse effects on flame-holding capability or thermal/structural integrity of the device. These requirements place somewhat conflicting constraints on the design of a viable fuel-injection scheme, and solutions to these problems are being actively sought internationally. A need exists for the development of a system that effectively integrates fuel injection and flame holding for supersonic combustion. Such a device would contribute significantly to the present research and industrial technology base [23].
In the recent work of Powell et al. [24], the many technological challenges that are still under investigation in the Hypersonic Technology (HyTech) program and the extent of advancement achieved in each area were presented. Among the discussed challenges are: the starting condition and mass capture in the inlet, the pressure ratio in the isolator, the piloting and flame holding, the fuel injection and mixing, the total pressure losses in the combustor, the frozen flow losses, the divergence losses, the nozzle thrust vector in the nozzle, the regeneratively-cooled structures and thermal management, the expected coking (deposition) of the hydrocarbon fuels being exposed to high temperatures during the endothermic reaction, the change in the composition of the cracked hydrocarbon fuels associated with the change in the ignition delay time that affects combustion stability, and the significant difference in engine operation during the ramjet and scramjet modes.

Combustor scaling represents another source of challenge, which should be seriously compromised by the non-linearity of chemical reaction times and dissipative processes. Therefore, it is critical that supersonic combustor testing be accomplished at or near full scale [25].

For the supersonic mixing studies, it is suggested to investigate the effect of the injection angle of the main fuel on the supersonic mixing and combustion characteristics. It is recommended to study the effect of the transverse normal ethylene and propane injections on the flame holding and combustion characteristics in order to investigate the relationship between the injection scheme and the flame holding and flow field and energy field features. It is suggested to simulate the supersonic combustion of the normal ethylene and propane injections with the pilot gaseous hydrogen. For the future studies, it is suggested to dedicate more effort trying to carry out the simulation of the supersonic combustion of liquid kerosene with gaseous hydrogen as a pilot fuel. The radiative interaction is also suggested to be included in the future studies due to the existence of the hydrocarbon combustion products, which are radiative participating medium.

1.3 Objectives of Present Study

The primary objective of the current study is to numerically examine the possibility of igniting hydrocarbon fuels in supersonic airstreams and maintaining the hydrocarbon flames in such hostile environments. The secondary objective of the study is
to investigate the effect of the combustor configuration, the main fuel equivalence ratio, and the pilot fuel equivalence ratio on the flame holding mechanism and the flow field and energy field characteristics.

The combustion characteristics of gaseous propane in supersonic airflow using the rearward-facing step that is swept inward form both end sides is studied. The effect of sweeping the rearward-facing step from both end sides, in the cavity configuration, on the flow field features of propane combustion is investigated.

Next, an extensive study for the flame holding and mixing and combustion characteristics of gaseous ethylene in supersonic airstreams is carried out. In this study, different combustor configurations, different main fuel equivalence ratios, and different pilot fuel injection equivalence ratios were employed. First, The effect of the combustor configuration on the temperature flow field and the flow structure is investigated by simulating two different combustor configurations, the rearward-facing step and the cavity. Next, the effect of the equivalence ratio of the main fuel injection on the general flow field features and energy field characteristics is studied. Lastly, the effect of the pilot fuel equivalence ratio on the flame holding mechanism, and the combustion and flow field qualities concludes the study. The equivalence ratios examined are ranged between 0 and 0.08.

1.4 Work Layout

The current study is presented in the following logical manner. An extensive literature survey for the related previous work is compiled in Chap. 2. The theoretical formulations and code description are provided in Chap. 3. Chapter 4 presents and discusses the results for the supersonic propane combustion while the obtained detailed results for the supersonic ethylene combustion are analyzed and discussed in Chap. 5. Finally, concluding remarks on the supersonic combustion of hydrocarbon fuels in scramjet engines are provided in Chap. 6.
Chapter II

LITERATURE SURVEY

2.1 Introduction

A supersonic combustion RAMJET or SCRAMJET has long been considered to be a feasible engine concept for hypersonic vehicles [7]. Figure 2.1 shows a schematic of a SCRAMJET engine concept where the aircraft underbody and engine designs are integrated together [26].

The shock waves formed by the vehicle forebody and the engine inlets serves as the engine compressor section while the engine exhaust and vehicle afterbody serve as the expansion nozzle to generate thrust from the gases burned in the combustor. The surface geometry would be chosen so that supersonic flow would be maintained throughout the internal passages of the engine avoiding large recovery of temperature and pressure from the free stream air [27]. The essential features of two-dimensional or planar geometry scramjet engines are diagrammed in Fig. 2.2 [26].

Figure 2.3 shows the Airframe-Integrated supersonic combustion ramjet (scramjet) along with a partial cross-section through a typical modular engine. The sidewalls of the inlet continue the compression process, which began on the vehicle forebody. The instream struts complete the compression process and also provide locations for global distribution of fuel. The particular concept depicted here shows a combination of perpendicular and parallel fuel injection, which would typically take place behind a rearward-facing step and at the base of the strut, respectively [28].

2.2 Injection Modes and Mixing

The thermodynamic conditions at the test section entrance of the Scramjet engine are representative of the conditions of the lower end of the hypersonic flight regime. For these vehicles it is anticipated that the fuel be used to cool components of the vehicle and of the engine and, thus, enter the test section at high temperatures (even a supercritical conditions), resulting in fast vaporization and mixing upon injection. The low range of hypersonic flight regime is, therefore, of particular interest, since the level of heating of the fuel will be relatively low, and thus longer residence time will be required for the fuel.
to achieve complete combustion within the engine combustor. The mixing-combustion coupling at these conditions is of great interest [21].

Supersonic combustion ramjet (scramjet) propulsion systems rely on injection and burning of fuel in very high speed flow fields. In such an environment the fuel remains inside the combustion chamber for such short durations that rapid mixing of the fuel into the freestream air is essential for an acceptable design [29]. Rapid mixing ensures the shortest possible combustor length and maximizes the heat release from the combustion, whereas a uniform distribution of fuel within the combustor optimizes combustion efficiency and minimizes the amount of air processed by the inlet that does not participate in the combustion. Clearly, an understanding of the fundamental fluid mechanics of compressible mixing is essential to a successful supersonic combustor design [30].

Fuel-air mixing in an air-breathing engine becomes increasingly inefficient at higher velocity, hence requiring a longer combustor length. Although this is caused by the reduced flow residence time inside the combustor and the compressibility effect that adversely affects the rate of mixing [31-33], a short combustor length is desirable because the thrust-to-drag ratio of an engine is roughly proportional to the ratio between the combustor diameter and length [34].

Injection and mixing enhancement play important roles in successfully designing a hypersonic air-breathing propulsion system. This is especially true when a liquid hydrocarbon fuel is used. Several fundamental studies have focused on liquid fuel injection from the walls of combustors or from bluff body flame-holders into subsonic or supersonic crossflow [35-37]. Several fuel injection schemes, such as angled injection [38], non-circular nozzles [39], and ramp injectors [40], have been studied in attempts to create deeper fuel penetration into the air stream for better mixing and to generate smaller droplets of the liquid spray for faster evaporation [41]. Various mixing enhancement schemes have been proposed including contoured injection orifices, flow field and shock oscillations, baroclinic vortex generation, and wall-mounted vortex generators [23].

If the heat release by the combustion process becomes greater than a critical value in a scramjet engine, the Mach number falls to unity and the flow becomes thermally choked [42]. This choked flow may, in turn, cause a normal shock to form at the engine inlet. This process, known as “unstart,” creates large amounts of drag and radically
reduces the performance of the engine at high flight Mach number [43]. The numerical results of Moon et al. [44] suggest that there would be two possibilities to trigger thermal choking, such as 1) strong turbulent mixing, and 2) instability of shear layer between incoming air and fuel jet. McDaniel and Edwards [45] studied the dynamic simulation of thermal choking in a nominally two-dimensional scramjet isolator/combustor configuration.

The fuel-injection modes are used to control heat release. At lower speeds (below Mach 5, and to some extent Mach 5-7, too much heat release too early in the combustor will result in thermal choking and inlet unstart. Parallel fuel injection, which is shown to have a slower-mixing process, is therefore used extensively to stretch out the combustion zone. Above Mach 7, thermal choking is much less likely to occur, and the faster-mixing perpendicular injection process is utilized to get faster combustion and higher performance. In order to quantify this mixing-controlled combustion philosophy, a considerable amount of research has been done on perpendicular and parallel mixing [24].

Different methods of liquid fuel injection have been investigated. Parallel flow mixes through the growth of the shear layer generated at the interface of the different components. It is observed that compressibility plays a major role in reducing the growth of the shear layer, thus requiring longer fluid residence time to insure good mixing in practical devices. As the compressibility increases, the spreading rate of the shear layer was observed to drop to about one quarter of the compressible shear layer growth for the same velocity and density ratios of the two mixing constituents. The convective Mach number (defined as a measure of the speed of the turbulent structures in the shear layer relative to the free stream) increases the stability of the large-scale turbulent structures, which are responsible for the turbulent shear layer growth. This is of particular significance in high-speed flows, where parallel injection is the preferred mode due to the lower total pressure relative to the other fuel injection and mixing options. An increase in the stability of the large vortical structures in the shear layers due to compressibility is observed even in situations where the turbulence is intentionally intensified. Growth of the shear layer was forced by a pulsating shock impinging on the shear layer in parallel compressible flows in high speed (i.e., Mach 3 and 5, respectively) as a destabilizing
mechanism leading to the growth of the shear layer and accelerated mixing. Only a negligible effect was obtained both in the near and far field. However, when a shock of the same strength impinged on the boundary layer of the two flows prior to their coalescence, an increase in the shear layer growth (14 to 26 percent) was experienced. Thus, an increase in the turbulence in the boundary layer upstream of the mixing station increased, causing an increase of as much as 26 percent in the shear layer growth. This indicated the significant role played by the small-scale turbulence in the mixing process. Introduction of axial vorticity was shown to improve mixing, which was also attributed to the small-scale turbulence effect on the growth of the shear layer and on the enhancement of turbulence in the shear layer. Mixing at a molecular level is, in particular, important in combustion applications when stoichiometric mixing is a prerequisite to initiate chemical reactions [21].

Mohieldin and Tiwari [46] studied numerically the advantage of using the tandem injection on the regular single step tangential injection regarding the mixing aspect in the flow field.

Studying the flow field behavior of the transverse injection of the fuel is one of the recent demanding research trends in the combustion field of the scramjet engine. This technique is used to increase the fuel-air mixing in order to achieve the required heat release pattern with the short combustion residence time associated with the high Mach number condition [6].

Figure 2.4 shows a schematic of the region surrounding a single perpendicular injector. Because the mainstream flow is supersonic, there is a bow shock off the underexpanded fuel jet and internal wave structure associated with the jet expansion. The boundary layer ahead of the jet separates, and there is a recirculation zone downstream of the injector as well. The details of these local zones are quite important to the ignition, flame holding, and combustion processes and therefore important to real combustor design [24].

Schetz et al. [47] presented a comprehensive review of the mixing of transverse jets and wall jets in supersonic flow. While the streamwise injection has the advantage of adding to the thrust component of the engine, many of the approaches utilized to improve the wall injection have been used successfully to enhance the fuel-air mixing [6].
A numerical study was conducted by Lee et al. [48] for the mixing and burning augmentation of the transverse injection in a scramjet combustor. Based on the fact that the main factor controlling the mixing characteristics in transverse injection is the backpressure around the injection hole, it was tried to make a flow expansion beside the injection hole with a cavity in order to reduce backpressure around the front hemisphere of injection hole. It was concluded that the near field has convection dominated regime whose mixing and burning processes are accelerated by convective flow, while the far field has diffusion dominated regime whose mixing and burning processes are dominated by mass diffusion.

The effect of the staged hydrogen fuel normal injection in supersonic air streams was studied numerically by Drummond and Weidner [49]. In comparison with the single normal injection, the staged normal injection produced a much larger region of separation around the injectors. The separated region becomes significantly larger with increased spacing, and the fuel-air ratio there moves closed to stoichiometric increasing the amount of reaction. Staged injections provided two important requirements for improved flame holding, a large separation that increases residence time of the fuel-air mixture, and a more favorable fuel-air ratio for reaction. Increasing the spacing between staged injectors was anticipated to improve these qualities even more.

The axially staggered laterally inline step-injector configuration was investigated by McClinton [50]. Both the top- and bottom-wall blocks incorporate a rearward-facing step located ahead of the injection orifices. The top wall step is located upstream of the bottom-wall step. Four fuel injectors were equally spaced in each wall. The results are compared with results of previous investigations made in this combustor model by using laterally staggered rather than opposed injectors. The opposed injector configuration eliminated the adverse lateral pressure gradient experienced at the downstream injectors in the staggered injector configuration and strengthened the gradient over that produced by single-wall injection.

The experimental study of King et al. [51] showed that the combination of a moderate pressure, sonic normal injection combined with a tangential slot flow is preferred for the mixing enhancement over the tangential slot injection alone. This
scheme produces total mixing layer spreading angles up to 70% greater, and hence more
total mixing layer growth, than the slot injector alone.

Transverse or inclined injection introduces different mixing mechanism. At a
macro-scale, axial vorticity is produced at the edges and above the jet as the main flow
surrounds the jet in an axial and transverse direction. These vortices break the plume and
entrain the injectant into the core flow. The level of mixing obtained by this strong
momentum exchange is traditionally quantified by the degree of penetration and
concentration decay of the jet injected into the main flow, usually air [21]. Studies
performed by Mays et al. [52] and Wood et al. [53] addressed the effect of small-scale
turbulence on transverse injection and mixing. It was suggested that the onset and
divergence of instability in the jet is ultimately responsible for the plume fracture. This
instability propagates upstream and produces additional turbulence in the core flow. Even
in supersonic flows, an upstream interaction exists, as the instability at the jet boundary
induces oscillations of the bow shock generated in front of the jet via the separated region
in front of the jet. In turn, these shock oscillations contribute to increase the vorticity in
the flow [21].

An important feature of the normal injection flow field is the gross penetration of
the jet into the flow. Baranovsky and Schetz [54] introduced the injection angle as a
separate parameter in the correlation, which was set to evaluate the penetration of liquid
jets. It was found that the upstream injection (injection angle is greater than 90° with
respect to the incoming air flow direction) can be used as a method to increase
penetration and residence time of a liquid fuel into a scramjet combustion chamber. It
was also found that the maximum penetration takes place at injection angle (θ) =135
degrees.

Flow field and combustion/ignition characteristics of a supersonic combustor with
a fuel injection strut were examined experimentally and computationally by Masuya et al.
[55]. Both normal and parallel injections were employed through the strut. Normal wall
injections were added to the strut injection. Pilot injections upstream of the strut and wall
injections were used. Plasma torch port is located on both sides of the strut to force
ignition. Mixing and combustion efficiencies for a more disturbing strut were higher than
those for a less disturbing strut due to more severe deceleration and disturbance of the
airstream. Mixing and combustion efficiencies of fuel injected from the struts were almost linearly increased with an increase of the flow rate ratio of the perpendicularly injected fuel to the total fuel. Fuel from the strut ignited at a lower air temperature than that from the wall in both the autoignition and the forced ignition conditions. The twin plasma torches with pilot injection could ignite perpendicular fuel jets of both paths without time lag, and they could also ignite parallel jets from the base of the strut. Ignition limits with the plasma torch were extended by increasing the pilot fuel flow rate.

Flame stabilization and combustion, along with wall friction and heat-transfer losses, are the major processes of concern in the supersonic combustor in addition to the fuel injection and mixing processes. Flame stabilization and combustion are intimately tied to the fuel injection, vaporization, mixing, and ignition processes as well as combustor geometry. As such, just about all of the experimental combustion data available are configuration dependent. Thus, flame stabilization is achieved by using a rearward-facing step and efficient combustion by initially eliminating and finally restricting the acceleration (or expansion) rate of the flow to prevent quenching of the reactions over a wide range of initial conditions [11].

Using the rearward-facing step in the supersonic combustors and injecting the fuel perpendicular or at least inclined to the main air flow have the advantage of holding the flame because of the existence of the separated and recirculating regions in the flow field as depicted in Fig. 2.4. This can help in solving, in part, the complication of holding the flame in supersonic engines due to the fact that the flow in such engines is not premixed which means that if bluff bodies are to be used as flame-holders they have to be large. This is highly undesirable in supersonic combustors due to very high drag. Therefore, this problem of flame holding could be solved using the rearward-facing steps in the combustors and/or the perpendicular fuel injection. This issue emphasizes the importance of flow field details around the fuel injectors [24].

Segal et al. [56] conducted an experimental study of transverse hydrogen injection and combustion behind a reward-facing step into a Mach 2 high temperature clean-air. The experiment was conducted in an electrically heated (not vitiated), continuous-flow facility to evaluate the effects of initial conditions and analyze the interaction between mixing and combustion in supersonic reacting flows. This work and the earlier non-
reacting data for the same combustor reported in [57] provide new experimental data for supersonic combustion of hydrogen using clean air. Matsuo and Mizomoto [5] studied the flow structure of supersonic flow of Mach 2.5 past a backward-facing step with perpendicular sonic injection from the bottom wall. They examined the effect of both the step height and dynamic pressure ratio of the jet flow to the main flow using the perfect gas condition in two-dimensional space. The effect of H$_2$-transverse injection on the characteristics of the flow field was investigated numerically by Berman et al. [58] using both adiabatic and constant temperature wall boundary conditions.

The experimental study of Jian-Guo et al. [59] concluded that the 90° rearward-facing step enhances the mixing pattern of the kerosene-hydrogen dual fuel system in comparison to that of the 45° step. This is attributed to the lower recovery temperature in the 45° step case, which leads to the poorer mixing of the pilot hydrogen and the supersonic air. It needed more hydrogen to produce enough radicals to ignite the kerosene spray.

The flow over a ramp induces a pair of counter-rotating stream-wise vortices as shown in Fig. 2.5 [60]. Supersonic flow over a ramp generates both shock and expansion waves. This leads to the generation of the vorticity by baroclinic torque. Baroclinic torque is exerted on a fluid flow whenever the density and pressure gradients are not parallel [61]. Numerous ramp designs have been investigated. In the work of Stouffer et al. [62] an array of compression and expansion style ramps were investigated whose geometry is shown in Fig. 2.6. In these studies, hydrogen was used as the fuel and air as the oxidizer. In these concepts, rapid turns in geometry induce formation of shocks, which for compression ramps occur at the base and for expansion ramps at the trough. Dramatic differences were found in mixing and combustion efficiency between these two styles. It is well known that, for the same ramp angle, vorticity shed from a compression ramp induces much stronger vorticity than that from an expansion ramps due to differences in projected stream area. Despite significantly improved fuel/air mixing from the compression ramps, the expansion ramps achieved higher combustion efficiency. This result may be expected because good combustion efficiency is achieved with mixing at small scales. The extremely strong vorticity of the compression style ramp, while

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increasing the fuel/air contact area also provides a centrifuge that diminishes opportunity for mixing.

Ramp fuel injectors have also been designed with sweep to control shock and expansion waves. Tests conducted at NASA Langley Research Center show that combustion efficiency of swept ramp injectors is much improved compared to those without sweep. The ramp with sweep approaches the combustion efficiency that is achieved with normal injection. The effect of ramp sweep was numerically investigated by Drummond et al. [63] and Donohue et al. [29], who also performed experimental planar laser induced iodine fluorescence measurements. Their calculations confirm the importance of using sweep for the ramp injectors.

There are a number of studies specifically related to the 3-D mixing flow field of ramp injectors. Hartfield et al. [64] presented measurements of injectant mole fraction in the flow field of a swept ramp with air injection using the same technique used by Donohue [33]. The results illustrated the strong effect that ramp generated vortices have on the mixing process. Waitz et al. [65] presented both numerical simulations and experimental measurements of total pressure and fuel concentration for helium injection behind an unswept ramp, which added the effect of baroclinic vortex generation when a low density fuel is used. Riggins et al. [66] presented numerical simulations of the mixing flow fields of both swept and unswept ramps with hydrogen injection into high temperature air and went on to calculate the reacting flow field as well using the SPARK code. The study showed substantially higher mixing as well as flow losses for the swept ramp case. It also showed increased penetration and spreading of the jet plume in the reaction case. Daso and Gross [67] computed the flow field behind swept and unswept ramps with air injection using the USA code and illustrated how side sweep of the ramp significantly increased the mixing downstream. A numerical study designed to investigate the relative importance of ramp generated vortices vs. baroclinic vorticity on supersonic mixing behind swept ramps was performed by Donohue et al. [68].

An experimental investigation was conducted by Fuller et al. [69] to compare the performance of the aero-ramp injector with a physical ramp injector to enhance mixing in supersonic flow. The scope of the investigation focused on jet penetration, mixing characteristics, and total pressure losses. The aero-ramp exhibited a significant increase
in jet penetration when the jet-to-free stream flux ratio was increased from 1.0 to 2.0; however, the physical ramp showed very little change. The aero-ramp produced superior mixing in the near field and slightly less than comparable mixing in the far field. Thus, the mixing performance decreased with increasing jet momentum for the physical ramp while it increased for the aero-ramp. The pressure losses induced by the physical ramp were more severe.

A numerical parametric study of the cantilevered ramp injector for various geometric parameters was conducted by Schumacher and Sislian [70]. Unlike the conventional ramp injectors, the sweeping of the sidewalls of the cantilevered ramp injector does not translate into appreciably superior mixing performance, due mainly to the increased strength of the reflected shock, which drives the fuel jet to the lower wall into regions of low vorticity.

Cox et al. [71] proposed a new injector concept for secondary gaseous injection into a supersonic crossflow to improve the fuel/air mixing. The basic idea is to arrange an array of flush-wall injectors in such a way as to induce large vortical structures in the main stream to increase entrainment and mixing. Both the experimental and computational results they got demonstrated the creation of large-scale vortices in the mixing region, as intended.

Shock waves have been used to enhance mixing. The fuel is injected in the intake region where the temperature and pressure are sufficiently low so that combustion does not occur. By injecting in the intake region, the fuel has time to mix before its pressure and temperature are finally raised as it enters the combustion chamber. This increase in pressure and temperature is generated by passing a shock through the mixture. Buttsworth [72] demonstrated that shock cannot only be used to promote ignition, but they can also be used to generate vorticity as they cross the fuel-air mixing region, and, thus, can be used to enhance mixing.

It is understood that there exists a strong interaction between mixing and combustion, even in the limiting cases when one or the other becomes rate controlling. Due to this coupling, observations from mixing in non-reacting flows are hard to extend directly to reacting flows. Furthermore, in many practical situations, the Damkohler number, defined as the ratio between the characteristic fluid residence time in the reaction
zone and the chemical reaction time scale, is $O(1)$. In such cases, the flow field may become either mixing or kinetic limited in localized regions; however, in general, combustion takes place in thick, highly turbulent burning regions. The mean and time varying parameters responsible for mixing are affected by heat release, which, in turn, affect the chemical kinetics; thus, mixing and combustion become closely coupled [56].

When heat release effects are included, significant modifications of the turbulent structures occur. It has been indicated that the heat released from chemical reactions both generates and suppresses turbulence. It is shown that the turbulent dilation and viscous dissipation in flames reduce small-scale turbulence, while the shear gradient effects, mainly of pressure and density, generate new large-scale structures [21].

The effect of small-scale turbulence on the mixing process in high-speed flows requires more detailed investigation. In particular, mixing at a molecular level, which indicates the ability to initiate chemical reactions, is of great interest. Concentration distribution is not sufficient to provide this information. Although it is recognized that a reacting flow field is substantially modified once exothermic reactions take place, mixing of non-reacting flows needs further investigation to provide further insight of the characteristics of the micro-mixing processes [21].

The effect of the chemical reaction on the flow field characteristics of the normal injection of sonic hydrogen downstream of a rearward-facing step in supersonic airstream was investigated in [73]. The comparison between the non-reacting and reacting flow fields showed that the combustion heat release precluded the flow expansion around the step edge; instead, the released heat was sufficient to cause a shock compression of the main flow immediately behind the step. The reacting jet has a completely different structure. In the non-reacting case, the jet has the characteristic barrel shape of an underexpanded jet, ending with a normal shock. Because of the heat release, the fuel jet penetrate sufficiently deeper into the main flow, approximately 80% more than in the non-reacting situation.

The effect of the heat released by combustion on the fuel/air mixing distribution in the supersonic reacting flow field was studied experimentally by Abbitt et al. [74]. Hydrogen was injected transversely as staged, underexpanded jets behind a rearward-facing step into a ducted Mach 2 air free stream. The pressure rise associated with the
heat release involved in the reaction forces a rapid lateral displacement of the fuel towards the side walls. A large amount of burning, therefore, occurs on the side walls. This would suggest that the mixing distributions observed in the non-reacting flow field was greatly altered. The wall limited the amount of spreading that would otherwise occur, and possibly induced some recirculation or deceleration of the flow, which could aid in flame holding.

Effervescent (or aerated-liquid, or barbotaged) atomization, characterized by introducing gas bubbles directly into a liquid flow immediately upstream of the injector orifice to generate a two-phase flow, has been extensively studied for quiescent environments [75-78]. Depending on the amount of gases added into the liquid jet, two primary mechanisms generate small droplets in the effervescent atomization process. It has been observed that droplet size could be reduced as the amount of gas added to the liquid flow increased. Based on this observation, there is considerable interest in examining the role of effervescent atomization in enhancing the mixing and vaporization processes in a scramjet combustor [79, 80].

In their recent work on the atomization performance of aerated-liquid jets, Lin et al. [81] applied the effervescent atomization technique to the problem of fuel injection into a supersonic crossflow. The spray penetration heights of aerated-liquid jets were studied experimentally using wide ranges of liquid properties, nozzle orifice diameters, jet-to-air momentum flux ratios, and barbotage gas-to-liquid mass ratios. Two different modes of spray structures for aerated-liquid jets in supersonic crossflows were identified—pure liquid mode spray and barbotage mode spray. It was observed that the overall breakup process for pure liquid mode spray is slow and that greater axial distance is required to generate fine droplets. On the other hand, liquid breakup processes for barbotage mode spray occur immediately after or even before the liquid is discharged. This is primarily due to the highly turbulent features of this inhomogeneous two-phase flow and the expansion caused by high-pressure barbotage gas. These two modes of spray appear randomly and alternatively for low levels of barbotage [41].

Avrashkov et al. [82] developed a system for the kerosene injection into a supersonic flow. This system is based on two main principles: firstly, the use of tubular micropylons, and, secondly, the saturation of fuel with gas bubbles. The use of
micropylon allows to arrange uniformly the fuel jets in the flow and to increase considerably their number. Immediately before the liquid kerosene injection, the saturation of fuel with gas bubbles (i.e., the bargotage) is made. On the whole, the use of tubular micropylons and liquid fuel bubbling permit to increase significantly the process of mixture formation under conditions of supersonic flow.

Critical issues regarding fuel injection and mixing in a scramjet combustor are discussed in details in the literature [6,83,84].

2.3 Auto and Forced Ignition

Ignition delays of conventional hydrocarbon fuels must be significantly reduced for successful supersonic combustion [85,86].

McClinton [87] showed that combination of the step-base and the perpendicular injection downstream of the step was effective in enhancing the ignition ability. The effect of a variety of parameters on the autoignition behavior was studied. The free-stream total temperature, wall temperature, and wall boundary layer energy deficiency have the greatest impact on autoignition. Injectors located within three step heights downstream of a step are shown to have very poor autoignition characteristics. But when the injectors are moved downstream, autoignition behavior is improved. Sweeping the step and fuel temperature produced only slight changes in autoignition behavior. Injection angle was shown to have a significant impact on autoignition: upstream injection improved ignition, and downstream angled injection impaired autoignition. Huber et al. [88] suggested possible autoignition source in the supersonic combustors and proposed a simple model to predict ignition limits in typical combustors. These candidates are the base region behind steps and struts, recirculation regions upstream of the fuel jets injected perpendicular to the airflow, and the stagnant region behind the bow shocks upstream of the fuel jets. The study reported that autoignition of fuel from struts occurred easier than that from the wall because the strut had a thinner boundary layer that resulted in a higher surface temperature than the wall.

Tomioka et al. [89] investigated the flow field at pre-ignition phase in a supersonic combustor with perpendicular injections behind a backward-facing step to understand the mechanism of the ignition enhancement observed in the ignition tests with the same combustor. It was concluded that the interaction of the separation region
upstream of the fuel jet and the two-dimensional step base-recirculating region, namely
the merging of these two regions, caused enlargement of the ignition region and the
enhancement of the ignition ability. Ignition parameters were compared for the cases with
and without the step. As a result, the interacted region in case with the step was found to
be more preferable ignition source due to its enlarged size.

Autoignition of hydrogen fuel injected into a scramjet combustor does not occur
at low flight Mach number and an igniter is required [87,90]. Several kinds of igniters
[91-95], have been tested. Among them, a plasma torch is one of the most promising
igniters for a supersonic combustor. It is not pyrophoric, toxic, or corrosive, and it is safe
and reliable to use in a propulsion system of the aerospace plane [94]. Kimura et al. [95]
first applied the plasma torch to ignite a fuel jet in supersonic airstream. Northam,
O’Brien, and their associates found that an argon-hydrogen plasma torch is an effective
igniter [96] and developed an uncooled long duration torch [97]. They showed a strong
sensitivity of the plasma igniter performance to the combustor geometry and/or fuel
distribution, and designed a new injector suitable for the plasma igniter [98,99]. Sato et
al. [100] developed and tested a new plasma torch with oxygen or air as a feedstock,
which may be advantageous from the view point of the total aerospace plane system.

The effects of various operational parameters of plasma torches as well as
combustor geometry and fuel injection location of the ignition of hydrogen were
experimentally studied in supersonic combustor by Masuya et al. [94]. The ignition
temperature was found almost linearly decreased as the input electric power increased.
Adding small fraction of hydrogen to the argon plasma torch igniter was found to
increase its effectiveness. The chemical effect of the plasma torch was considered to be
the main reason of this improvement.

Two simultaneous ignition sources, a spark plug and a plasma torch mounted in
the cavity floor, were used in the combustion of liquid JP-7 in the scramjet USAF
combustor used by Mathur et al. [41]. It was noticed that turning off the ignition sources
in the cavity did not have any detrimental effect on the combustion.

The issue of the ignition delay of hydrocarbon endothermic fuels was investigated
by Hawthorn and Nixon [101]. They studied the ignition delay of propane-air and
methylocyclohexane-air mixtures and compared them to hydrogen-air and methane-air
mixtures. It was found that the ignition delays of propane and methycyclohexane fuels are greater than those for hydrogen at temperatures below 1800 F, but significantly lower than those for methane. For temperatures above 1800 F, it appears that these hydrocarbons may have ignition delays comparable to that of hydrogen.

The ignition delay of RP-1 (kerosene) was reduced by adding an accelerant (Alex® nano aluminum powder) as indicated in the work of Tepper and Kaledin [102]. This accelerant was found to reduce the ignition delay, while increasing the volumetric energy density of the hydrocarbon, which is an added benefit.

Ignition characteristics of a scramjet combustor with a strut may be different from those without a strut. The ignition characteristics of fuel from the strut were compared with those of fuel injected only from the walls [90,94,100]. Installation of struts divide the combustor into several flow paths, ignition of fuel jets in each flow path would occur independently. At least one igniter should be attached on each stream tube [55].

2.4 Vitiated and Clean Incoming Air

In order to provide the proper ground-based facilities for testing the supersonic combustors, the test stagnation conditions must be on the level that matches the flight conditions. Therefore, it is necessary to heat the incoming supersonic air. Typical heating techniques used to generate this high enthalpy include electric arcs, combustion of hydrogen or methane fuels in air with oxygen replenishment, or storage heaters. The use of an electric arc heater results in air dissociation and the generation of significant amount of nitrogen oxides, as well as a depletion in the net level of oxygen below 21% by volume. In combustion heaters, the flow constituents are a function of the fuel used; for example, with hydrogen burner H₂O is a primary contaminant, or with a methane heater a combination of both H₂O and CO₂ are the primary contaminants. Due to the presence of these test flow contaminants, the combustion characteristics in a ramjet or scramjet engine can potentially be different than results obtained in clean air or actual flight [103].

Differences between testing in air and vitiated air could be due to differences in thermodynamic properties and chemical kinetic effects. Thermodynamic effects include differences between the heat capacities of H₂O and CO₂ compared to N₂. The heat capacities for both H₂O and CO₂ are substantially higher than N₂. Therefore, for the same
amount of water formed, the temperature rise in vitiated air will be less than that in air. The temperature rise in vitiated air would also be less than that in air due to dissociation of some of the additional H₂O in the vitiated air. Chemical kinetic effects will also be different due to the presence of CO₂ and additional H₂O in the vitiated air as well as additional chemical kinetic reaction [104].

Various studies, [105-110], have explored the effect of NO, H₂O, and CO₂ contaminants on combustion processes, primarily with hydrogen fuel with application to hypersonic propulsion systems. These include both experimental and computational studies. A general trend from these works is that H₂O and CO₂ have a minimal influence on the kinetics of hydrogen-air combustion while NO serves to reduce both ignition and reaction times. The range of temperature and pressure investigated and the database with fuels other than hydrogen are limited. Lai and Thomas [103] investigated numerically the effect of NO, H₂O and a combination of H₂O and CO₂ on combustion of various fuels including hydrogen, ethane and methane with air. Srinivasan and Erickson [110] studied the influence of the effects of vitiation for a relatively simple flow configuration but with a full 3-D computational flow model including mixing, finite-rate reactions, and appropriate thermodynamic properties. Srinivasan and Erickson [104] used the same simple 3-D combustor model to simulate the influence of vitiated air, as compared to air, in the combustion of hydrogen injected at an angle of 30° into a confined supersonic flow with equivalence ratio approaching unity. Computations have been made for air and vitiated air with the same set of initial (except for the molar composition) and boundary conditions. Many numerical works have reported the effect of vitiated air via H₂O and radicals. Bakos and Morgan [111] conducted an experimental and numerical investigation to study the effects of test air contamination by atomic oxygen on hydrogen fueled scramjet combustion in hypervelocity environments with Mach 5 test flow.

In the past, many researchers have used vitiated air, numerically and experimentally, to calculate ignition delay time, ignition temperature, and combustion efficiency. Experimentally, vitiation often occurs in chemically heated facilities, in the form of water vapor or hydrocarbons reaction products. Mitani et al. [112] investigated experimentally the effect of vitiation on the combustion performance of scramjet engines at Mach 6. Both Vitiated Air Heater (VAH, V-mode) and Storage Air Heater (SAH, S-
radical pool, which could decrease the overall timescales of hydrocarbon consumption. Furthermore, endothermic fuel reactions can be expected to improve the fuel’s combustion properties, if for no other reason than the fuel enters in a hot vaporized state. Moreover, the mixing length of a supersonic combustor is theoretically proportional to the square root of the molecular weight of the fuel. Therefore, the large amounts of hydrogen generated from endothermic reactions such as reforming might also be expected to also improve the fuel’s combustion properties [119].

Quite a large number of liquid fuels and fuel pilots for scramjets have been tested in connected-pipe combustor and free-jet engine tests [120-124] in an attempt to find a fuel that is energy-density efficient, would burn to near completion in the residence times available (typically < 1.5 ms), and also be logistically suitable. Unfortunately, those fuels, fuel blends, and pilots that did perform well were not logistically suitable, i.e., they contained toxic, pyrophoric, or carcinogenic components that were unacceptable. Monopropellant pilots, which are logistically suitable, were also tested, but could not sustain the desired degree of heat release [125]. Thus, there still exist a need to develop a high-energy density, storable liquid fuel or fuel that is both highly reactive and safe [14].

Silane (SiH₄) is a pyrophoric gas that can be added to hydrogen to decrease ignition delay times of the fuel. Morris [126] made an experimental investigation into the ignition limits of different mixtures of silane and hydrogen. It was concluded that silane is a useful additive to produce ignition in hydrogen when the intake temperature of the combustion chamber are below that where spontaneous combustion of hydrogen would normally occur. Furthermore, the addition of silane will also decrease the ignition delay time.

2.5.1 The Problem of Cooling in High-Speed Vehicles and The Role of Fuel

As air breathing-engine-propelled vehicle speeds increase, thermal problems multiply because of the effect of stagnation temperature. While total cooling needs increase, the most critical regions are the leading edges and the engines. Although thermal effects can be somewhat accommodated by improved materials and passive cooling, sustained hypersonic flight in the atmosphere requires a substantial heat sink. Compared to a mechanical refrigeration system or a non-combustible coolant, the fuel is the best source of cooling [127].
In the high Mach number region of the flight envelope (M>4), aerodynamic heating is too great for conventional structural materials to survive without active cooling. The fuel not only must have a good heat-of-combustion but also must provide the necessary heat sink for the cooling system [128].

Higher aircraft speeds also have a direct impact on the operating environment a jet fuel will encounter. The higher speeds mean higher air stagnation temperatures, which increase the aircraft cooling requirements and prevents the use of air as a coolant. Thus, increasing engine thrust-to-weight ratio and aircraft speed result in large heat loads that must be managed with the main coolant available on the aircraft--the fuel [129].

The fuel in modern military aircraft is the primary coolant for on-board heat sources. It is used to cool aircraft components such as the engine lubricant oil, hydraulic fluid, environmental control system (ECS), avionics and electrical systems, and at high Mach numbers, the airframe. As aircraft and engine technology have advanced from the F-4 to tomorrow's advanced fighter, the heat sink requirements of the fuel have increased significantly. The engine is the main heat source for the aircraft at Mach 3 and below, but the ECS is becoming an increasingly important part of the heat management problem. Fuels used in high-speed aircraft will have to absorb large amounts of excess heat for aircraft thermal management purposes. This will result in the fuels being heated to supercritical conditions [129].

Fuel is circulated through hot sections of the aircraft, usually back into the tanks, and finally to the engine where it is burned. This "recuperative" approach has the benefit that thermal energy dumped into the fuel is then eventually recovered as additional thrust [130].

2.5.2 Endothermic Fuels, The Promising Fuel for Hypersonic Combustion Systems

Definitions of and differences between cryogenic and endothermic systems: The "Cryogenic" fuels are the fuels that have a negative, less than zero, "Boiling Point." Therefore, in order to use these fuels as liquids, they must be cooled beyond the boiling point and storage environments must satisfy this condition. Examples for the cryogenic fuels and their corresponding boiling point temperature are the liquid hydrogen H₂ (-423 F) and liquid methane CH₄ (-259 F).
The "endothermic" fuels are the fuels that extract heat while forming from their initial components. Therefore, the decomposition of these fuels into the initial components requires energy for its accomplishment and by that a quantity of heat can be absorbed from the surrounding environment causing the required thermal loading management of the vehicle. An example for the endothermic fuels is the methylcyclohexane MCH (C\(_6\)H\(_{11}\)CH\(_3\)). The boiling point of MCH is 213 °F, which means that it is a liquid in the normal ambient conditions.

**Cryogenic fuels: advantages and disadvantages:** The cryogenic fuels have high energy contents and thermal tolerance. Figure 2.7 shows that hydrogen has almost three times higher energy per unit mass than other fuels [130].

The temperature limit of a fuel is a key consideration for its selection as a high-speed transport fuel. Figure 2.8 shows that hydrogen has the highest temperature limit over other fuels [130]. On the other hand, Fig. 2.9 indicates that cryogenic fuels have relatively poor energy contents per unit volume, which is an undesirable property that is magnified by their storage requirements [130].

Cryogenic fuels must be viewed with extreme caution because of the severe constraints that they place on the design of the aircraft and because of the high cost of transporting, storing, and delivering them. Hydrogen or methane handling facilities at just a few U.S. airports would be very costly to install and maintain, and of course these fuels raise serious safety questions. From the military standpoint, cryogenic fuels appear impractical because, again, military operations must not be tendered by a need for costly and exotic infrastructures, and by all means not by an uncertain and vulnerable supply of mobility fuels. Nevertheless, serious consideration is being given to such option and it is possible that successful large-scale applications using hydrogen or methane might eventually be developed [130].

**Endothermic fuels: the phenomenon and advantages:** An innovative approach based on more conventional types of fuels takes advantage of the fact that some hydrocarbons, when they degrade at high temperatures, do so cleanly, i.e., without forming carbonaceous surface deposits. Instead, they break down to smaller hydrocarbons that are then circulated to the combustor. The chemical breakdown itself absorbs heat, thus providing another useful thermal management process. A number of these "endothermic"
fuels are known, and some are under serious study. All of the known endothermic fuel reactions require a catalyst to make them proceed and absorb extra heat at moderate temperatures. Hence, variants such as the catalytic heat exchanger are being considered in future aircraft concepts. While the endothermic fuel technique introduces a new element of complexity into aircraft design (and particularly new maintenance requirements and reliability concerns), it has obvious advantages over the use of cryogenic fuels. There are indications that, free of certain environmental and chemical influences, most hydrocarbons tend to have good high-temperature tolerance [130].

Cryogenic fuels can contribute only sensible and latent heat, whereas certain hydrocarbon fuels can in addition provide cooling through endothermic reactions. Hydrocarbons can undergo both thermal and catalytic reactions. Theoretically, the total heat-sink capacities for hydrocarbon fuels range from about 50% to 112% of the cooling capacity of hydrogen (on a "%" heat of combustion basis) with laboratory proven capabilities up to about 85% [127].

One example of an endothermic reaction is the dehydrogeneration of methylcyclohexane to toluene and hydrogen as shown here:

\[ C_{7}H_{14} \rightarrow C_{7}H_{8} + 3H_{2} \]  \hspace{1cm} (2.1)

This reaction, which has a chemical endotherm of 940 Btu/lb, was identified as a potential source of cooling in earlier investigations of endothermic fuels. However, a catalyst is required for this reaction to occur at a rate that will produce the necessary cooling. Catalysts composed of platinum supported on high surface area alumina have been shown to work well in this application [131,132].

The cracking reactions, which convert high molecular weight paraffins into mixtures of lighter olefins and paraffins, can be conducted either with or without solid catalysts. Catalytic cracking is carried out at relatively low temperatures, 400-550°C, in the presence of acidic compounds such as zeolites [133]. Thermal cracking, on the other hand, is a gas phase reaction and requires higher temperatures, above 500°C, for the reaction to occur at useful rates. Although catalytic cracking and thermal cracking reactions both produce a mixture of low molecular weigh hydrocarbons; they occur by different mechanisms and result in different product distributions. The catalytic mechanism occurs by way of carbenium ion intermediates on the catalyst surface and
produces high concentrations of C3 and C4 products and very few C1 and C2 products. On the other hand, the thermal cracking reaction occurs by a free radical mechanism and results in high concentrations of C2 and C3 compounds [134].

In the laboratory investigations of Wickham et al. [134] the effect of adding a chemical initiator on the rate of thermal cracking of both normal and isoparaffin fuels. It was found that at all temperatures the addition of up to 2 wt% percent of the initiator produced measurable increases in cracking rate. For example at 500°C, this initiator increased the rate of n-heptane cracking by a factor of six, whereas at 550°C the initiator produced over a factor of two improvements in rate. It was found that the initiator only accelerates the cracking rate and does not alter the overall thermal cracking mechanism.

The thermal decomposition of three high-energy density hydrocarbon fuels; RP-1, JP-10, and quadricyclane was examined by Wohlwend et al. [135]. Stability measurements performed in this study indicated that RP-a was the most stable at the conditions investigated, followed closely by JP-10. Quadricyclane is the least stable, degrading at relatively low temperatures compared to JP-10 and RP-1. It was concluded that quadricyclane would not be a capable if providing significant fuel system cooling (due to its thermal instability) if reaction times or temperature were excessive.

The endothermic fuels have the following technical, commercial, and safety advantages:

- Continued availability
- Relatively inexpensive
- Condensed phase under standard temperature and pressure (STP)
- Higher latent heat of vaporization
- Safe handling and storage
- High energy content per unit volume
- No ignition limitations under subsonic combustion conditions
- Non-cryogenic;
  - Insulation not required
  - Vapor recovery not required
  - Conventional Army/Commercial (A/C) fuel system
  - A/C turn-around time not governed by fuel
Conventional fuel handling/logistics;
Off-site production
Launch side hardening easier
Available enabling technologies
Potentially smaller vehicles

Hydrogen has very low density, and it has boil-off problems, leading to packaging challenges that derive up structural mass and required overall volume for a given mission. Cryogenics such as hydrogen and methane will also have obvious handling problems. In contrast, hydrocarbons are slower burning and have between two-fifth and one-third the energy per unit mass compared to hydrogen; however, with up to 11 times the storage density, they have over 3.5 times more energy content per unit volume [136]. The properties of various hydrocarbons are summarized in Table 2.1, contrasted with cryogenic hydrogen in both liquid and slush form, [137-140]. Hydrocarbons contain approximately 15-20% hydrogen, and so they actually store hydrogen at up to twice the density of pure cryogenic hydrogen [141].

Conventional hydrocarbon fuels can be divided into two basic categories: methane, with energy density of 50 MJ/kg and specific gravity of about 0.4 (and also cryogenic storage requirements), and the JP hydrocarbons, with nearly twice the density but only 40 MJ/kg specific energy content. Interestingly, even endothermic fuels such as methylcyclohexane (MCH) have about the same storage properties and combustion energy content as the JP fuels, through they may have advantages in recuperating combustion heat. Hydrogen as either liquid or slush has about the same energy content, with a slight difference due to the heat of fusion, but slush has about a 15% higher density than the liquid form.

Clear technological, economical, and operational advantages exist when liquid hydrocarbon fuels, such as kerosene, are used in comparison with hydrogen-based systems for the development of small hypersonic vehicles. However, the flow features in a supersonic ramjet combustor, primarily the short residence time of a fuel-air mixture, which is $<10^{-3}$ S, along with the multistage physical-chemical mechanism of liquid hydrocarbon fuel burning, increase the difficulties of ignition and flame stabilization. If the selected fuel is amenable to operate at supercritical conditions, a significant decrease
in the time required for the liquid fuel breakup and vaporization can be achieved. Further, if chemical decomposition accompanies these transformations, the potential formation of hydrogen or other active radicals will result in increased reactivity of the mixture and a reduction in the combustion length [142].

Moreover, endothermic fuel reactions can be expected to improve the fuel's combustion properties, if for no other reason than that the fuel enters in a hot, vaporized state. Furthermore, the mixing length of the supersonic combustor is inversely proportional to the gas diffusion coefficient [22]. The gas diffusion coefficient is in turn inversely proportional to the square root of the molecular weight of the diffusing components. Therefore, the large amounts of hydrogen generated from endothermic reactions such as reforming might also be expected to improve the fuel combustion characteristics by lowering the average fuel molecular weight [143].

The use of hydrocarbon fuels in volume limited systems will require an ignitor and some form of combustion enhancement. One approach is to use part of the air to burn all of the fuel in a subsonic pre-burner. Another approach is to use form of pyrophoric material as an ignitor at low temperatures and a flame-holder or combustion enhancement aid at high temperatures where residence times become shorter and kinetics dominates the flame propagation [14].

Over the past 15 years a significant amount of experimental research work has been done on the injector performance and combustion stability using kerosene (RP-1) as the fuel of rockets. This work encompassed a large variety of injection schemes, chamber dimensions, and operating conditions [144].

In the analysis conducted by Lewis [141] the fundamental question of whether the packaging benefits of high-density hydrocarbon fuels outweigh the high-energy content of hydrogen fuels. For a cruiser operating in the Mach 8-10 corridor, in which it is desired to maximize cruise range for a given total takeoff weight, the results seems to be that the aerodynamic and volumetric advantages of storable hydrocarbons are about equivalent or superior to the specific impulse ($I_{sp}$) advantages of hydrogen in determining cruise range.

In the work of Edwards and Maurice [119], several hydrocarbon fuels/fuel systems challenges for hypersonic cruise and space access vehicles were discussed under
the HyTech program. These challenges include extension of fuel heat sink capability, improvement of hydrocarbon combustion properties, fuel system fouling mitigation, and fuel system integration.

Heneghan et al. [145] developed a high-thermal-stability JP-8+100 hydrocarbon fuel, which provides a 55°C (100°F) increase in the bulk maximum temperature (from 325°F to 425°F) and improves the heat sink capability by 50-percent over conventional JP-8 fuel.

A general purpose CFD model has been proposed by Zhou and Krishnan [146] for the heat/mass transfer analysis of endothermic fuel flows under high pressures and heterogeneous catalysis mechanisms. This model was incorporated into a multidimensional CFD code, CFD-ACE. The model was demonstrated for the catalytic endothermic reaction of MCH dehydrogenation to Toluene.

Special attention is directed towards the simulation of the combustion flow field of gaseous methane and gaseous ethylene which are considered to be the light-hydrocarbon fuels resulting from the cracking of the heavy-hydrocarbon fuel, kerosene.

Ethylene C$_2$H$_4$ is a primary fuel itself and is also produced in large amounts during the combustion of methane CH$_4$, ethane C$_2$H$_6$ and other higher hydrocarbons [147]. Ethylene is chosen in the hydrocarbon-fueled scramjet engines because it is used as a surrogate test fuel for hydrocarbon fuels.

Sun et al. [148] investigated experimentally the effects of the equivalence ratio and static temperature of premixed air-gasoline mainstream on the flame propagation speed and ignition delay.

In the experimental work of Vinogradov et al. [149], liquid JP and gaseous ethylene were injected in the isolator upstream of the combustion chamber in a Mach 1.6 airflow behind a thin pylon to determine the ability of the pylon to improve penetration and mixing. The liquid fuel injection behind the pylon increased the fuel penetration to be entrained by the high velocity airflow core resulting in improved mixing, offering the possibility of reduced combustion chamber length. Injecting behind the pylon increased the normalized wall pressure distribution indicating higher rates of heat release in the far field as an indication of improved combustion efficiency. The behind-pylon ethylene injection indicated a substantial increase in penetration over the basic wall injection case.
2.6 Flame Holding Mechanisms For Liquid Hydrocarbon Combustion

Fuel-air mixing, flame holding, pressure losses, and thermal loading are among the major issues that need to be resolved for the successful design and implementation of hydrocarbon-fueled supersonic combustion ramjet (scramjet) engines. A need exists for the development of a system that effectively integrates fuel injection and flame holding for supersonic combustion [152]. A study by Yu et al. [153] in an unheated Mach 2 flow, with fuel injection upstream of a variable cavity length-to-depth ratio (L/D), suggested that small-aspect-ratio cavities provide better flame holding capability than longer cavities with inclined aft ramp angles.

In the experimental study of Mathur et al. [152] the cavity-based flame-holder with low-angle flush wall fuel injection upstream of the cavity was successfully demonstrated in a model scramjet combustor using gaseous ethylene. The study showed that ignition and combustion produced a precombustion shock train, resulting in dual-mode combustor operation. The shock train became stronger and the starting location of the shock train moved progressively upstream with increasing fuel-air equivalence ratio. The cavity-based flame holding concept proved very effective over a wide range of operating conditions and combustor fuel-air equivalence ratios.

The cavity can be used to set up a pilot flame reducing the induction time associated with ignition of fuel-air mixture. Such a method can be useful for maintaining stable flame holding at low equivalence ratio in scramjet operation or minimizing the effect of shock trains. In the work of Situ et al. [154], the preliminary tests of fuel-rich hot gas as reacting jets were performed without liquid fuel jets. A dual cavity was employed as the main flame holding mechanism. The pilot energy of fuel-rich hot gas injected into the supersonic combustor was produced by a dependent pre-burner. The kerosene in the pre-burner was ignited to produce fuel-rich hot gas, which was discharged via six injectors divided equally into two groups: right upstream of the first cavity pointed at 35 degrees with respect to the bottom wall in flow direction, and at the bottom wall of the first cavity parallel to the main stream respectively.

Another fuel-riched hot gas combustion study was conducted by Situ et al. [155]. The major goal of the study was to investigate the characteristics of kerosene-fueled supersonic combustion in dual-combustors. An experimental study was carried out to
observe the effect of the fuel air equivalence ratio on supersonic combustion efficiency and total pressure recovery coefficient, and to investigate where and under which conditions the flame zone is supersonic. Liquid kerosene was injected into a semi-dependent subsonic dump combustor. Then, the fuel-riched hot gas was injected in parallel to the freestream through a slot nozzle injector located at the bottom wall of supersonic combustor.

The results of the early tests conducted by Kay et al. [156,157] clearly demonstrated that the supersonic combustion of various hydrocarbon fuels could be achieved; although for many test conditions, special externally mounted piloting devices were required to initiate and stabilize the flame.

Bonghi et al. [158] injected liquid toluene at 5H down stream of a step of height H in a Mach 2.5 flow at 300 K and 1000 K using a parallel hydrogen-pilot flame. Toluene (C₆H₅CH₃) is one of the components of catalytically cracker methylcyclohexane (MCH), a candidate fuel for supersonic combustion applications. Segal and Young [21] using the same previous configuration injected the toluene from a reservoir at 300 K, and thus, absorbed energy from the surroundings to vaporize and further heat to the local temperature. The large recirculation region formed by hydrogen-pilot combustion extends beyond the liquid injection station, 5H, and thus a substantial amount of the injected liquid reaches the region of stabilization of the pilot flame. When the amount of liquid increases above a certain quantity, it quenches the pilot flame. The amount of liquid fluid that can be injected without inducing quenching was found to be dependent strongly on the equivalence ratio of the pilot flame and, in smaller proportion, on the air stagnation temperature. It was found that as the pilot energy level increases the amount of toluene that can be injected (while maintaining a stable flame) can also be increased. Beyond a certain value, however, the ratio of energy levels decreases again, as more liquid is injected and the amount that reaches the region of stabilization of the pilot flame increases, inducing quenching. This effect is enhanced by the effect of heat release on the structure of the flow field. A larger deposition of heat in the combustion region caused a pressure increase followed by an enlargement of the recirculation region and a reduction in the local velocity, which favors upstream interaction, further facilitating the arrival of
liquid in the recirculation region and quenching of the pilot flame. The increase in the stable flame margin with the air stagnation temperature, $T_0$, was evident.

Vinogradov et al. [159] used various combinations of strut and wall injection of both pilot-hydrogen and liquid kerosene to obtain stable combination at kerosene equivalence ratios as low as 0.6 and pilot equivalence ratios as low as 0.1 for Mach 6 flight conditions. Bonghi et al. [158] evaluated the piloted energy needed to maintain stable combustion of liquid toluene using a rearward-facing step as the main flame holding mechanism with a gaseous hydrogen-pilot flame in a Mach 2.5 airflow. Kay et al. [4] used a gaseous ethylene pilot to stabilize the combustion of a primary fuel, injected both upstream and downstream of the pilot, for a Mach 3 airflow.

The piloted-supersonic combustion experiments strongly recommended that hydrogen piloting is highly effective for a variety of fuels including methane and kerosene. A monopropellent, OTTO fuel, was successfully used as an effective pilot in the scramjets [14]. Other results showed that silane/hydrogen mixtures were effective pilots for ethylene and kerosene combustion [20].

It was shown in the work of Chang and Lewis [160] that piloting the Jet-A-fueled scramjet engines with silane is beneficial in decreasing the combustor length necessary to complete and in reducing the drag. The addition of 10% silane to jet-A fuel reduces the reaction length to 5% of the original length required at 1 atmosphere, 1000 K, and 2000 m/s.

In their experimental study, Kay et al. [4] used three wall-mounted pilots, which serve to initiate the combustion process and stabilize the flame. Staged combustion, whereby the engine fuel is injected at three axial stations corresponding to the pilot location and two downstream stations, is employed to distribute the combustor heat release. This leads to high combustion efficiency while controlling the combustor pressure distribution and preventing combustor-inlet interaction that could unstart the inlet. Also, by tailoring the fuel distribution, it is possible to operate as a dual-combustion scramjet where the combustion process is either all supersonic or mixed supersonic/subsonic, depending on overall equivalence ratio and flight Mach number. They used gaseous ethylene to simulate the ignition characteristics of vaporized Jet-A (JP-5) fuel and limited tests were made using Jet-A. Supersonic combustion tests were
performed using gaseous ethylene fuel with primary fuel injection along and with staged fuel injection over a wide range of spacings between the primary and secondary injection stages. In addition to the ethylene-fueled combustor performance tests, they performed significant combustor testing using Jet-A, a liquid hydrocarbon, as the primary fuel while the pilot injected as a liquid from the parametric piloting test hardware. In later tests, the fuel-cooled piloting hardware was used and the fuel was preheated within the pilot cooling passage, as it would be in an actual engine, to a thermodynamic state such that it flash-vaporized upon injection into the combustor.

Jian-Guo et al. [59] investigated the effect of the hydrogen pilot injection on the ignition of liquid kerosene in Mach 2.5-supersonic combustor. They concluded that without additional ignitor, a proper combination of pilot hydrogen and recessed flame-holder may ignite kerosene and maintain sustained combustion. The minimum equivalence ratio for pilot hydrogen to sustain combustion was found to be 0.03. The effect of increasing the total temperature for the incoming supersonic air from 1470 K to 1700 K was not found of a significant effect implying that the characteristics evaporation time for kerosene is smaller than the mixing time and characteristics reaction time. The evaporation of kerosene is not the controlling factor. They also concluded that the 90° rearward-facing step enhances the mixing pattern of the kerosene-hydrogen dual fuel system in comparison to that of the 45° step. This is attributed to the lower recovery temperature in the 45° step case, which leads to the poorer mixing of the pilot hydrogen and the supersonic air. It needed more hydrogen to produce enough radicals to ignite the kerosene spray.

Through the experiments of Yu et al. [161] the combustion of kerosene in two supersonic test combustors using pilot hydrogen was studied. The integrated modules of pilot and flame-holder using recessed cavity with different geometry were designed and tested. Effect of pilot injection scheme, cavity geometry, and combustor scaling on minimally required pilot hydrogen equivalence ratio were systematically examined. Results show that the stream wise pilot injection is not the most effective scheme for the promotion of kerosene ignition. Also, the cavity depth and length have significant effect on ignition and flame sustaining, while the slanted angle of aft wall is less important.
In an effort to reduce the combustor length, Yu et al. [34] conducted experimental study to evaluate the flame holding and mixing enhancement characteristics of supersonic reacting flow over acoustically open cavities. Several wall cavities having various size and aspect ratios were subjected to supersonic open-flow flame experiments. The results showed that cavities with a short aspect ratio provided good flame holding, whereas those with a relatively long aspect ratio shortened that flame length substantially via acoustic excitation. In all cases that utilized cavities, the combustor pressure and the exit recovery temperature were increased suggesting enhanced volumetric heat release. The subject of the cavity flows and their relevance to flame holding in supersonic combustion engines was surveyed in [162-164].

An unsteady flow analysis on the effect of cavity length to depth ratio and cavity aft wall angle has been studied by Baurle et al. [165] to determine the important characteristics that influence cavity flame holding effectiveness.

Burnes et al. [166] investigated the use of combustor wall cavities not only to provide stable flame holding but also to enhance fuel-air mixing in supersonic combustors. Several different configurations of acoustically open cavities were placed inside a supersonic combustor. For certain cavity configurations, supersonic flow over the cavity generated large coherent structures via flow-induced cavity resonance. On one hand, fuel injection directly into the cavity suppressed the flow oscillations even in the case of the most unstable cavity and inhibited coherent structure formation downstream. This injection scheme would be ideal for cavities that will function as stable flame-holders. On the other hand, fuel injected into the wake of the cavity was entrained into the coherent structures, and showed the evidence of mixing enhancement. The presence of large coherent structures periodically occurring in the wake of the cavity showed that turbulent compressible mixing in an enclosed supersonic duct is significantly affected by flow-induced cavity resonance. This opens up the possibility of organizing the coherent "vortical" structures in a scramjet flow field and controlling the combustion inside the vortices to shorten the combustor length and improve engine performance.

The results of Gruber et al. [167] indicates that the aft ramp angle plays a strong role in determining the character of the shear layer that spans the length of the cavity. Reduction in the aft ramp angle to below 90° yields more stable, two-dimensional flow
fields. Reductions in the aft ramp angle result in higher drag coefficient and shorter residence times within the cavity.

A computational study of an ethylene-fueled scramjet combustor employing an aerodynamic ramp fuel injector and a cavity flame-holder was performed in the work of Eklund et al. [168]. It was found that the position and strength of the three-dimensional pre-combustion shock train and the combustor heat release distribution were strongly coupled, which complicated the modeling of the flow field.

2.7 Importance of Modeling and Simulation

The supersonic combustion ramjet (scramjet) is expected to be the most effective propulsion system for the Single Stage To Orbit (SSTO) transportation vehicles and hypersonic transportation vehicles of the next Generation. Many studies on scramjet components such as inlet, combustor, and nozzle have been carried out to obtain a better understanding of the performances of the individual components, [169-172]. However, it is expected that intensive interactions among these components will occur in real engines. For example, a rise in pressure due to combustion causes separation which propagates upstream into the inlet and changes the inlet back pressure, which may result in unstart condition in the inlet. In the case of interactions, the total performance of the engine cannot be evaluated based on the linear combination of the obtained performance of the individual components. Thus, tests of the models of the whole engine are necessary to elucidate the interactions among these components and the overall performance of the whole engine [173]. Testing of the models of whole engine requires rather big and expensive wind-tunnel facilities. Thus, only a limited number of results on whole engine tests have been reported [20,117].

The design of future hypersonic propulsion system will depend heavily on computational fluid dynamics (CFD) because of the difficulties associated with testing combustors in ground-based facilities. If used properly, CFD can be a strong tool in conjunction with experiments. Computational solutions have the great advantages that aspects of the flow field can be switched on and off to isolate the mechanism of an observed phenomenon. For instance, chemistry may be turned on in a computed flow to determine its influence, boundary layers may be switched from laminar to turbulent, and perturbations can be introduced in upstream calculations to isolate cause and effect.
Computational solutions also permit a flow field to be assessed without intrusion, and numerical measurement can be made to the resolution of the grid. This capability has been used very effectively to identify details of shock-shock interaction, shock-boundary-layer interactions, supersonic shear layers, and combustion systems that could not possibly be measured experimentally. A particularly promising example is the use of CFD investigations of ionized or electrically charged gases to explain reported aerodynamic and propulsion benefits [25].

Multiphase combustion is such a complex phenomenon that it warrants focused research using modeling and numerical simulations. Though physical experiments are the ultimate test to study the performance of combustion/propulsion systems, they are often extremely expensive and complicated, and at times are not even possible. This is due to the hostile environments, complicated interactions, and couplings. On the one hand, these couplings make it impossible to study the effect of one parameter at a time in a physical experiment of this nature. On the other hand, numerical experiments open an avenue for isolating and understanding the influence of different parameters on complex combustion situations. Furthermore, these can serve as means of evaluating scaling laws, which would be extremely difficult and expensive to determine from physical experiments alone. Modeling also provides a potential design tool for future combustion and propulsion systems. However, this is not a simple or straightforward extension of computational fluid dynamics (CFD) by including a few more terms in the governing equations [174].

Numerical simulation is time consuming even with ultrafast modern computers. The fuels of choice, e.g., hydrocarbons or metal slurries, will have a large number of kinetic steps and species involved in their combustion. The computational time increases as the square of the number of species, and calls for reduced chemistry based on sound logic. The presence of solid particles, such as soot or unburned fuel droplets, and their transport in the turbulent flow field complicates the situation even further, and requires extremely small grid sizes. Ultimately, the results of these complex numerical simulations should be made available in the form of user-friendly models for the designer.
Strong interaction of the computational combustion community with experimentalists is needed in order to assure meaningful model validations, and to generate more reliable and advanced models to aid in the design of complex combustion/propulsion systems of the future.

Computational fluid dynamics (CFD) simulations have become invaluable in the design process due to the high costs and long turnaround times encountered in experimental programs and due to the inability to reproduce all desired flow field conditions in present laboratory facilities. Fundamental numerical techniques for the calculation of compressible flow fields have been available for some time, but the computational resources required for making accurate 3-D simulations of complex flow fields have become more generally available for design purposes only relatively recently. This is, for the most part, due to the many dramatic improvements that have occurred in the performance of computer hardware, but is also due to progress in the development of efficient and accurate numerical techniques and algorithms. Advances in areas such as grid generation, development of higher order schemes, and turbulence modeling make reasonably accurate simulations of extremely complex flow fields now possible. It is important to point out that if CFD codes are to be incorporated into a design process, the need for experimental validation is a necessity, a point that is sometimes under-emphasized [23].

One of the advantages of CFD simulations over standard experimental data sets is that all flow field properties are available everywhere in the flow field so that any desired quantity can be extracted from the CFD results. Both detailed information about particular flow field features and global information, such as conservation consistency checks and overall performance quantities, can be calculated from the numerical data set [23].

The design of fuel injection configurations like the ones considered in the scramjet engines rely on the understanding of extremely complex flow fields with features such as: turbulent mixing, combustion reactions, strong three-dimensionality, compressibility effects, boundary layers, and flow separations. The ability to study such flow fields experimentally has been limited because of the difficulty in gaining access into the harsh, yet easily perturbed environment of a supersonic flow field. Understanding
the geometrical complexity of such flows has been limited by the fact that most traditional quantitative measurement techniques are pointwise techniques. Theoretical studies in the past have been stalled by the difficulties in dealing with the highly non-linear set of equations that describe the physics of these flow fields. Numerical approaches give reasonable, and often very accurate, solutions to problems such as these that are not solvable analytically. Recently, due to the development in non-intrusive laser diagnostics measurement techniques and to advances in the field of computational fluid dynamics, the ability to study such flow fields has been greatly improved [23].

Recent advances in numerical simulation techniques and theoretical studies offer new descriptions of the physical phenomena in high-speed flows including mixing and combustion interactions and the onset and development of instabilities and vorticity, both in non-reacting and chemically reacting flows. Although numerical simulations offer much physical insight and a great level of detail, the experimental validation of both the theoretical models and the numerical algorithms is largely lacking due to difficulties in measuring essential parameters in these flow fields, such as velocity, temperature, and pressure characteristics. Furthermore, there are numerous modeling issues, which are largely unresolved and need insight from experimental observation. Existing experimental facilities are, in general, dedicated to study of only a limited range of topics because of extreme conditions of high enthalpy flow, including an overview of the demands of availability of existing facilities. Certain facilities, capable of reproducing high enthalpy conditions, can operate for only short time durations, insufficient to achieve stable thermal conditions. Other existing facilities are, in general, limited in terms of their experimental flexibility [21].

To efficiently simulate the piloted-scramjet engines, a reasonable kinetic model has to be implemented in the CFD code. The simple global kinetic models may be inadequate to study piloting problems, since they neglect intermediate combustion products, which are essential to the phenomenon [14]. At the same time, the computational cost of a given reaction mechanism depends primarily on the number of species included, rather than the number of reactions [175]. Therefore it is recommended to use a kinetic scheme with a minimum number of species and reactions that is effectively yet capable of modeling the chemistry with reasonable accuracy for the
expected combustion conditions. In the dual-fuel cases, in which pilot hydrogen is injected to support the ignition of ethylene and kerosene hydrocarbon fuels, the combustion of pilot hydrogen has to be accounted for in the chemistry part of the simulation. This necessitates inclusion of the hydrogen combustion in the used kinetic scheme. Fulfilling this task makes the selection of the chemistry scheme being more tightened to achieve both the minimum possible number of species and the involvement of hydrogen combustion as one of the elementary reactions of the scheme.

Singh and Jachimowski [13] developed a reduced 10-species, 10-step (with backward reactions) kinetic model for ethylene combustion, which compared favorably with the results calculated with the detailed mechanism of Jachimowski [176]. This reduced model is also suggested for assembling reaction mechanisms of heavy hydrocarbons such as propane, butane, n-heptane, etc.

Different CFD techniques used for Scramjet engine analysis were presented in the work of White et al. [177]. Various levels of approximation to the Reynolds-averaged Navier-Stokes equations, by which the flow field through a scramjet engine can be described, were mentioned. It included using the Parabolized Navier-Stoked (PNS) equations, reducing the geometry assumption to two-dimensional planar or axisymmetric flow, and using the Euler/Boundary-Layer Superposition approach. The application of the CFD techniques to scramjet engine analysis was highlighted by presenting examples of, and a discussion of, the techniques applied to the analysis of the various engine components; the inlet, the combustor, and the nozzle.

For the support of the design of a fixed geometry scram intake two-dimensional Navier-Stokes calculations have been performed by Bissinger [178]. Unstructured-grid Navier-Stokes (UNS) methodology is well suited to the analysis of scramjet combustor flow fields in view of its ability to deal with complex injection geometries and to adaptively refine the grid in critical regions such as flame zones. UNS applications to scramjet combustor flow have been limited in view of the need to deal with complexities associated with combustion and turbulence modeling, which are better established in structured flow solvers. Lee et al. [179] used UNS code to investigate the scramjet combustor field for swept ramp fuel injectors. They summarized the progress achieved in implementation of the grid adaptive methodology.
In the work of Kodera et al. [180] the hybrid grid method to compute supersonic reacting flow rate was applied to internal reacting flows of a scramjet engine at flight Mach number of 8. The details of reacting internal flow field such as boundary layer separation, mixing, ignition and combustion as well as engine performance such as thrust and combustion efficiency were investigated. Ungewitter et al. [181] upgraded the k-ε turbulence model by improving the compressibility correction and transitional modeling. A more stable Gauss-Seidel implicit solver was incorporated into the unstructured Navier Stokes code and a new variable element grid methodology was employed which improved the resolution in several key areas while maintaining a minimum number of cells.

Chakravarthy et al. [182] presented the progress they recently achieved in the turbulence modeling closure. Their contribution focused on the improvements to the classical models and the usage of the hybrid Reynolds Average Navier Stokes Equations/Large Eddy Simulation (RANS/LES) methods. They presented their simulation data for a couple of supersonic flow case studies that are: swept ramp injection into a supersonic flow, and two-hole transverse sonic injections downstream of a rearward-facing step in supersonic flow field. The calculations produced using the new closure compared favorably with existing relevant experimental data.

Quantifying the level of confidence, or accuracy, of computational fluid dynamics (CFD) codes and numerical solutions has recently received increased attention in the research and engineering application literature. The issues of credibility, validation, and verification of the CFD codes were discussed intensively in [183-188].

A fine enough mesh with a good enough quality must be used to ensure that there are not significant variations in the solution when either the number or the placement of the mesh points is varied. Otherwise it is impossible to distinguish modeling errors from numerical errors. The mesh refinement and optimization were studied in [189-190].

The accessibility of the CFD tools on the Internet was discussed in [191]. A concept was presented for evolving the current RocketWeb™ Internet Analysis System into a comprehensive design process, capable of seamlessly integrating the diverse design and analysis tools necessary to create robust designs. The resulting system would result in a rigorous, controlled design process capable of reducing both design cycle time and cost.
Table 2.1 Energy properties of H\textsubscript{2} and hydrocarbon fuels data complied from Refs. [137-140]

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Energy/Mass, MJ/kg</th>
<th>Energy/Volume, MJ/l</th>
<th>STP Density, Kg/m\textsuperscript{3}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid H\textsubscript{2}</td>
<td>116.7</td>
<td>8.2</td>
<td>71</td>
</tr>
<tr>
<td>Slush H\textsubscript{2}</td>
<td>116.6</td>
<td>9.8</td>
<td>82</td>
</tr>
<tr>
<td>Methane</td>
<td>50.0</td>
<td>20.8</td>
<td>424</td>
</tr>
<tr>
<td>n-Heptane</td>
<td>44.6</td>
<td>30.3</td>
<td>717</td>
</tr>
<tr>
<td>JP-4</td>
<td>43.5</td>
<td>33.1</td>
<td>760</td>
</tr>
<tr>
<td>JP-5</td>
<td>43.0</td>
<td>35.1</td>
<td>815</td>
</tr>
<tr>
<td>JP-7</td>
<td>43.9</td>
<td>34.7</td>
<td>790</td>
</tr>
<tr>
<td>JP-8</td>
<td>43.2</td>
<td>35.0</td>
<td>809</td>
</tr>
<tr>
<td>Jet A</td>
<td>43.4</td>
<td>34.6</td>
<td>799</td>
</tr>
<tr>
<td>Kerosene</td>
<td>42.8</td>
<td>34.2</td>
<td>800</td>
</tr>
<tr>
<td>MCH</td>
<td>43.4</td>
<td>33.4</td>
<td>770</td>
</tr>
</tbody>
</table>

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Fig. 2.1 Schematic diagram of the scramjet engine configuration [26].

Fig. 2.2 Essential features of two-dimensional or planar geometry scramjet engines [26].
Fig. 2.3 Airframe-integrated scramjet along with a partial cross-section through a typical modular engine [28].

Fig. 2.4 Schematic of the region surrounding a single perpendicular injector [28].
Fig. 2.5 Generation of counter-rotating streamwise vorticity by ramp fuel injector [60].

Fig. 2.6 Scramjet fuel-injector compression and expansion ramps [60].
Fig. 2.7 Energy content per unit mass for different avionic fuels [130].
Fig. 2.8 Temperature limit for different avionic fuels [130].
Fig. 2.9 Energy content per unit volume for different avionic fuels [139].
CHAPTER III
THEORETICAL FORMULATIONS

3.1 Introduction
The Computational Fluid Dynamics "CFD" Code used in the present study is the FLUENT commercial code. FLUENT is a general-purpose computer program for modeling fluid flow, heat transfer, and chemical reaction [192].

FLUENT models a wide range of phenomena by solving the conservation equations for mass, momentum, energy, and chemical species using a control volume based finite difference method. The governing equations are discretized on a curvilinear grid to enable computations in complex irregular geometries. A non-staggered system is used for storage of discrete velocities and pressures. Interpolation is accomplished via a first-order, Power-Law scheme or optionally via higher order upwind schemes. The equations are solved using SIMPLE-like algorithms with an iterative line-by-line matrix solver and multigrid acceleration.

3.2 Governing Equations
For all flows, FLUENT solves conservation equations for mass and momentum. For flows involving heat transfer or compressibility, an additional equation for energy conservation is solved. For flows involving species mixing or reactions, a species conservation equation is solved or, if the PDF model is used, conservation equations for the mixture fraction and its variance are solved. Additional transport equations are also solved when the flow is turbulent.

3.2.1 The Mass Conservation Equation
The equation for conservation of mass, or continuity equation, can be written as follows:
\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = S_m
\] (3.1)

Equation (3.1) is the general form of the mass conservation equation and is valid for incompressible as well as compressible flows. The source \( S_m \) is the mass added to the continuous phase from the dispersed second phase (e.g., due to vaporization of liquid droplets) and any user-defined sources.
3.2.2 Momentum Conservation Equations

Conservation of momentum in the \( i \) direction in an inertial (non-accelerating) reference frame is described by [193]

\[
\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_i}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + F_i
\]  

(3.2)

where \( p \) is the static pressure, \( \tau_{ij} \) is the stress tensor (described below), and \( \rho g_i \) and \( F_i \) are the gravitational body force and external body forces (e.g., that arise from interaction with the dispersed phase) in the \( i \) direction, respectively. \( F_i \) also contains other model-dependent source terms such as porous-media and user-defined sources.

The stress tensor \( \tau_{ij} \) is given by

\[
\tau_{ij} = \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \frac{2}{3} \mu \frac{\partial u_i}{\partial x_i} \delta_{ij}
\]  

(3.3)

where \( \mu \) is the molecular viscosity and the second term on the right hand side is the effect of volume dilation.

3.2.3 The Energy Equation

The general form of the energy equation is:

\[
\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}(u_i (\rho E + p)) = \frac{\partial}{\partial x_i} \left( k_{\text{eff}} \frac{\partial T}{\partial x_i} - \sum_{j'} h_{j'} J_{j'} + u_j (\tau_{ij})_{\text{eff}} \right) + S_h
\]  

(3.4)

where \( k_{\text{eff}} \) is the effective conductivity \( (k + k_t, \text{ where } k_t \text{ is the turbulent thermal conductivity, defined according to the turbulence model being used}), \) and \( J_{j'} \) is the diffusion flux of species \( j' \). The first three terms on the right-hand side of Eq. (3.4) represent energy transfer due to conduction, species diffusion, and viscous dissipation, respectively. \( S_h \) includes heat of chemical reaction, and any other volumetric heat sources defined.

In Eq. 3.4,

\[
E = h - \frac{p}{\rho} + \frac{u_i^2}{2}
\]  

(3.5)

where sensible enthalpy \( h \) is defined for ideal gases as

\[
h = \sum_{j'} m_{j'} h_{j'}
\]  

(3.6)
In Equation (3.6), $m_j$ is the mass fraction of species $j$ and

\[ h_j = \int_{T_{\text{ref}}}^{T} c_{\rho,j} \, dT \quad (3.7) \]

where $T_{\text{ref}}$ is 298.15 K.

Equation (3.4) includes pressure work and kinetic energy terms, which are often negligible in incompressible flows.

The viscous dissipation terms, which describe the thermal energy created by viscous shear in the flow, is included in Eq. (3.4). Viscous heating will be important when the Brinkman number, $Br$, approaches or exceeds unity, where

\[ Br = \frac{\mu U_e^2}{k \Delta T} \quad (3.8) \]

and $\Delta T$ represents the temperature difference in the system. The effect of enthalpy transport due to species diffusion is included in Eq. (3.4) through the term $\frac{\partial}{\partial x_i} \sum_j h_j \dot{J}_j$.

The source of energy, $S_h$, in Eq. (3.4) includes the source of energy due to chemical reaction:

\[ S_{h,\text{reaction}} = \sum_j \left[ \frac{h_j^0}{M_j} + \int_{T_{\text{ref}}}^{T} c_{\rho,j} \, dT \right] R_j \quad (3.9) \]

where $h_j^0$ is the enthalpy of formation of species $j$ and $R_j$ is the volumetric rate of creation of species $j$.

When one of the radiation models is used, $S_h$ in Eq. (3.4) also includes radiation source terms. It should be noted that the energy sources, $S_h$, also include heat transfer between the continuous and the discrete phase.

### 3.3 Basic Physical Models for Flow and Heat Transfer

#### 3.3.1 Turbulence Models

In turbulent flows, the velocity at a point is considered as a sum of the mean (ensemble-averaged) and fluctuating components:

\[ u_i = \bar{u}_i + u_i \quad (3.10) \]
Substituting expressions of this form into the instantaneous momentum equations (and dropping the overbar on the mean velocity, \( \bar{u} \)) yields the ensemble-averaged momentum equations:

\[
\frac{\partial}{\partial t}(\rho \bar{u}_i) + \frac{\partial}{\partial x_j}(\rho \bar{u}_i \bar{u}_j) = \frac{\partial}{\partial x_j} \left( \mu \left[ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] - \frac{2}{3} \rho \mu \frac{\partial u_i}{\partial x_j} \right) - \frac{\partial p}{\partial x_i} + \rho g_i + F_i + \frac{\partial}{\partial x_j}(-\bar{\rho} \bar{u}_i \bar{u}_j) \quad (3.11)
\]

Equation (3.11) has the same form as the fundamental momentum balance with velocities now representing ensemble-averaged (or mean-flow) values. The effect of turbulence is incorporated through the "Reynolds stresses", \( \bar{\rho} \bar{u}_i \bar{u}_j \). FLUENT relates the Reynolds stresses to mean flow quantities via one of three turbulence models:

1. The \( k-\varepsilon \) model
2. The RNG \( k-\varepsilon \) model
3. The Reynolds Stress Model (RSM)

The process of selecting a turbulence model for a given turbulent flow problem is greatly facilitated when having a good understanding of the salient features of the flow in question. Based on this understanding, it should then be considered which model would be more suitable. To do so, the capabilities and limitations of the individual models must be known. This section provides an overview of the models and general guidelines that helps choosing the correct turbulence model for the flow to be modeled.

The standard \( k-\varepsilon \) model proposed by Jones and Launder [194] as been the workhorse of engineering turbulence models for more than two decades. It falls in the category of "two-equation" turbulence models based on an isotropic eddy-viscosity concept. As such, it is more universal than other low-order turbulence models such as algebraic ("zero-equation") and one-equation models. Robustness, economy, and reasonable accuracy for a wide range of turbulent flows explain its popularity in industrial flow and heat transfer Simulations. It is a semi-empirical model, and the derivation of the model equations, including the various model constants, relies on phenomenological considerations and empiricism.

The Renormalization Group (RNG) \( k-\varepsilon \) model also belongs to the \( k-\varepsilon \) family of models. The model equations in their RNG form are similar to those for the standard \( k-\varepsilon \) model. There are major differences, however, between the RNG and standard \( k-\varepsilon \) models.
The RNG model was derived using a more rigorous statistical technique, and its model constants are derived "analytically."

The Reynolds Stress Model (RSM) is the most elaborate turbulence model that FLUENT provides. Eschewing the isotropic eddy viscosity hypothesis, the RSM closes the Reynolds stresses by solving their transport equations (six additional equations in 3D, in comparison with $k-\varepsilon$ models). As such, the RSM accounts for the history and transport of the Reynolds stresses in a rigorous manner. The effects of streamline curvature, swirl, and rotation are all directly accounted for by the transport equations for the Reynolds stresses.

3.3.2 Compressible Flows

Compressibility effects are encountered in gas flows at high velocity and/or in which there are large pressure variations. When the gas flow velocity approaches or exceeds the speed of sound or when the pressure change in the system ($\Delta p/p$) is large, the variation of the gas density with pressure has a significant impact on the flow velocity, pressure, and temperature. Compressible flows create a unique set of flow physics, which should be well known to provide the special input requirements and solution techniques that are described in this section.

Compressible flows can be characterized by the value of the Mach number

$$M = \frac{u}{c}$$

(3.12)

where $c$ is the speed of sound in the gas:

$$c = \sqrt{\gamma RT}$$

(3.13)

and $\gamma$ is the ratio of specific heats ($C_p/C_v$).

When the Mach number is less than one, the flow is termed subsonic. At Mach numbers much less than one (e.g., $M < 0.3$ or so), compressibility effects are negligible and the variation of the gas density with pressure can safely be ignored in the flow modeling. When the Mach number approaches unity, however, compressibility effects become important. The flow will choke at Mach 1.0. When the Mach number exceeds 1.0, the flow is termed supersonic. Supersonic flows may contain shocks and expansion fans which can impact the flow pattern significantly and which require compressibility in
the FLUENT model. FLUENT provides a full range of compressible flow modeling capabilities for subsonic, transonic, and supersonic flows.

Compressible flows are typically characterized by the total pressure \( P_0 \) (isentropic stagnation pressure) and total temperature \( T_0 \) (isentropic stagnation temperature) of the flow. These quantities can be related to the static pressure and temperature via the following relationships:

\[
\frac{P_a}{P_s} = \left[1 + \frac{\gamma - 1}{2} M^2 \right]^\frac{\gamma}{\gamma - 1}
\]

\[
\frac{T_a}{T_s} = \left[1 + \frac{\gamma - 1}{2} M^2 \right]
\]

These unique relationships describe the variation of the static pressure and temperature in the flow as the velocity (Mach number) changes under isentropic (loss-free, constant enthalpy) conditions.

For a given pressure ratio from inlet to exit, for example, Eq. (3.14) can be used to estimate the exit Mach number (which would exist in a one-dimensional isentropic flow). For air, Eq. (3.14) predicts a choked flow (Mach number of 1.0) at an isentropic pressure ratio, \( P_s/P_0 \), of 0.5283. This choked flow condition will be established at the point of minimum flow area (e.g., in the throat of a nozzle). In the subsequent area expansion the flow may either accelerate to a supersonic flow in which the pressure will continue to drop, or the flow may return to subsonic flow conditions, decelerating with a pressure rise. When a supersonic flow is exposed to an imposed pressure increase, a shock will occur, with a sudden pressure rise and deceleration accomplished across the shock.

Compressible flows are described by the standard continuity and momentum equations solved by FLUENT, and there is no need to activate any special physical models (other than the compressible treatment of density as detailed below). The energy equation solved by FLUENT, Eq. (3.4), correctly incorporates the coupling between the flow velocity and the static temperature, and should be activated whenever a compressible flow is solved. In addition, you should activate the optional viscous dissipation terms in Eq. (3.4), which become important in high-Mach-number flows.

For high-Mach-number flows, compressibility affects turbulence through so-called "dilatation dissipation," which is normally neglected in the modeling of
incompressible flows [195]. Neglecting the dilatation dissipation fails to predict the observed decrease in spreading rate with increasing Mach number for compressible mixing and other free shear layers. To account for these effects in the \( \kappa-\varepsilon \) models in FLUENT, the dilatation dissipation term, \( Y_M \), is included in the \( \kappa \) equation. This term is modeled according to a proposal by Sarkar and Balakrishnan [196]:

\[
Y_M = \rho e^2 M_t^2
\]  

(3.16)

where \( M_t \) is the turbulent Mach number, defined as

\[
M_t = \sqrt{\frac{\kappa}{a^2}}
\]  

(3.17)

where \( a = \sqrt{\gamma RT} \) is the speed of sound. This compressibility modification always takes effect when the compressible form of the ideal gas law is used.

### 3.3.3 Chemical Species Transport and Reacting Flow

FLUENT models chemical species transport and chemical reactions using the reacting flow models described in this section. The mixing and transport of chemical species are modeled by solving conservation equations describing convection, diffusion, and reaction sources for each component species.

When you choose to solve conservation equations for chemical species, FLUENT predicts the local mass fraction of each species, \( m_i \), through the solution of a convection-diffusion equation for the \( i \)th species. This conservation equation takes the following general form:

\[
\frac{\partial}{\partial t}(\rho m_i) + \frac{\partial}{\partial x_i}(\rho u_i m_i) = -\frac{\partial}{\partial x_i} J_{i,j} + R_r + S_r
\]  

(3.18)

where \( R_r \), is the mass rate of creation or depletion by chemical reaction and \( S_r \), is the rate of creation by addition from the dispersed phase. An equation of this form will be solved for \( N-1 \) species where \( N \) is the total number of fluid phase chemical species present in the system.

The diffusion flux, \( J_{i,j} \), may optionally be augmented by a thermal diffusion term, \(-D_{i}^{T} \frac{1}{T} \frac{\partial T}{\partial x_i}\) (also called Soret diffusion).

where \( D_{i}^{T} \) is the diffusion coefficient for species \( i \).
In turbulent flows, FLUENT computes the mass diffusion in the form:

\[ J_{i,j} = -\left( \rho D_{i,m} + \frac{\mu_r}{Sc_r} \right) \frac{\partial m_{i,j}}{\partial x_i} \]  

(3.19)

where \( S_{ct} \) is the effective Schmidt number, \( \frac{\mu_r}{\rho D_i} \) (with a default setting of 0.7).

For many multi-component mixing flows, the transport of enthalpy due to species diffusion \( \nabla \cdot \left[ \sum_{k=1}^{n} (h_k) J_{k,i} \right] \) can have a significant effect on the enthalpy field and should not be neglected. In particular, when the Lewis number \( Le = \frac{\rho D}{k / c_v} \) is far from unity, and when the species involved have significantly differing heat capacities, this term cannot be neglected.

The reaction rates that appear as source terms in Eq. (3.18) are computed from Arrhenius rate expressions or by using the eddy dissipation concept due to Magnussen and Hjertager [197]. Models of this type are suitable for a wide range of applications including laminar or turbulent reaction systems, and combustion systems including premixed or diffusion flames.

The source of chemical species \( i' \) due to reaction, \( R_{r,i} \), is computed as the sum of the reaction sources over the \( k \) reactions that the species may participate in:

\[ R_{i'} = \sum_{k} R_{r,i,k} \]  

(3.20)

where \( R_{r,i,k} \) is the rate of creation/destruction of species \( i' \) in reaction \( k \). Reaction may occur in the continuous phase between continuous phase species only, or at surfaces resulting in the surface deposition or evolution of a chemical species. The reaction rate, \( R_{r,i,k} \), is controlled either by an Arrhenius kinetic rate expression or by the mixing of the turbulent eddies containing fluctuating species concentrations.

The Arrhenius reaction rate is computed as:

\[ R_{r,i,k} = -\nu_{r,i,k}^* M_i T^b_i A_k \prod_{j \in \text{reactants}} C_j^{r_{i,j}} \exp\left(-\frac{E_k}{RT}\right) \]  

(3.21)

where \( \nu_{r,i,k}^* = \) molar stoichiometric coefficient for species \( i' \) in reaction \( k \) (positive values for reactants, negative values for products)
$M_{i'} = \text{molecular weight of species } i' \text{ (kg/kmol)}$

$\beta_k = \text{temperature exponent (dimensionless)}$

$A_k = \text{pre-exponential factor (consistent units)}$

$C_{j'} = \text{molar concentration of each reactant species } j' \text{ (kmol/m}^3\text{)}$

$\nu_{j',k} = \text{exponent on the concentration of reactant } j' \text{ in reaction } k$

$E_k = \text{activation energy for the reaction (J/kmol)}$

The values for $\nu_{i',k}$, $\beta_k$, $A_k$, $\nu_{j',k}$, and $E_k$ are defined in the problem setup.

The influence of turbulence on the reaction rate is taken into account by employing the Magnussen and Hjertager model. In this model, the rate of reaction $R_{i',k}$ is given by the smaller (i.e., limiting value) of the two expressions below:

$$R_{i',k} = -\nu_{i',k} M_{i'} A \rho \frac{E}{k} \frac{m_R}{v_{R,k} M_R}$$  \hspace{1cm} (3.22)

$$R_{i',k} = -\nu_{i',k} M_{i'} A B \rho \frac{E}{k} \frac{\sum_{p} m_p}{\sum_{p} \nu_{p,k} M_p}$$  \hspace{1cm} (3.23)

where $m_p = \text{mass fraction of any product species, } P$

$m_R = \text{mass fraction of a particular reactant, } R$

$R = \text{reactant species giving the smallest value of } R_{i',k}$

$A = \text{an empirical constant equal to 4.0}$

$B = \text{an empirical constant equal to 0.5}$

The eddy breakup model relates the rate of reaction to the rate of dissipation of the reactant and product containing eddies. $\kappa/\epsilon$ represents the time scale of the turbulent eddies following the eddy break up model of Spalding. The model is useful for the prediction of premixed and diffusion problems as well as for partially premixed reacting flows.

In turbulent reacting flows, FLUENT calculates the reaction rates from the Arrhenius expression (Eq. (3.21)) and the eddy breakup model (Eqs. (3.22) and (3.23)). The limiting (slowest) rate is used as the reaction rate and the contribution to the source terms in the species conservation and enthalpy equations are calculated from this reaction.
rate. Energy released by or required for the chemical reaction is accounted for in the source term of the enthalpy equation as shown in Eq. (3.9).

The introduction of the kinetic term into the rate expression for turbulent flows is useful as it can act as a cut-off to the mixing controlled rate when chemistry is very slow. However, in many practical situations, the eddy breakup model describes the limiting rate.

If the fuel is introduced to an oxidant, spontaneous ignition does not occur unless the temperature of the mixture exceeds the activation energy threshold required to maintain combustion. In the simulation an ignition source has to be supplied to initiate combustion. This ignition source may be a heated surface that heats the gas mixture above the required threshold level. Often, however, it is the equivalent of a spark: an initial solution state that causes combustion to proceed. This "fuel spark" or "initial solution state" is supplied by patching a hot temperature into a region of the model that contains a sufficient fuel/air mixture for ignition to occur. Often, there may be a need to patch both the temperature and the fuel/oxidant/product concentrations to produce ignition in the model. The initial patch has no impact on the final steady-state solution-no more than the location of a match determines the final flow pattern of the torch that it lights.

3.4 Thermal Model

3.4.1 Density: Ideal Gas Law for Compressible Flows

For compressible flows, the gas law has the following form:

$$\rho = \frac{P_{op} + p}{RT}$$

where $p$ is the local relative (or gauge) pressure predicted by FLUENT and $P_{op}$ is defined as the Operating Pressure in the Operating Conditions panel.

3.4.2 Composition-Dependent Thermal Conductivity for Multicomponent Mixtures

When the ideal gas law is used with multi-component flow field, the composition-dependent thermal conductivity based on kinetic theory is calculated as

$$k = \sum_{i'} \frac{X_{i'} k_{i'}}{\sum_{j'} X_{j'} \phi_{i', j'}}$$

where
\[
\phi_{i,j} = \frac{1}{8 \left( 1 + \frac{M_i}{M_j} \right)^{1/2}} \left[ 1 + \left( \frac{\mu_i}{\mu_j} \right)^{1/2} \left( \frac{M_j}{M_i} \right)^{1/4} \right]^{-2}
\]

(3.26)

and \( X_r \) is the mole fraction of species \( i' \).

### 3.4.3 Composition-Dependent Viscosity for Multicomponent Mixtures

When the ideal gas law is used with multi-component flow field, the composition-dependent thermal conductivity based on kinetic theory is calculated as

\[
\mu = \sum_r \frac{X_r \mu_r}{\sum_j X_j \phi_{i,j}} \quad \text{(3.27)}
\]

where

\[
\phi_{i,j} = \frac{1}{8 \left( 1 + \frac{M_i}{M_j} \right)^{1/2}} \left[ 1 + \left( \frac{\mu_i}{\mu_j} \right)^{1/2} \left( \frac{M_j}{M_i} \right)^{1/4} \right]^{-2}
\]

(3.28)

and \( X_r \) is the mole fraction of species \( i' \).

### 3.4.4 Specific Heat Capacity as a Function of Composition

The species heat capacity is defined as a function of temperature in a polynomial form as follows:

\[
C_p(T) = A_1 + A_2 T + A_3 T^2 + \ldots \quad \text{(3.29)}
\]

where coefficients \( A_i \)'s are characteristic data for each species.

The mixture's specific heat capacity is calculated as a mass fraction average of the pure species heat capacities as follows:

\[
c_p = \sum_r m_r c_{p,i'}
\]

(3.30)

### 3.5 Grid Generation
The grid is a discrete representation of the continuous field phenomena that is modeled and the accuracy and numerical stability of the simulation depend on the choice of the grid. In other words, the density and distribution of the grid lines determines the accuracy with which the model represents the actual physical phenomena.

In FLUENT, the control volume method, sometimes referred to as the finite volume method, is used to discretize the transport equations. In the discrete form of the equations, values of the dependent variables appear at control volume boundary locations (cell faces). These values have to be expressed in terms of the values at the nodes of neighboring cells in order to obtain algebraic equations. This task is accomplished via an interpolation practice, also called a "differencing scheme." The choice of differencing scheme not only affects the accuracy of the solution but also the stability of the numerical method.

The default differencing scheme used in FLUENT is the so-called power-law scheme. This scheme is derived from the exact analytical solution to the one-dimensional convection-diffusion equation. The power-law scheme is very stable and gives physically meaningful (bounded) solutions but, in certain situations, is susceptible to numerical diffusion effects. These effects, as mentioned earlier, are maximums when the flow is aligned at 45 degrees to the grid lines and there are significant gradients in the direction normal to the flow. Higher-order methods which are less susceptible to numerical diffusion, but also less stable compared to the power-law scheme, are also available in FLUENT.

It should be noted that recent research in CFD has focused on unstructured grids, where the grid points are placed in the flow field in a very irregular fashion; this is in contrast to a structured grid, which reflects some type of consistent geometrical regularity. Among the advantages of the unstructured grid meshes over the structured ones are the allowance for the maximum flexibility in matching mesh cells with the boundary surfaces and for putting cells where needed [193].

Both the structured and unstructured meshes are generated using "Gambit," which is the grid generation package of the flow solver "Fluent."

The meshes used in the present study are unstructured. The faces are meshed using the "Tri-Pave" scheme, which means that the mesh includes only triangular mesh.
elements that are interconnected in an irregular fashion to construct the unstructured meshing of the faces. The volume meshing emanates from the mesh elements of the faces and branches downward filling the whole volume and connecting the faces using the "T-Grid" scheme through which GAMBIT creates a mesh that consists primarily of the tetrahedral mesh elements but may include hexahedral, pyramidal, and wedge elements where appropriate.

Figure 3.1 shows an example for an unstructured face meshing using "Tri-Pave" scheme. Figure 3.2 shows the general shape of the tetrahedral mesh elements that are created in the volume if none of the faces are meshed prior to the application of the "T-Grid" scheme or if all pre-meshed faces are meshed by means of a Tri-Pave scheme.

3.6 Method of Solution

3.6.1 Basics of the Overall Solution Algorithm

The coupled solver in FLUENT solves the governing equations of continuity, momentum, and (where appropriate) energy and species transport simultaneously as a set, or vector, of equations. Governing equations for additional scalars will be solved sequentially (i.e., segregated from one another and from the coupled set).

The system of governing equations for a single-component fluid, written to describe the mean flow properties, is cast in integral, Cartesian form for an arbitrary control volume $V$ with differential surface area $dA$ as follows:

$$\frac{\partial}{\partial t} \int_V W dV + \int_V \{ F - G \} dA = \int_V H dV$$

(3.31)

where the vectors, $W$, $F$, and $G$ are defined as

$$W = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix}, \quad F = \begin{bmatrix} \rho v \\ \rho u + p_i \\ \rho v + p_j \\ \rho w + p_k \\ \rho v E + p v \end{bmatrix}, \quad G = \begin{bmatrix} 0 \\ \tau_{xi} \\ \tau_{yi} \\ \tau_{zi} \\ \tau_{ij} + q \end{bmatrix}$$

(3.32)

and the vector $H$ contains source terms such as body forces and energy sources.

Here $\rho$, $v$, $E$, and $p$ are the density, velocity, total energy per unit mass, and pressure of the fluid, respectively. $\tau$ is the viscous stress tensor, and $q$ is the heat flux.
Total energy $E$ is related to the total enthalpy $H$ by

$$E = H - \frac{P}{\rho}$$  \hspace{1cm} (3.33)

where

$$H = h + \frac{|v|^2}{2}$$  \hspace{1cm} (3.34)

Each iteration consists of the steps illustrated in Fig. 3.3 and outlined below:

1. Fluid properties are updated, based on the current solution. (If the calculation has just begun, the fluid properties will be updated based on the initialized solution.)
2. The continuity, momentum, and (where appropriate) energy and species equations are solved simultaneously.
3. Where appropriate, equations for scalars such as turbulence and radiation are solved using the previously updated values of the other variables.
4. When interphase coupling is to be included, the source terms in the appropriate continuous phase equations may be updated with a discrete phase trajectory calculation.
5. A check for convergence of the equation set is made.

These steps are continued until the convergence criteria are met.

### 3.6.2 Residual Reporting

The process of obtaining a converged solution is of great importance in FLUENT simulations. So that in order to monitor this process, FLUENT provides a running report of the residuals for each equation at each iteration. The residuals are a measure of how closely each finite difference equation is balanced, given the current state of the solution. In this section, a definition of the residuals is given.

At each iteration of the solution algorithm, FLUENT reports a residual for each equation that has been solved. These residuals provide a measure of the degree to which each equation is satisfied throughout the flow field. FLUENT computes residuals for each conservation equation by summing the imbalance in the equation for all cells in the domain. A detailed description of the calculation of the residuals is provided below.
At the end of each iteration, the residual sum for each of the conserved variables is computed and stored, thus recording the convergence history. This history is also saved in the data file. The residual sum is defined below.

On a computer with infinite precision, these residuals will go to zero as the solution converges. On an actual computer, the residuals decay to some small value ("round-off") and then stop changing ("level out"). For "single precision" computations (the default for workstations and most computers), residuals can drop as many as six orders of magnitude before hitting round-off. Double precision residuals can drop up to twelve orders of magnitude.

A residual for the coupled solvers is simply the time rate of change of the conserved variable \( W \). The RMS residual is the square root of the average of the squares of the residuals in each cell of the domain:

\[
R(W) = \left( \sum \left( \frac{\partial W}{\partial t} \right)^2 \right)^{1/2}
\]

(3.35)

Equation (3.35) is the unscaled residual sum reported for all the coupled equations solved by Fluent's coupled solver.

In general, it is difficult to judge convergence by examining the residuals defined by Eq. (3.35) since no scaling is employed. Fluent scales the residual using a scaling factor representative of the flow rate \( \phi \) through the domain. This scaled residual is defined as

\[
\frac{R(W)_{\text{iteration } N}}{R(W)_{\text{iteration 5}}}
\]

(3.36)

The denominator is the largest absolute value of the residual in the first five iterations.

The scaled residuals described above are useful indicators of solution convergence. It is sometimes useful to determine how much a residual has decreased during calculations as an additional measure of convergence. For this purpose, Fluent allows to normalize the residual (either scaled or unscaled) by dividing by the maximum residual value after \( M \) iterations.

Normalization of the residual sum is accomplished by dividing by the maximum residual value after \( M \) iterations:
Normalization in this manner ensures that the initial residuals for all equations are of $O(1)$ and is sometimes useful in judging overall convergence. By default, $M = 5$, making the normalized residual equivalent to the scaled residual.

3.6.3 Judging Convergence

A FLUENT calculation is converged when all governing equations are balanced at each point in the solution domain. This section provides guidance on how to judge the convergence of the solution via residual values and how to monitor the progress towards convergence via residual histories and histories of solution variables.

The residuals for each flow variable give a measure of the magnitude of the error in the solution at each iteration. As discussed in the preceding section, these residuals are normalized unless being set as un-normalized. Generally, a solution is well converged when the normalized residuals are on the order of $10^{-3}$. An important exception is the enthalpy residual, which should be about $10^{-6}$.

In addition, the residuals of the species transport equations need to decrease to $1 \times 10^{-5}$ to $1 \times 10^{-6}$ when solving problems involving mixing of two species of very different molecular weights (e.g., H$_2$ and WF$_6$). If the residuals have decreased to this level, are monotonically decreasing, and the flow field looks unchanged from the solution 50 iterations earlier, then the solution can be called "converged." Sometimes it might not be needed to generate a completely converged solution, if the basic features of the flow field could be picked up right away. When quantitative results are sought, however, complete convergence of the solution is essential.

In the present study convergence is primarily judged by reaching unchanged values for the most important flow field parameters such as temperature, pressure, velocity magnitude, and species mass fractions. These parameters are averaged over all grid cells at different cross flow planes along the combustor length using the mass weighted-approach. At the convergence condition these averages show unchanged values with the solution iterations.
The conservation of mass and energy are checked as another means for examining the convergence. The imbalance in the mass flow rate and the rate of heat flux relative to the total inputs of mass flow rate and heat flux rate respectively are accepted if less than 1% under the convergence condition.

3.7 Physical Models

Four physical models are used in the present study that includes; rearward-facing step, swept rearward-facing step, cavity with no-pilot injection, cavity with pilot injection models. The configurations used in this case study are that used by Owens et al. [198,199] with slight differences in the dimensions applied. Figures 3.8-3.11 present the four models with the full dimensions. The case studied feature the symmetry condition at the mid-span plane; therefore, just one half of the physical domain is simulated to minimize the computational time.

3.7.1 Rearward-Facing Step Configuration

In the configuration used in this study the rearward-facing step is located at the upper longitudinal wall. The 3-D schematic diagram for this configuration is demonstrated in Fig. 3.8(a). The step height (H) is 10mm. Gaseous ethylene, as the main fuel, is injected at four step heights downstream of the step normal to the incoming supersonic air stream. The onset of thermal choking was delayed by diverging the test section starting at 19H downstream of the step with a 3-deg half angle. The total length of the domain is 350mm with an inlet test section of 25.4x25.4 mm². The full dimensions of the combustor at the symmetry plane are shown in Fig. 3.8(b). An unstructured grid with a size of 389,251 cells is used in simulating this case study.

3.7.2 Swept Rearward-Facing Step Configuration

This configuration resembles that used in the rearward-facing case study except for some differences. The inlet test section dimensions, the step height and its location, the main injection diameter and its location, and the pilot injections diameter are exactly as those used in the ethylene case. The total length of the domain is 220mm. The onset of thermal choking was delayed by diverging the test section starting at 6H downstream of the step with a 3-deg half angle. The step implemented in the propane case study is swept from both end sides starting at 15 mm downstream of the combustor inlet creating as extra means of vorticity that aims at enhancing the fuel-air mixing. Gaseous pilot propane
is injected parallel to the incoming air stream via two holes with 1 mm diameter each that are centered at the base of the step. The incoming air is a 1.751-Mach flow to simulate the enthalpy level of the typical flight conditions at the combustor inlet. The incoming air is clean (no vitiation used). The schematic diagram for the propane combustion case is presented in Fig. 3.9. An unstructured grid with a size of 207,125 cells is used in simulating this case study.

3.7.3 Cavity with No Pilot Injection Configuration

In the configuration used in the present study the rearward-facing step is located at the upper longitudinal wall. A 15°-wedge is located downstream of the step and upstream of the main normal injection. The combination of the rearward-facing step and the wedge forms a cavity-like configuration that helps in enhancing the fuel-air mixing in addition to initiate and stabilize the main flame. This is demonstrated in Fig. 3.10. The unstructured grid used to simulate this case study is of a size of 245,702 cells.

3.7.4 Cavity with Pilot Injection Configuration

The only difference between this configuration and the cavity with no pilot injection configuration is in the injection of the gaseous pilot ethylene parallel to the incoming air stream via three holes that are equally distributed at the base of the step. The 3-D schematic diagram of this configuration and the combustor full dimensions at the symmetry plane are presented in Figs. 3.11(a) and 3.11(b) respectively. The unstructured grid used to simulate this case study is of a size of 245,702 cells.

3.8 Boundary and Initial Conditions

Once the governing flow equations are defined, then the real driver for any particular solution is the boundary conditions. This has particular significance in CFD; any numerical solution of the governing flow equations must be made to see a strong and compelling numerical representation of the proper boundary conditions [193].

The inflow boundaries are supersonic, so the total and static pressures, the total temperature, and the species mass fractions are specified. For these supersonic inflow boundaries, uniform conditions were assumed for the primitive parameters. The outflow boundaries are supersonic so all flowfield variables are allowed to float. They are calculated using linear extrapolation based on the flowfield values at the internal points.
No-slip boundary condition is dictated at all walls and step boundaries; meaning that zero relative velocity between the surface and the gas immediately at the surface is assumed and the temperature of the fluid layer immediately in contact with the surface equals the wall temperature. All surfaces are assumed adiabatic with zero temperature gradient at the walls.

To start the calculations, initial conditions for the pressure, temperature, species mass fractions, and turbulence parameters in the whole flowfield must be stipulated. The choice of the initial conditions should not affect the final steady-state answer. In theory, these initial conditions can be purely arbitrary. In practice, they should be chosen intelligently to expedite the final steady-state answer, and hence shortening the computer execution time [193]. For all case studies in the present investigation, the initial conditions were set by applying free-stream air inlet conditions throughout the entire flow field.
Fig. 3.1 An unstructured face meshing using "Tri-Pave" scheme.

Fig. 3.2 T-Grid meshing scheme.
Fig. 3.3 Overview of the solution process.

- Update properties.
- Solve continuity, momentum, energy, and species equations simultaneously.
- Solve turbulence and other scalar equations.
- Converged?
- Stop
Fig. 3.4(a) Schematic diagram for the rearward-facing step configuration.

Fig. 3.4(b) Schematic diagram for the step configuration at the symmetry plane with full-dimensions.
Fig. 3.5 Schematic diagram for the swept rearward-facing step configuration.

Fig. 3.6 Schematic diagram for the cavity with no pilot injection configuration.
Fig. 3.7(a) Schematic diagram for the cavity with pilot injection configuration.

Fig. 3.7(b) Schematic diagram for the cavity with pilot injection configuration at the symmetry plane with full-dimensions.
Because of the turbulent nature of the case study, the influence of turbulence on
the reaction rate is taken into account by comparing the Arrhenius reaction rate and the
two eddy-dissipation reaction rates. Out of the three mentioned rates the limiting
(slowest) rate is used as the reaction rate and the contributions to the source terms in the
species conservation and energy equations are calculated from this reaction rate.

The following global one-step reaction of propane is used to calculate the
Arrhenius reaction rate in the present study:

\[ \text{C}_3\text{H}_8 + 5\text{O}_2 \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O} \]  \hspace{1cm} (4.1)

The Arrhenius reaction rate constants for the chemistry scheme are listed below,

Pre-exponential factor = 4.836e+09
Activation energy = 1.256e+08 [J/kgmol]
Temperature exponent = 0

The renormalized group (RNG) form of the \( \kappa-\varepsilon \) turbulence model is used. The
turbulence near-wall is treated using the two-layer zonal model.

Because the flow is compressible and a multicomponent mixture, it is modeled as
an ideal gas and the density is calculated as a composition-dependent property. A
composition-dependent specific heat capacity is defined for the multicomponent mixture
material while temperature-dependent heat capacities for the individual species are
specified. The solver computes the mixture’s specific heat capacity as a mass fraction
average of the pure species heat capacities. The viscosity and thermal conductivity are
defined as composition-dependent properties.

The coupled solver is used with the explicit formulation and the steady state
approach. The second order upwind scheme is used for discretization of the flow,
turbulence kinetic energy, and turbulence dissipation rate equations.

4.3 Grid Independence Study

Unstructured grid mesh is used to simulate this case study. The full details for the
mesh elements, and the faces and volume-meshing scheme were previously reported in
Sec. 3.5.

For the sake of eliminating the factor of the effect of the grid refinement on the
accuracy of the results, the grid independence study was performed. Two grid sizes were
implemented. Unstructured grid mesh with 207,125 tetrahedral cells was used reaching
the converged solution followed by its adapted version that is composed of 402,873 tetrahedral cells. The converged solution was also obtained using the larger grid.

The longitudinal distribution of the calculated averaged upper-wall absolute pressure along the combustor length is plotted for both grid sizes to judge for the independence of calculated results on the grid refinement. Twelve cross flow lines marking the intersection of the combustor upper wall and the corresponding cross flow planes are defined along the upper wall length. The twelve cross flow planes are defined at \( X = 0.001, 0.015, 0.020, 0.025, 0.030, 0.031, 0.070, 0.090, 0.120, 0.150, 0.180, \) and 0.219m. The points on the curves of Fig. 4.1 represent the area weighted averages of absolute pressure at all grid cells of the twelve intersection lines for both grid meshes used. The solid line represents the calculated values obtained using the small grid size while the dotted line represents those of the large grid size.

The area-weighted average of a quantity \( \Phi \) is computed by dividing the summation of the product of the selected field variable and facet area by the total area of the surface as follows:

\[
\frac{1}{A} \sum_{i=1}^{n} \phi_i |A_i| = \frac{1}{A} \int \phi dA
\]

Figure 4.1 shows a comparison between the averaged upper-wall absolute pressures for both grids used. An excellent coincidence between the two curves is manifested. The maximum pressure difference between the two curves with respect to the maximum average upper-wall pressure value in the whole field is 2.89% at the axial location of \( X = 70 \) mm. Achieving the grid independence study, the remaining of the calculations was conducted using the small grid and these results are presented here.

4.4 Results

4.4.1 Symmetry Plane Results

The flow field features and the combustion characteristics are discussed through the presentation of flow contours at the symmetry plane as depicted in Figs. 4.2-4.5.

The contours of the absolute pressure throughout the combustor symmetry plane are presented in Fig. 4.2. The combination of the expansion and shock waves along the combustor length is shown. The Prandtl-Meyer expansion waves are formed right at the step corner \( (X=0.030m) \). The contour values show the pressure decrease associated with
these expansion waves. The high-pressure fuel injection in the low-pressure combustor environment causes the fuel to expand, penetrating down the combustor height. The fuel expansion is followed by the barrel shock confining the fuel plume and raising up the pressure through the normal injection plane. The interaction of the fuel injection and the incoming supersonic air brings about the bow shock that extends diagonally downstream the step base area hitting the lower combustor wall at $X=0.090\text{m}$. A series of reflection waves off the upper and lower combustor walls is observed by following the change in the values of the pressure contours around $X=0.136\text{m}$ for the upper wall and $X=0.092\text{m}$ and $0.184\text{m}$ for the lower wall. The pressure drop in the regions upstream and downstream of the normal injection location is responsible for creating vortices and recirculation zones that entrain the incoming supersonic air to be mixed with the pilot fuel injection forming a combustible mixture. The ignition of this combustible mixture yields high temperature medium that facilitates the ignition of the normal injection and supports and maintains the main flame extending downstream towards the combustor exit.

Figures 4.3 and 4.4 show the temperature and CO$_2$ contours respectively at the symmetry plane. The step base area exhibits a medium of high temperature and high combustion products concentration that surrounds the upstream side of the normal injection. This region is brought by the ignition of the combustible mixture formed in the step base area and the consequent release of heat of combustion. This high temperature region represents the main flame holding mechanism in the investigated configuration. It is worth nothing that in the main flame area extending downstream of the normal injection, the flame possesses its highest temperature and combustion products concentration in the far field domain towards the combustor exit and attached to the upper wall. The area closer to the downstream of the injection location characterizes lower temperature and products concentration. This observation is one of the inherent effects of the side sweeping of the step that pushes the flow field downstream substantially releasing the heat of combustion in the far field domain. For such flow field it is recommended to optimize the combustor length to ensure the complete combustion and consequently the full liberation of the chemical energy stored in the fuel before exiting the combustor.
The distribution of the Mach number contours at the symmetry plane is presented in Fig. 4.5. The dominance of the supersonic flow in the combustor is exhibited except in few pockets in the upper part of the combustor. The recirculations upstream and downstream of the normal injection in the upper area of the combustor slow down the flow in these regions creating two subsonic pockets. The 3°-divergence of the upper wall expands the flow in the upper part of the combustor creating a slight supersonic flow just upstream of the reflection waves off the upper wall at X=0.136m. The compression of this weak supersonic flow brings about the third subsonic flow area in the far domain close to the upper wall. Further downstream the flow expansion continues and the flow exits the combustor slightly supersonic in the upper domain with the exit Mach number increasing towards the combustor lower wall. The previous flow description well matches the typical aerodynamics of such flow field.

4.4.2 Cross Flow Results

The flow field features and the combustion characteristics at two cross flow planes, at X=0.031m and 0.070m, are depicted in Figs. 4.6-4.12. These cross flow planes are used to present the flow nature inside the flame holding area, which is the step base area, and at the normal injection station, respectively.

Figure 4.6 shows the temperature contours inside the step base area at X=0.031m. The two pilot injections are fully surrounded by high temperature medium that extends downstream to approach the upstream side of the normal injection as discussed in Fig. 4.3. The effect of the side sweeping of the step is apparent in keeping the high-temperature-combustion gases produced by the ignition of the pilot injections concentrated towards the middle area of the combustor with relatively lower temperature gases at the side walls of the combustor.

Figures 4.7 and 4.8 show the velocity vectors and stream line contours at two cross flow locations, X=0.031m and 0.070m, inside the step base area and at the normal injection location, respectively. The two plots show the interaction between the incoming supersonic airflow, coming normal the page, and the pilot and main injections, respectively. Due the symmetry of the configuration the streamlines were added to just one half of the domain. The vortices formed around the fuel injection help in promoting the air-fuel mixing and consequently lead to more efficient combustion. The high-
pressure normal injection adds to the momentum of the recirculations surrounding it creating two strong vortices as shown in Fig. 4.8.

Figure 4.9 shows the Mach number contours at the normal injection cross flow plane. Once the fuel is injected at high pressures it expands in the surrounding lower-pressure medium. This is evident from the increase of the Mach number in this area that reaches a value around Mach 3. Due to the effect of the barrel and bow shocks surrounding the normal fuel injection, the flow is compressed decreasing its Mach number. Passing the area of shocks and due to the interaction between the supersonic incoming airflow and the normal fuel injection, the cross flow again accelerates and increases the Mach number.

The effects of the expansion and shock areas on the cross flow absolute pressure and static temperature distributions along the normal injection plane are shown in Figs. 4.10 and 4.11, respectively. The advancement of the two pilot flames towards the normal injection plane causes the two high temperature regions to permanently surround the normal injection as shown in Fig. 4.11. This is a very supportive tool for the ignition of the normal injection. The regions close to the sidewalls of the combustor exhibit lower temperature levels as previously explained in Fig. 4.6. Figure 4.12 presents the CO₂ mass fraction contours at the normal injection plane showing the high combustion products concentration surrounding the normal injection.

4.4.3 Pilot Injection Plane Results

The velocity vectors and stream lines contours, the temperature and CO₂ mass fraction contours at the pilot injection plane, Y=0.0304m, are presented in Figs. 4.13-4.15. The interaction of the incoming supersonic air flow, that spills over the swept sidewalls of the combustor, and the pilot and normal fuel injections causes the flow recirculations in the pilot and main injection zones as shown in Fig. 4.13. The pilot flames initiated at the pilot injection locations and extended downstream surrounding the main normal injection, at X=0.070m and Z=0, are manifested in Figs. 4.14 and 4.15. The high-temperature and high combustion products concentrations featuring the pilot flame area are clearly seen. As previously explained, sweeping of the combustor sidewalls forces the hot and highly concentrated combustion gases towards the combustor centerline while the combustor side areas characterize lower temperature and products
concentration as shown in Figs. 4.14 and 4.15. The high temperature and combustion products concentration in the far field domain towards the combustor exit are clear, which confirms the recommendation of using longer combustors with the swept step configuration.

4.4.4 Upper-Wall Averaged Results

The average distributions of the static temperature and absolute pressure at the combustor upper-wall are depicted in Fig. 4.16. The way the average temperature and pressure are calculated is previously presented while discussing the grid independence study at the beginning of this chapter.

The slight increase in the upper wall temperature downstream of the combustor inlet is due to the surface frictional heating. The flow expansion due to the side sweeping of the step decreases the temperature of the upper wall downstream reaching the step edge where the pilot flame is initiated. This is responsible for the temperature increase that reaches the first temperature peak around the pilot injection ports, X=0.031m. The incoming supersonic air spills over the sidewalls of the swept step and expands mixing with the high-temperature pilot flame combustion products in the step base area. This leads to the reduction of the average upper-wall temperature downstream the step area approaching the low-temperature normal fuel injection location, X=0.070m. The ignition of the normal fuel injected leads to the second increase in the upper-wall average temperature downstream of the injection station. The flow compression through the shock wave reflected off the upper wall around X=0.136m contributes to increasing the rate of the temperature increase at this location. The high temperature in the far field domain towards the upper wall explains the increase of the temperature at the combustor exit.

The physics explained in the temperature field applies to the pressure field except that the high-pressure peak coincides with the normal injection location, X=0.070m.

The propane study yielded the following conclusion. The swept step showed the ability to hold the propane flame in the supersonic air stream without extinction. It was found that the side weeping of the combustor exhibits the high temperature and combustion products concentration in the far field domain while the area downstream of the normal injection location characterizes lower temperature and products concentration. It is recommended to optimize the combustor length to ensure the complete combustion.
and consequently the full liberation of the chemical energy stored in the fuel before the fuel exits the combustor.
Fig. 4.1 Comparison between longitudinal average upper-wall absolute pressure distributions for both grid sizes, grid independence study.
Fig. 4.2 Absolute pressure contours at the symmetry plane.
Fig. 4.3  Static temperature contours at the symmetry plane.
Fig. 4.4  CO₂ combustion product mass fraction contours at the symmetry plane.
Fig. 4.5  Mach number contours at the symmetry plane.
Fig. 4.6 Static temperature contours at X=0.031m cross flow plane.
Fig. 4.7 Velocity vectors and streamlines contours at X=0.031m cross flow plane.
Fig. 4.8 Velocity vectors and streamlines contours at X=0.070m cross flow plane.
Mach No.

40  2.967
39  2.907
38  2.846
37  2.786
36  2.725
35  2.665
34  2.605
33  2.544
32  2.484
31  2.423
30  2.363
29  2.302
28  2.242
27  2.182
26  2.121
25  2.061
24  2.000
23  1.940
22  1.880
21  1.819
20  1.759
19  1.698
18  1.638
17  1.577
16  1.517
15  1.457
14  1.396
13  1.336
12  1.275
11  1.215
10  1.154
  1.094
  1.034
  0.973
  0.913
  0.852
  0.792
  0.731
  0.671
  0.611

Combustor Height, M

0.005 0.01 0.015 0.02 0.025 0.03 0.035

Combustor Width, M

-0.01 -0.005 0 0.005 0.01

X=70mm cross plane

Fig. 4.9  Mach number contours at X=0.070m cross flow plane.
Fig. 4.10 Absolute pressure contours at X=0.070m cross flow plane.
Fig. 4.11 Static temperature contours at X=0.070m cross flow plane.
**Fig. 4.12** CO$_2$ combustion product mass fraction contours at X=0.070m cross flow plane.
Fig. 4.13 Velocity vectors and streamlines contours at the pilot injection plane, $Y=0.0304$ m.
Fig. 4.14  Static temperature contours at the pilot injection plane, Y=0.0304 m.

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Fig. 4.15 CO$_2$ combustion product mass fraction contours at the pilot injection plane, Y=0.0304 m.
Fig. 4.16 Average upper-wall absolute pressure and static temperature distribution along the combustor length.
CHAPTER V

ETHYLENE SUPERSONIC COMBUSTION

5.1 Introduction

A detailed description of the physical model, the boundary and initial conditions, and the important flow parameters characterizing the case study are presented in the physical model description. The definitions of the terms used in the presentation of the results and their calculation procedures are then offered. The most significant results that can best reflect the flow field characteristics of the supersonic ethylene combustion conclude the course of this chapter. The results presented in this chapter are divided into three sub-sections. First, the effect of the combustor configuration on the combustion characteristics and flame holding of the supersonic ethylene flame is presented. Second, a discussion on the effect of the equivalence ratio of the main fuel injection on the combustion flow field is followed. The chapter is concluded by analyzing the effect of the equivalence ratio of the pilot fuel injection on the flame holding mechanism, and the general features of the flow and energy fields.

5.2 Physical Models and Flow Calculations Description

The supersonic ethylene combustion flow field is investigated through three physical models; rearward-facing step, cavity without pilot injection, and cavity with pilot injection respectively. The configurations of the three physical models are described in details in Sec. 3.7. In the present section, the flow field properties and the detailed description of the physical models used in the calculations are provided.

The three investigated physical models share the following flow features. The incoming supersonic airflow is vitiated with H₂O mass fraction of 0.17 and the typical O₂ concentration in air. The incoming air total temperature and pressure are 1800 K and 431.7 kPa respectively. The normal ethylene main injection is gaseous with static temperature of 300 K, and equivalence ratio of 0.6 calculated based on the total amount of the incoming supersonic airflow. For the pilot injection cases, the parallel ethylene pilot injection is gaseous with static temperature of 500 K, and equivalence ratios of 0.02,
0.03, 0.045, 0.06, and 0.08 calculated based on the total amount of the incoming supersonic airflow.

The pressure inlet boundary conditions are specified for the incoming air inlet, and both the pilot and main ethylene injections. The flow outlet is supersonic and specified as pressure outlet boundary that uses first order extrapolation for all parameters from the adjacent inflow cells. At the supersonic inflow boundaries, the total and static pressures, the total temperature, and the species mass fractions are specified. For these supersonic inflow boundaries, uniform conditions are assumed for the primitive parameters. All walls and step boundaries are treated as no-slip adiabatic surfaces. Applying free-stream inlet conditions throughout the entire flow field sets the initial conditions.

Because of the turbulent nature of the case study, the influence of turbulence on the reaction rate is taken into account by comparing the Arrhenius reaction rate and the two eddy-dissipation reaction rates. Out of the three mentioned rates, the limiting (slowest) rate is used as the reaction rate and the contributions to the source terms in the species conservation and energy equations are calculated from this reaction rate.

The following global one-step reaction of ethylene is used to calculate the Arrhenius reaction rate in the present study:

\[ C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O \] (5.1)

The Arrhenius reaction rate constants for the chemistry scheme are listed below,

- Pre-exponential factor = 2e+12
- Activation energy = 1.256e+08 [J/kgmol]
- Temperature exponent = 0

The renormalized group (RNG) form of the k-ε turbulence model is used. The turbulence near-wall is treated using the two-layer zonal model.

Because the flow is compressible and a multicomponent mixture, it is modeled as an ideal gas and the density is calculated as a composition-dependent property. A composition-dependent specific heat capacity is defined for the multicomponent mixture material while temperature-dependent heat capacities for the individual species are specified. The solver computes the mixture's specific heat capacity as a mass fraction.
average of the pure species heat capacities. The viscosity and thermal conductivity are defined as composition-dependent properties.

The coupled solver is used with the explicit formulation and the steady state approach. The second order upwind scheme is used for discretization of the flow, turbulence kinetic energy, and turbulence dissipation rate equations.

5.3 Definitions

5.3.1 Stagnation Pressure Efficiency and Entropy Production

Across a scramjet combustor, the loss in the stagnation pressure is of a fundamental interest, and may introduce an efficiency based on such loss as follows [143]:

$$\eta_{pt} = \frac{P_{out}}{P_{inlet}} = \pi$$ (5.2)

where $\eta_{pt}$, $P_T$, and $\pi$ are the stagnation pressure efficiency, the total pressure, and the total pressure ratio respectively and the subscripts “inlet” and “outlet” refer to the combustor inlet and outlet station respectively.

The relationship of interdependence of the total pressure ratio $\pi$ and the entropy production $\Delta S$ is defined as [26]:

$$\pi = \frac{P_{out}}{P_{inlet}} = e^{-\left(S_{outlet} - S_{inlet}\right)/R}$$ (5.3)

where $S$ and $R$ are the entropy and the gas constant respectively and the subscripts “inlet” and “outlet” refer to the combustor inlet and outlet station respectively.

This means that the total pressure ratio $\pi$ depends exponentially upon the entropy increase. In other words, the total pressure ratio should be expected to decrease very rapidly as entropy, the natural indicator of the effects of dissipation or flow losses, increases. From Eq. (5.3), the entropy production is defined as:

$$\Delta S = (S_{outlet} - S_{inlet}) = R \ln \left(\frac{P_{inlet}}{P_{outlet}}\right)$$ (5.4)

5.3.2 Kinetic Energy Efficiency

The concept of kinetic energy efficiency $\eta_{KE}$, expounded in Refs. [200-202], can be used to obtain the following definition:
where $m_{C,H_4, inj}$ is the injected fuel flow rate,

$$m_{C,H_4} = \int \rho Y_{C,H_4} (\vec{V} \cdot \vec{n}) dA,$$

$\rho$, $Y_{C,H_4}$, $\vec{V}$, and $A$ are the local fuel density, fuel mass fraction, normal velocity vector, and cross section area, respectively.

### 5.3.4 Fuel Penetration and Rate of Fuel Decay

The penetration of the fuel jet is measured at the point in the cross flow plane of the normal fuel injection, $X=0.070m$, where the maximum fuel mole fraction has dropped to 0.005 [52]. Since fuel mole fraction distribution at the normal fuel injection cross flow plane marks the maximum fuel concentration at the line of symmetry, the fuel penetration is defined by plotting the fuel mole fraction distribution versus the combustor height at the cross flow line that marks the intersection of the symmetry plane and the normal fuel injection cross flow plane. For easily discussing the penetration results, the penetration values are presented while measured from the upper-wall of the combustor at the normal injection location.

The rate at which the maximum fuel concentration at each cross section decays with axial distance is a good indication of the overall mixing rate of the jet [52]. The fuel mole fraction contours at sixteen cross flow planes, at $X=0.001$, 0.015, 0.030, 0.031, 0.039, 0.048, 0.0566, 0.065, 0.070, 0.110, 0.150, 0.190, 0.220, 0.260, 0.300, and 0.349m respectively, are plotted which showed the maximum fuel mole fraction to be located at the combustor centerline. Accordingly, the combustor symmetry plane is used to define the value of maximum fuel mole fraction at the sixteen lines making the intersection of the symmetry plane with the corresponding sixteen cross flow plane that are mentioned earlier. The longitudinal distribution of the maximum fuel mole fraction, at each cross flow plane, through the combustor length is plotted to evaluate the overall mixing rate of the fuel jet.

### 5.3.5 Upper-Wall Average Absolute Pressure and Static Temperature Distribution

For the heat transfer and design considerations, the longitudinal distribution of the average absolute pressure and static temperature along the upper-wall of the combustor are calculated. Sixteen cross flow planes are defined at $X=0.001$, 0.015, 0.030, 0.031, 0.039, 0.048, 0.0565, 0.065, 0.070, 0.110, 0.150, 0.190, 0.220, 0.260, 0.300, and
that extends to towards the upstream side of the normal injection. The temperature contours depicted in Fig. 5.2(a) show the high-temperature gases in the step base area. These high-temperature gases help in initiating the ignition of the normal fuel injection and maintaining its flame. This represents the flame holding mechanism of the step configuration.

The interaction between the flow recirculations in the step base area and the incoming supersonic airflow creates a two counter-flow vortices as shown in Fig. 5.3(a) which presents the velocity vectors and streamline contours at a cross flow plane inside the step base area, at X=0.040m. The vortices in the step base area direct the flow outward in the direction of the combustor sidewalls. These vortices are responsible for promoting the fuel/air mixing in the lateral direction inside the step base area and consequently maintaining an efficient combustion in this area. This is evident in the temperature contours at the same cross flow plane that is depicted in Fig. 5.4(a), which shows the high temperature area that extends throughout the width of the combustor surrounding the step edge, Y=0.025m.

The flow field features and energy field characteristics at Y=0.0304m lateral flow plane that lies in the middle of the step base area and extends longitudinally through the combustor length are shown in Figs. 5.5(a) and 5.6(a). This lateral flow plane marks the pilot injection plane for the cases with pilot injection. The flow field in this plane features a pair of counter flow vortices created in the step base area and surrounding the normal fuel injection as shown in Fig. 5.5(a). Downstream the normal fuel injection, another vortical region exists that directs the flow at the wakes of the injection location towards the combustor sidewalls. As explained before, these sets of vortices are effective in enhancing the fuel/air mixing in the regions both upstream and downstream of the normal injection station. The permanent high temperature regions surrounding the normal injection station are evident in Fig. 5.6(a), which are due to the vortices formed in their respective areas as explained before.

The flow field features and energy field characteristics of the step configuration that are presented at the symmetry plane, at X=0.040m cross flow plane inside the step base area, and at Y=0.0304m lateral flow plane exhibited the manifested flame holding capability of the step configuration in the supersonic air streams.
The injection of the under-expanded high-pressure normal fuel injection, at X=0.070m, in the low-pressure supersonic air medium originates the strong two pair of vortices surrounding the sides of the normal fuel injection as shown in Fig. 5.7(a). These vortices push the flow towards the combustor sides. The interaction between the flow recirculations surrounding the normal fuel injection and the incoming supersonic airflow creates the two counter-flow vortices that are shown in Fig 5.7(a). Fig. 5.8(a) presents the cross flow temperature contours at the normal injection plane. It shows the high-temperature areas at the sides of the normal fuel injection especially towards the combustor sidewalls. These hot gases contribute to the holding mechanism of the flame.

When comparing the velocity vectors and streamlines contours for the wedge configuration, Fig. 5.1(b), to that of the step configuration that is previously explained, Fig. 5.1(a), it is shown that the existence of the wedge expands the recirculations to predominate the step base area. This yields a better fuel/air mixing scheme and consequently a more efficient combustion. This is manifested in the higher temperature levels in the step base area of the wedge configuration as depicted in Fig. 5.2(b) compared to that of the step configurations, Fig. 5.2(a). Another advantage for the wedge configuration, which distinguishes it from the step configuration, is the pocket of high temperature gases that is trapped between the wedge straight surface and the normal fuel injection. This area takes over the role of a permanent energy source that supports the ignition of the normal fuel injection. The better combustion characterization for the wedge configuration is not only limited to the step base area but is presented in the downstream flow field as well by observing the higher temperature levels in the case of the wedge configuration compared to those of the step configuration in the downstream flow field.

The wider vortices in the step base area in the wedge configuration over that of the step configuration, as shown in Fig. 5.1(a) and (b), stretches the cross flow in the step base area towards the bottom wall. This is evident when comparing the velocity vectors and streamline contours of both configurations at X=0.40m cross flow plane that are presented in Fig. 5.3(a) and (b). The preference of the wedge configuration over the step configuration in supporting the ignition and the flame holding of the normal fuel injection is demonstrated when observing the more homogenous temperature distribution and
higher temperature levels pertinent to the wedge configuration in the cross flow plane, 
X=0.40m, over that of the step configuration as shown in Figs. 5.4 (a) and (b).

When comparing Figs. 5.5(a) and (b), which present the velocity vectors and streamline contours for both the step and wedge configurations at the Y=0.0304m lateral flow plane, it is shown that the existence of the wedge downstream of the step stretches the two small counter flow vortices created in the step configuration to fully and laterally occupy the entire cavity area. Therefore, the wedge configuration creates more homogenous flow medium that enhances the combustion characteristics in this area. This is obvious by observing the higher and more homogenous temperature distribution in the step base area (the cavity area) in the case of the wedge configuration over that in the step configuration as shown in Figs. 5.6(a) and (b), which present the temperature contours at the Y=0.034m lateral flow plane. Again the influential effect of the wedge in both flow regions upstream and downstream of the normal fuel injection is presented by observing the higher temperature levels in the entire flow field especially in the region surrounding the normal fuel injection. This observation stresses on the superiority of the wedge configuration as a flame holding mechanism over that of the step configuration.

The comparison between the velocity vectors and streamline contours for both configurations is done by observing Figs. 5.7(a) and (b), which present these vectors and contours at the normal injection station, X=0.70m. The wedge existence enlarges the recirculations area in the normal direction. This can be evaluated by locating the meeting point of the two counter flow vortices that marks the interaction between the normal injection and the incoming supersonic airflow. For the step configuration, this point is at Y=0.01m compared to Y=0.007m for the wedge configuration. Comparing the temperature contours for both configurations at the same cross flow plane, as shown in Figs. 5.8(a) and (b) shows the positive effect of the wedge in increasing the temperature of the gases surrounding the normal fuel injection plume compared to that of the step configuration. This is translated in more potential for holding the flame in the supersonic air streams.

One more comparison between the temperature flow fields of the step and wedge configurations in the downstream cross flow location at X=0.220m is presented in Figs.
5.9(a) and (b). These figures show the overall higher temperature levels exhibited when using the wedge configuration over that of the rearward-facing step configuration.

The advantage of the wedge configuration over the step configuration is clearly shown when comparing the axial combustion efficiency for both configurations as depicted in Fig. 5.10. The remarkable difference at the normal fuel injection location emphasizes the supportive effect of the wedge that is just upstream of the normal fuel injection, on burning more quantity of fuel compared to that of the step configuration.

Figure 5.11 shows the fuel penetration for both configurations under investigation. The wedge configuration exhibits more fuel penetration through the combustor height than that offered by the step configuration. This can be attributed to the effect of the wedge, which enlarges the recirculations in the normal direction, as shown in Figs. 5.7(a) and (b), and consequently permits the deeper fuel penetration compared to that of the step configuration. This observation is another advantage that is added to the wedge configuration.

The comparison between the rates of decay of the fuel concentration for both configurations is presented in Fig. 5.12. In the step base area, the rate of fuel entrained to this area, due to the created vortices, is higher than the rate of fuel depletion by combustion. This is the reason for the increase in the fuel mole fraction in this area for both configurations. Due to the fact that the general combustion efficiency for the wedge configuration is higher than that of the step configuration, as explained in Fig. 5.10, the rate of fuel depletion by combustion in the wedge configuration is higher than that in the step configuration and consequently its rate of increase of the fuel concentration is lower than that of the step configuration. This leads to the conclusion of the better mixing capabilities of the wedge configuration compared to that of the step configuration in the main flame holding region, the step base area. In the downstream of the normal injection station the rate of mixing in the middle of the combustor is shows in favor for the wedge configuration but in the far field domain the step configuration shows higher mixing capabilities, which enables its fuel concentration to converge towards the respective value of the wedge configuration at the exit of the combustor. This shows the good mixing capabilities of the step in the far field domain.
The upper-wall average static temperature distributions across the combustor length for both configurations are presented in Fig. 5.13. The wedge configuration exhibits higher upper-wall temperature along the combustor length than that of the step configuration. The same behavior is observed when comparing the flow field average static temperature distributions for both configurations as depicted in Fig. 5.14. It is worth of noting to observe the convergence of the values of the average temperatures for both configurations, as compared in Figs. 5.13 and 5.14, at the combustor exit. This observation stresses on the enhancement of the mixing capabilities of the step configuration in the far field domain reaching that of the wedge configuration, as discussed previously.

The longitudinal distributions of the average absolute pressure for the two configurations under investigation both at the upper-wall and in the flow field are depicted in Figs. 5.15 and 5.16 respectively. The two figures show that, although the pressure flow field is less sensitive to the configuration effect than the temperature flow field, as presented in Figs. 5.13 and 5.14, but yet the wedge configuration shows higher-pressure values in the region around the normal injection location.

Although the average absolute pressure values at the combustor exits for both configurations do not have that much difference, but due to the higher average Mach number at the combustor exit of the wedge configuration over that of the step configuration, the wedge-exit stagnation pressure is higher than that of the step. This leads to the higher stagnation pressure efficiency for the wedge configuration, which values 44.68%, while that of the step is 43.098%. This implies that the wedge configuration exhibits lower stagnation pressure loss than that associated with the step configuration. The same efficiency measure can be noticed by comparing the entropy production for both configurations, which amounts 254.97 and 261.65 J/kg. K for the wedge and step configurations respectively. According to the definition of the kinetic energy efficiency presented in Sec. 5.3.2, the wedge configuration showed higher kinetic energy efficiency than the step configuration. The kinetic energy efficiency for the wedge configuration is 45.327% while its contemporary value for the step configuration is 43.679%.
The comparisons presented in Figs. 5.1-5.16 and that are held between the efficiencies' values confirm the general advantage of the wedge configuration over the rearward-facing step configuration with regard to holding the flame in the supersonic airstreams, producing overall higher temperature medium throughout the combustor, and exhibiting lower flow losses and higher combustor efficiency.

5.4.2 Effect of Main Fuel Equivalence Ratio

In this section, the effect of the equivalence ratio (ER) of the normal fuel injection on the general flow field and combustion characteristics of the wedge configuration is presented. Two ER values of 0.60 and 0.45 for the normal fuel injection, calculated based on the mass flow rate of the total incoming supersonic airflow, are used with no pilot injection. The ER value is set by changing the main fuel injection pressure. Increasing the fuel injection pressure increases the ER through the increase in the fuel mass flow rate. The comparison between the flow field features, the energy field characteristics, and the efficiencies levels of the two case studies is held. The only changing parameter in this comparison is the ER value while all other boundary conditions and solution parameters are set the same.

When comparing the velocity vectors and streamlines contours of the ER of 0.60, Fig. 5.1(b), with that of the ER of 0.45, Fig. 5.1(c), it is shown that, using the lower ER, the fuel entrained in the step base area forms a single recirculation region that fills in the entire step base area while increasing the fuel injection pressure, ER of 0.60, more fuel is entrained in the step base area that intensifies the recirculations but confines it in a smaller region that is close to the normal injection location. One more observation that worth of noting is the effect of the higher injection pressure, higher ER, in stretching the recirculation region in the vertical direction towards the combustor lower wall. This is shown in the deflection of the incoming supersonic air stream downward towards the combustor lower wall. The reason for this behavior is the higher penetration for the normal fuel injection in the case of the higher ER value as shown in Fig. 5.17, which depicts the comparison between the fuel penetration patterns of the two ER values. The temperature contours at the symmetry plane for the ER values of 0.60 and 0.45 are presented in Figs. 5.2(b) and (c) respectively. The comparison between the two temperature fields shows the better temperature distribution in the step base area in the
lower ER case. It is also noticed that the higher injection pressure has a less advantageous effect in reducing the temperature in the area close to the wedge angled-surface, compared to that exhibited by the lower ER case, while it has a more advantageous effect in the vertical stretching the high temperature medium backing the upstream side of the normal fuel injection. This forms a supportive means of maintaining the main flame while facing the high-speed incoming air. Another advantage for the higher ER case is the pocket of high temperature gases that is trapped between the wedge straight surface and the normal fuel injection. This area plays the role of a permanent energy source that supports the ignition of the normal fuel injection. In the downstream flow field, the higher ER case exhibited, in general, higher temperature levels compared to those of the lower ER case.

The vertically widened vortices in the step base area in the higher ER case over that of the lower ER case, as seen in Figs. 5.1(b) and (c), stretches the cross flow in the step base area downward towards the bottom wall. This would be clearly observed when comparing the velocity vectors and streamlines contours of both ER cases at X=0.40m cross flow plane as presented in Figs. 5.3(b) and (c). The additional fuel entrained in the step base area, in the case of the higher ER, with its relatively low temperature breaks the temperature homogeneity featured in the lower ER case, Fig. 5.4(c), to produce a temperature spectrum with low values in the middle of the combustor and high values towards the combustor sidewalls. This is shown in Figs. 5.4(b) and (c). Although the high ER case lacks the homogenous temperature distribution in the step base area, it posses higher temperature levels in both the step base area and the lower half of the combustor as shown in Figs. 5.4(b) and (c).

Figures 5.5(b) and (c) present the velocity vectors and streamline contours for both ER cases at the Y=0.0304m lateral flow plane, it is shown that the additional entrained fuel in the step base area, due to the higher injection pressure, develops a couple of vortices in the middle of the lateral plane. This couple of vortices lumps laterally towards the combustor sidewalls to form a recirculation that fully occupy the entire step base area. Moreover, the higher injection pressure, higher ER case, lessens the intensity of the vortices formed in the down stream proximity of the normal injection station. These flow field differences are noticed when comparing Figs. 5.5(b) and (c).
The temperature flow fields for the two ER cases, Figs. 5.6(b) and (c), present the same observation reported in the X=0.040m cross flow plane, which states that although the high ER case lacks the homogenous temperature distribution in the step base area, it exhibits higher temperature levels in both of the sides of the step base area and the combustor flow field downstream of the normal fuel injection location, as shown in Figs. 5.6(b) and (c).

The comparison between the velocity vectors and streamline contours for both ER’s at the normal injection station, X=0.070m, is held by observing Figs. 5.7(b) and (c). The low-pressure region formed in the neighborhood of the normal injection location creates the strong flow recirculations that intensify with the increase of the injection pressure, increasing ER, especially in the combustor upper-wall area surrounding the injection port. This brings about a better vortical pattern in the normal injection plane in the case of the higher ER as shown in Figs. 5.7(b) and (c). Comparing the temperature contours for both ER cases at the same cross flow plane, as shown in Figs. 5.8(b) and (c), it is shown that the area surrounding the normal fuel injection port features higher temperature gases in the higher ER case compared to that of the lower ER value. This helps in igniting the normal fuel injected and enhancing the potential for holding the flame in the supersonic air streams. Moreover, the higher ER case presents higher temperature levels in the bottom half of the combustor that shares in elevating the average temperature in the cross flow plane of the normal fuel injection.

The comparison between the temperature flow fields of the two ER cases in the downstream cross flow location at X=0.220m is presented in Figs. 5.9(b) and (c). These figures show the overall higher temperature levels exhibited when using the higher ER. This is attributed to the higher amount of heat released in the flow field as a result of the more fuel injected in the case of the bigger ER.

In the comparisons held between the 0.60 and 0.45-ER cases in all planes; the symmetry plane, the X=0.040m and X=0.070m cross flow planes, and the Y=0.0304m lateral flow plane, the higher ER case showed less homogenous combustion characteristics in the step base area that is presented in the less homogenous temperature distribution in the entire step base region. At the same time, the comparisons held at the symmetry and lateral planes show higher temperature levels in the downstream flow field.
level of losses compared to those associated with the 0.45-ER case. The kinetic energy efficiency of the 0.60-ER case is 45.327% while the contemporary value of the 0.45-ER is 42.844%.

The comparisons presented in Figs. 5.1-5.9 (b) and (c) and Figs. 5.17-5.23 and that held between the values of the efficiencies shows the positive effect of increasing the ER of the normal fuel injection on the general flow field features and energy field characteristics in the combustor except in the step base area in which the lower ER features better temperature distribution and higher combustion efficiency.

5.4.3 Effect of Pilot Injection Equivalence Ratio

The effect of the pilot injection equivalence ratio ($ ER_p $) on the flame holding mechanism and combustion characteristics of ethylene in supersonic air streams is studied. The only changing parameter in this study is the value of the $ ER_p $ while keeping all other boundary conditions and flow parameters the same. Changing the $ ER_p $ is achieved by changing the pilot injection pressure. The $ ER_p $ is directly proportional to the injection pressure, which means increasing the pilot injection pressures leads to the increase in the $ ER_p $. There are seven values for the $ ER_p $ investigated and these are 0, 0.01, 0.02, 0.03, 0.045, 0.06, and 0.08. The $ ER_p $ for each one of the three-fuel pilot injections is calculated based on the total amount of the incoming supersonic airflow and the fuel mass flow of each individual pilot injection.

The flow field features and energy field characteristics of the different $ ER_p -$case are discussed and compared to determine the optimum $ ER_p $ that achieves the aspired goals of holding the flame and enhancing the combustion characteristics. The injection pressure that yields 0.01 $ ER_p $ could not resist the backpressure in the step base area. The boundary condition for the absolute injection pressure is 92705.8 Pa while the average backpressure for the flow field surrounding in pilot injection ports in the cavity area is 95798.6 Pa; therefore, reversed flow through the pilot injection ports dominated the flow field. This is demonstrated in Figs. 5.24(a), (b), and (c), which show the velocity vectors and streamlines contours at the three fuel injection ports. The streamlines clearly show the reversed flow getting out of the injection ports. This observation nullified the possibility of using 0.01-$ ER_p $ in the pilot injection study. Consequently, the 0.01-$ ER_p $-case
was excluded from the comparison study of the pilot equivalence ratio. Figure 5.25 presents the reversed flow through the central pilot injection port at the symmetry plane.

The comparisons between the velocity vectors and the temperature contours of the six pilot injection equivalence ratios of 0.0, 0.02, 0.30, 0.045, 0.06, and 0.08 are held at different flow planes, the symmetry plane, the X=0.040m plane, the pilot injection plane, and the X= 0.070m plane.

The effect of ER_p on the flow field features in the step base area is presented in Figs. 5.26(a)-(f). The pilot injection adds to the momentum of the recirculations in the cavity area. This stretches the vortical structure to dominate the entire cavity area and intensifies the recirculations. There is a common pattern noticed in the figure, that is the progressive vertical confinement of the vortices, which recirculate inside the cavity region, with the increase of the value of the ER_p except at 0.02-ER_p. This can be perceived by defining the vertical location of the tangent of the outer most recirculating streamline that deflects and revolves inside the cavity region. For ER_p of 0.0, 0.02, 0.30, 0.045, 0.06, and 0.08, the vertical locations of the tangents are 0.01265, 0.01353, 0.01112, 0.0106, 0.0103, and 0.00926 m respectively, measured from the combustor upper wall of the cavity region.

This observation demonstrates the passive effect for the pilot injection on the flow field quality in the cavity region. This negatively affects the fuel/air-mixing scheme in the region, which is expected to provide the holding mechanism for the flame of the normal injection. The only exception for this general observation is the 0.02-ER_p-case. This stretches the recirculation region both axially, through the combustor length to occupy bigger area in the cavity region, and vertically, through the combustor height to improve the interaction with the incoming supersonic air flow. This is presented in Fig. 5.26(b).

The effect of the ER_p on the fuel penetration at the normal injection plane is presented in Fig. 5.27. The ER_p decreases the penetration of the normal fuel in the incoming supersonic airflow, which reduces the available chances for the fuel/air mixing in the main-flame region downstream of the normal injection station. This should negatively affect the combustion characteristics of the main flame extending downstream towards the combustor exit. The only exception for this trend is the 0.02-ER_p-case, which
features the highest fuel penetration value matching that of the 0.0-ER_p-case. This is another precursor for the superiority of the 0.02-ER_p-case in the range of ER_p’s examined.

The effect of the ER_p on the quality of the fuel/air-mixing scheme is shown in Fig. 5.28, which presents the rates of decay of the fuel along the combustor length for the six ER_p under investigation. This figure shows that the increase of the ER_p decreases the rate of decay of the fuel concentration (i.e., the slope of the lines) in the cavity region while it does not affect it downstream the normal injection station. It is also shown that downstream of the normal injection location, the level of initial mixing is higher in the cases of the smaller ER_p (i.e., the lines are shifted downward in the vertical direction). The progressive confinement of the recirculations in the cavity region with the increase of the ER_p, as shown in Fig. 5.26, leads to the decrease in the decay of the fuel concentration and as a result affects the mixing rate in the cavity region negatively. The 0.02-ER_p-case possesses the best mixing quality in the cavity region among all other cases with pilot injection. In the region downstream of the normal injection and due to the increased quantity of pilot fuel injected, the initial mixing is seen to be higher in the cases of lower ER_p without affecting the rate of decay of the fuel concentration. Comparing the rate of fuel decay for 0.0-ER_p and 0.02-ER_p-cases in the downstream flow field shows that although the 0.02-ER_p-case exhibits higher initial level of fuel mole fraction, it offers a higher mixing rate (higher line slope) that converges its fuel mole fraction value towards its lower counterpart value of the 0.0-ER_p-case far downstream at the combustor exit. This adds another feature for the 0.02-ER_p-case.

The temperature contours at the symmetry plane for the investigated ER_p-cases are exhibited in Figs. 5.29(a)-(f). The no-pilot case presents the highest levels of temperature distribution in both flow field regions, the cavity region and the downstream region. The excessive addition of the relatively low-temperature-pilot injection in the small cavity area quenches the flame entrained inside the cavity region, by the vortical effect in this region. This effect reduces the overall temperature levels in the cavity region that extends to surround the upstream part of the normal injection. This leads to deterioration in the combustion characteristics of the normal fuel injection. This is obviously noticeable when comparing the levels of the temperature contours in the cavity and downstream flow fields of the 0.03-ER_p, 0.045-ER_p, 0.06-ER_p, and 0.08-ER_p-cases,
with those of 0.0-ER<sub>p</sub>-case as presented in Figs. 5.29(a),(c)-(f). The 0.02-ER<sub>p</sub>-case is excluded from the general observation mentioned in the previous statement. The comparison between the temperature contours at the symmetry plane for the 0.02-ER<sub>p</sub> and 0.0-ER<sub>p</sub>-cases reveals an advantage for the 0.02-pilot injection equivalence ratio case over the 0.0-ER<sub>p</sub>-case and all examined ER<sub>p</sub>-cases. This is shown in Figs. 5.29(a), (b). Although the 0.02-pilot injection reduces the temperature in the area occupied by the relatively lower-temperature pilot injection, the three pilot flames extend downstream towards the normal injection and the energy liberated by the pilot flames elevates the temperature levels in the upper part of the cavity region and at the vicinity of the normal injection. This behavior generally increases the temperature of the upstream face of the normal injection, which enhances the flame holding mechanism of the normal fuel injection.

The effect of the pilot equivalence ratio on the general energy field at the symmetry plane, which is discussed above, is now presented at the pilot injection plane. This is presented by comparing the temperature contours depicted in Figs. 5.30(a)-(f) for the six investigated pilot injection cases. The suppressive effect of the pilot injection on the temperature field in both of the cavity and downstream regions is clear when comparing Figs. 5.30(a) and (c)-(f). The positive effect of the 0.02-ER<sub>p</sub> on elevating the temperature levels in the cavity area is shown in Figs. 5.31(a), and (b) which presents the temperature contours in the pilot injection plane with a focus on the region surrounding the normal injection. The 0.02-ER<sub>p</sub>-case exhibits an advantage over the 0.0-ER<sub>p</sub>-case by offering a temperature increase of 200° in the combustor central area, which is supporting the upstream side of the normal injection and around 120° temperature increase at the sides of the combustor. This observation represents the main advantage of the 0.02-ER<sub>p</sub>-case over the 0.0-ER<sub>p</sub>-case in promoting the flame holding mechanism in the cavity region.

The temperature contours at X=0.040m inside the cavity for the six ER<sub>p</sub>-cases under investigation are shown in Figs. 5.32(a)-(f). The superiority of the 0.02-ER<sub>p</sub>-case is affirmed when comparing its temperature levels at this cross flow location to those of the 0.0-ER<sub>p</sub>-case as presented in Figs. 5.32(a) and (b). The 0.02-ER<sub>p</sub>-case possesses higher temperatures at the upper part and the sides of the combustor. This high temperature flow
marches downstream to envelope the upstream side to the normal fuel injection. This behavior stands in favor of the 0.02-ER_p-case while comparing it to the 0.0-ER_p-case in regard to the quality of the flame holding mechanism. The deterioration of the combustion characteristics in the cavity area with the progressive increase of the ER_p is shown when comparing the decreasing temperature levels exhibited in Figs. 5.32(c)-(f), which are pertinent to 0.03-ER_p, 0.045-ER_p, 0.06-ER_p, and 0.08-ER_p-cases respectively, and those of the base line case, 0.0-ER_p, which are presented in Fig. 5.32(a).

The temperature contours at the normal injection plane, X=0.070m, for the six ER_p-cases under investigation are presented in Figs. 5.33(a)-(f). In this figure, the positive effect of the pilot-injection equivalence ratio is revealed. Examining the values of the temperature contours shows that increasing the ER_p increases the temperature level in the upper part of the combustor surrounding the normal injection. It is noticed that 0.03-ER_p-case exhibits the highest temperature level (3355 K) among the other investigated ER_p-cases. Although further increase in the ER_p decreases the maximum temperature level, the area inhabited by the high temperature values is getting larger especially in the 0.06-ER_p-case which reports the highest area-weighted average static temperature in the X=0.070m cross flow plane.

The longitudinal distribution of the area-weighted average flow field static temperature is plotted in Fig. 5.34 for the ER_p under investigation. For easily analyzing the effect of the ER_p on the temperature flow field along the combustor, the data of Fig. 5.34 is presented in Table 5.1. Examining the values of the flow field average temperature reported in Fig. 5.34 and Table 5.1 shows that part of the relatively lower-temperature pilot fuel injected in the small cavity region ignites releasing the energy of combustion that raises the temperature in the cavity area. This is the reason for the increase of the average temperature of the 0.02-ER_p over that of the no-pilot injection case, 0.0-ER_p-case at X=0.040m as shown in Fig. 5.34 and Table 5.1. Further increase in the relatively low-temperature pilot injection does not sufficiently provide high quantity of energy of combustion that can counteract the quenching effect of the pilot fuel injected in the cavity region. This leads to the continuous temperature decrease in the cavity region with further increase in the pilot injection equivalence ratio, ER_p, as presented in Fig. 5.34 and Table 5.1 at X=0.040, and 0.060m. The pilot fuel that does not ignite in the
cavity region marches downstream along the combustor and part of it starts igniting in the high-temperature side areas of the combustor at the normal injection station. The 0.06-ER_p-case shows the highest average temperature at the normal injection plane, X=0.070m. Further increase in the ER_p entrains more quantity of pilot fuel whose heat absorption effect is higher than the heat liberated by its combustion and as a result the average flow temperature decreases for the 0.08-ER_p-case at X=0.070m plane. The partial consumption through combustion of the remaining fuel pilot injection that is entrained in the flow field narrows the temperature difference shown at X=0.110m plane. Further downstream, the balancing effect of heat liberation through the ignition of the pilot fuel and the heat absorbed by the extra non-ignited fuel keeps the 0.02-ER_p-case featuring the highest flow field average static temperature reaching the combustor exit as shown in Fig. 5.34 and Table 5.1. A thorough examination of the average flow field temperature shows that 0.02-ER_p-case represents the optimum pilot fuel injection choice that can achieve the highest temperature in the flame holding region, cavity area, and downstream of the combustor.

The continuous liberation of the heat due to the partial combustion of the pilot fuel, that did not ignite in the cavity area and is entrained in the flow downstream the combustor, interprets for the increase of the flow field area-weighted average absolute pressure with the increase in the value of the ER_p as depicted in Fig. 5.35. Although the entrained pilot fuel keeps igniting through its way downstream the combustion, the largest amount of pilot fuel ignites at the normal injection location. This brings about the large difference in the average pressure values that take place at the normal injection location, X=0.070m. This difference converges in the downstream of the combustor. A slight increase in the flow pressure at the combustor exit with the increase of the ER_p leads to a slight increase in the stagnation pressure efficiency, as depicted in Fig. 5.36, a slight decrease in the entropy production, as depicted in Fig. 5.37, and a slight increase in the kinetic energy efficiency, as depicted in Fig. 5.38.

Increasing the pilot injection equivalence ratio, ER_p, increases the amount of fuel that does not ignite in the cavity region and is entrained in the flow field to be ignited in part downstream the combustor. As the combustion efficiency is defined to be inversely proportional to the quantity of fuel unburned, the combustion efficiency decreases with
the increase in the ER_p as shown in Fig. 5.39. This figure emphasizes on the advantage of
the 0.02-ER_p-case over the other competing pilot injection cases by featuring the highest
combustion efficiency in the flame holding region, the cavity area. This combustion
efficiency is close to that of the no-pilot injection case, 0.0-ER_p.

Taking into consideration both of the flame holding capabilities and the
combustion and flow field qualities, the 0.02 case showed the optimum ER_p value that
can achieve the trade off between the mentioned objectives. This conclusion is reached
after carefully analyzing the data presented in Figs. 5.24-5.39.

The main findings attained out of the ethylene study can be summarized in the
following points. The step configuration with no pilot injection can afford the flame
holding mechanism in the supersonic air stream by creating the flow recirculations in the
step base area and featuring permanent high temperature region surrounding the normal
fuel injection. The step configuration showed good mixing capabilities in the far field
domain. The wedge configuration proved superiority over the generic rearward-facing
step configuration in holding the ethylene flame in the supersonic airstreams, producing
overall higher temperature medium throughout the combustor, and exhibiting lower flow
losses and higher combustor efficiency. The increase in the equivalence ratio of the
ethylene normal fuel injection enhances the general flow field features and energy field
characteristics in the combustor except in the step base area where the lower equivalence
ratio features better temperature distribution and higher combustion efficiency.

Although the wedge with no pilot injection configuration presents the highest
level of temperature distribution in the cavity and downstream regions, the 0.02-pilot
equivalence ratio increases the temperature of the upstream face of the normal injection
and enhances the flame holding mechanism. 0.02-pilot equivalence ratio presented the
optimum pilot injection case that can promote the flame holding mechanism and keep
good combustion and flow field qualities. While the further increase of the pilot injection
equivalence ratio quenches the high temperature gases in the cavity region, which leads
to the deterioration of the flame holding mechanism, the excessive pilot fuel injected
expresses its effect by increasing the average flow field static temperature and absolute
pressure in the far field domain.
Table 5.1 Values of the longitudinal distribution of the area-weighted average flow field static temperature for different pilot equivalence ratios

<table>
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<th>ER</th>
<th>0.001</th>
<th>0.015</th>
<th>0.030</th>
<th>0.031</th>
<th>0.040</th>
<th>0.060</th>
<th>0.070</th>
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<td>2333</td>
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<td>2303</td>
<td>2417</td>
<td>2344</td>
<td>2318</td>
</tr>
<tr>
<td>0.03</td>
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<td>1754</td>
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<td>1270</td>
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<td>1787</td>
<td>2003</td>
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<td>2269</td>
<td>2401</td>
<td>2337</td>
<td>2316</td>
</tr>
<tr>
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<td>1937</td>
<td>2245</td>
<td>2388</td>
<td>2332</td>
<td>2315</td>
</tr>
</tbody>
</table>
Fig. 5.1  Velocity vectors and streamlines contours at the symmetry plane.
0.60-Step, Nopilot

0.60-Wedge, Nopilot
Fig. 5.2 Temperature contours at the symmetry plane.
Combustor Height, m

Combustor Width (m)

(a) 0.60-step, nopilot

(b) 0.60-wedge, nopilot

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Fig. 5.3  Velocity vectors and streamlines contours at $X=0.040\text{m}$ plane.
Static Temp*

31 3272
30 3251
29 3222
28 3183
27 3147
26 3096
25 3022
24 2897
23 2835
22 2773
21 2699
20 2648
19 2611
18 2595
17 2523
16 2398
15 2273
14 2149
13 2024
12 1899
11 1774
10 1649
9 1524
8 1467
7 1455
6 1437
5 1400
4 1327
3 1288
2 1278
1 1275

0.60-Step, Nopilot
X = 40mm Cross Plane

(a) 0.60-step, nopolit

Static Temp*

31 3272
30 3251
29 3222
28 3183
27 3147
26 3096
25 3022
24 2897
23 2835
22 2773
21 2699
20 2648
19 2611
18 2595
17 2523
16 2398
15 2273
14 2149
13 2024
12 1899
11 1774
10 1649
9 1524
8 1467
7 1455
6 1437
5 1400
4 1327
3 1288
2 1278
1 1275

0.60-Wedge, Nopilot
X = 40mm Cross Plane

(b) 0.60-wedge, nopolit
Fig. 5.4  Temperature contours at X = 0.040m plane.
Combustor Length, m

(a) 0.60-step, nopilot

(b) 0.60-wedge, nopilot

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Fig. 5.5 Velocity vectors and streamlines contours at the pilot injection plane, $Y=0.0304m$.  

(c) 0.45-wedge, nopilot
Static Temp.
26  3364
25  3301
24  3180
23  3125
22  3079
21  3004
20  2985
19  2940
18  2864
17  2822
16  2780
15  2762
14  2754
13  2569
12  2383
11  2198
10  2012
  9  1827
  8  1641
  7  1456
  6  1270
  5  1085
  4  899
  3  714
  2  528
   1  343

(a) 0.60-step, nopilot

Static Temp.
26  3364
25  3301
24  3180
23  3125
22  3079
21  3004
20  2985
19  2940
18  2864
17  2822
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13  2569
12  2383
11  2198
10  2012
  9  1827
  8  1641
  7  1456
  6  1270
  5  1085
  4  899
  3  714
  2  528
   1  343

(b) 0.60-wedge, nopilot
Fig. 5.6  Temperature contours at the pilot injection plane, $Y=0.0304\text{m}$.

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Fig. 5.7 Velocity vectors and streamlines contours at the normal injection plane, X=0.070m.

(c) 0.45-wedge, nospilot

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Fig. 5.8 Temperature contours at the normal injection plane, X=0.070m.
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Fig. 5.9  Temperature contours at X=0.220m.
Fig. 5.10  Comparison between the combustion efficiency of the step and wedge configurations.

Fig. 5.11  Comparison between the fuel penetration of the step and wedge configurations.

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Fig. 5.12  Comparison between the rate of fuel decay of the step and wedge configurations.
Fig. 5.13 Comparison between the upper-wall average static temperature distribution of the step and wedge configurations.

Fig. 5.14 Comparison between the flow field average static temperature distribution of the step and wedge configurations.
Fig. 5.15 Comparison between the upper-wall average absolute pressure distribution of the step and wedge configurations.

Fig. 5.16 Comparison between the flow field average absolute pressure distribution of the step and wedge configurations.
Fig. 5.17  Comparison between the fuel penetration of the 0.45-ER and 0.60-ER wedge configuration cases.

Fig. 5.18  Comparison between the rate of fuel decay of the 0.45-ER and 0.60-ER wedge configuration cases.

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Fig. 5.19  Comparison between the combustion efficiency of the 0.45-ER and 0.60-ER wedge configuration cases.
Fig. 5.20 Comparison between the upper-wall average static temperature distribution of the 0.45-ER and 0.60-ER wedge configuration cases.

Fig. 5.21 Comparison between the flow field average static temperature distribution of the 0.45-ER and 0.60-ER wedge configuration cases.
Fig. 5.22 Comparison between the upper-wall average absolute pressure distribution of the 0.45-ER and 0.60-ER wedge configuration cases.

Fig. 5.23 Comparison between the flow field average absolute pressure distribution of the 0.45-ER and 0.60-ER wedge configuration cases.

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Fig. 5-24  Reversed flow at the pilot injection ports for 0.01-ERP, pilot inj. plane.

Fig. 5-25  Reversed flow at the pilot injection ports for 0.01-ERP, sym. plane.
Fig. 5.26  Velocity vectors and streamlines contours at the symmetry plane for different pilot equivalence ratios.
**Fig. 5.27** Effect of the pilot injection equivalence ratio on the fuel penetration.

**Fig. 5.28** Effect of the pilot injection equivalence ratio on the rate of decay of the fuel.
Fig. 5.29  Temperature contours at the symmetry plane for different pilot equivalence ratios.
Static Temp.

(a) \( \phi_p = 0.0 \)

(b) \( \phi_p = 0.02 \)

(c) \( \phi_p = 0.03 \)
Fig. 5.30  Temperature contours at the pilot injection plane, Y=0.0304m, for different pilot equivalence ratios.
Fig. 5.31 Comparison between the temperature contours of 0.0-ER, and 0.02-ER,-cases focusing on the cavity region.
(a) $\phi_p = 0.0$

(b) $\phi_p = 0.02$

(c) $\phi_p = 0.03$

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Fig. 5.32 Temperature contours at X=0.040m cross flow plane for different pilot equivalence ratios.
Fig. 5.33 Temperature contours the normal injection plane, X=0.070m, for different pilot equivalence ratios.

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Fig. 5.34 Comparison between the flow field average static temperature distributions for different pilot equivalence ratios.

Fig. 5.35 Comparison between the flow field average absolute pressure distributions for different pilot equivalence ratios.
Fig. 5.36 Effect of pilot injection equivalence ratio on the stagnation pressure efficiency.

Fig. 5.37 Effect of pilot injection equivalence ratio on the entropy production.

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Fig. 5.38 Effect of pilot injection equivalence ratio on the kinetic energy efficiency.

Fig. 5.39 Effect of pilot injection equivalence ratio on the combustion efficiency.
CHAPTER VI

CONCLUDING REMARKS

A numerical study has been conducted to investigate the mixing and combustion enhancements in scramjet engines, which are characterized by the supersonic combustion flow fields. The primary objective of the current study is to numerically examine the possibility of igniting hydrocarbon fuels in supersonic airstreams and maintaining the hydrocarbon flames in such hostile environments. The secondary objective of the study is to investigate the effect of the combustor configuration, the main fuel equivalence ratio, and the pilot fuel equivalence ratio on the flame holding mechanism and the flow field and energy field characteristics.

The four physical models used in the current study are the unswept generic rearward-facing step, the side swept rearward-facing step, the wedge with no pilot injection, and the wedge with pilot injection configurations. The Computational Fluid Dynamics "CFD" Code used in the present study is the FLUENT commercial code, which is a control volume based finite difference method. FLUENT is a general-purpose computer program for modeling fluid flow, heat transfer, and chemical reaction. FLUENT solves the Reynolds average Navier-Stokes equations. It models a wide range of phenomena by solving the conservation equations for mass and momentum. For flows involving heat transfer or compressibility, an additional equation for energy conservation is solved. For flows involving species mixing or reactions, a species conservation equation is solved. Additional transport equations are also solved when the flow is turbulent. The governing equations are discretized on a curvilinear grid to enable computations in complex irregular geometries. A non-staggered system is used for storage of discrete velocities and pressures. Interpolation is accomplished via a first-order, Power-Law scheme or optionally via higher order upwind schemes. The equations are solved using SIMPLE-like algorithms with an iterative line-by-line matrix solver and multigrid acceleration. The coupled solver is used with the explicit formulation and the steady state approach. The second order upwind scheme is used for discretization of the flow, the turbulence kinetic energy, and the turbulence dissipation rate equations.
All physical models feature the following: the incoming airflow is supersonic, and the main fuel is injected normal to the incoming airflow. For the cases with pilot injections, the pilot fuel is injected parallel to the incoming airflow upstream of the main normal fuel injection. The pressure inlet boundary conditions are specified for the incoming air inlet, and both the pilot and main fuel injections. The flow outlet is supersonic and specified as pressure outlet boundary. All walls and step boundaries are treated as no-slip adiabatic surfaces. Applying free-stream inlet conditions throughout the entire flow field sets the initial conditions.

The influence of turbulence on the reaction rate is taken into account by considering the limiting (slowest) rate out of the three rates of the Arrhenius reaction rate and the two eddy-dissipation reaction rates. A global one-step reaction of the investigated fuel is used to calculate the Arrhenius reaction rate. The renormalized group (RNG) form of the $k$-$\varepsilon$ turbulence model is used. The turbulence near-wall is treated using the two-layer zonal model. Because the flow is compressible and a multicomponent mixture, it is modeled as an ideal gas and the density, the specific heat, the viscosity, and the thermal conductivity are calculated as composition-dependent properties.

At the beginning of the investigation, liquid kerosene was used, which is the closest formula to the jet fuels that are most likely to be used in the hydrocarbon-fueled scramjet engines. After using different reduced kinetic schemes for kerosene that have the hydrogen combustion as one of the elementary reactions, the difficulty of igniting the liquid kerosene while injecting pilot gaseous hydrogen ceased the study. The issue of the combustion simulation of two different fuel injections with two different fuel types and flow phases in supersonic airstreams was realized to be numerically hardly achieved. Thereafter, attention has been directed towards the simulation of ethylene and propane as gaseous hydrocarbons in supersonic air flow fields.

The combustion characteristics of gaseous propane in supersonic airflow using the rearward-facing step that is swept inward form both end sides is studied. The effect of sweeping the step on the flow field features of propane combustion is investigated.

Next, an extensive study for the flame holding and mixing and combustion characteristics of gaseous ethylene in supersonic airstreams is carried out. In this study, different combustor configurations, different main fuel equivalence ratios, and different
pilot fuel injection equivalence ratios were employed. First, the effect of the combustor configuration on the temperature flow field and the flow structure is investigated by simulating two different combustor configurations, the rearward-facing step and the cavity. Next, the effect of the equivalence ratio of the main fuel injection on the general flow field features and energy field characteristics is studied. Lastly, the effect of the pilot fuel equivalence ratio on the flame holding mechanism, and the combustion and flow field qualities concludes the study. Six pilot injection equivalence ratios are studied, 0.0, 0.02, 0.03, 0.045, 0.06, and 0.08.

The propane study yielded the following conclusions. The swept step showed the ability to hold the propane flame in the supersonic air stream without extinction. It was found that the side sweeping of the combustor exhibits the high temperature and combustion products concentration in the far field domain while the area downstream of the normal injection location characterizes lower temperature and products concentration. It is recommended to optimize the combustor length to ensure the complete combustion and consequently the full liberation of the chemical energy stored in the fuel before the fuel exits the combustor.

The main findings attained from the ethylene study can be summarized in the following points. The step configuration with no pilot injection can afford the flame holding mechanism in the supersonic air stream by creating the flow recirculations in the step base area and featuring permanent high temperature regions surrounding the normal fuel injection. The step configuration showed good mixing capabilities in the far field domain. The wedge configuration proved superiority over the generic rearward-facing step configuration in holding the ethylene flame in the supersonic airstreams, producing overall higher temperature medium throughout the combustor, and exhibiting lower flow losses and higher combustor efficiency. The increase in the equivalence ratio of the ethylene normal fuel injection enhances the general flow field features and energy field characteristics in the combustor except in the step base area where the lower equivalence ratio features better temperature distribution and higher combustion efficiency.

Although the wedge with no pilot injection configuration presents the highest level of temperature distribution in the cavity and downstream regions, the 0.02-pilot equivalence ratio increases the temperature of the upstream face of the normal injection
and enhances the flame holding mechanism. The 0.02-pilot equivalence ratio presented the optimum pilot injection case that can promote the flame holding mechanism and keep good combustion and flow field qualities. While the further increase of the pilot injection equivalence ratio quenches the high temperature gases in the cavity region, which leads to the deficiency of the flame holding mechanism, the excessive pilot fuel injected shows its positive effect by increasing the average flow field static temperature and absolute pressure in the far field domain.

For the supersonic mixing studies, it is suggested to investigate the effect of the injection angle of the main fuel on the supersonic mixing and combustion characteristics. It is recommended to study the effect of the transverse normal ethylene and propane injections on the flame holding and combustion characteristics in order to investigate the relationship between the injection scheme and the flame holding and flow field and energy field features. It is suggested to simulate the supersonic combustion of the normal ethylene and propane injections with the pilot gaseous hydrogen. For the future studies, it is suggested to dedicate more effort trying to carry out the simulation of the supersonic combustion of liquid kerosene with gaseous hydrogen as a pilot fuel. The radiative interaction is also suggested to be included in the future studies due to the existence of the hydrocarbon combustion products, which are radiative participating mediums.
REFERENCES


CURRICULUM VITA
for
AHMED A. TAHA

DEGREES:

- Doctor of Philosophy (Mechanical Engineering), Old Dominion University, Norfolk, VA, Dec. 2002
- Master of Science (Mechanical Power Engineering), Cairo University, Cairo, Egypt, June 1994
- Bachelor of Science (Mechanical Power Engineering), Cairo University, Cairo, Egypt, July 1988

PROFESSIONAL CHRONOLOGY:

- Mechanical Engineering Dept., Old Dominion University, Norfolk, VA. Research and Teaching Assistant, Aug. 1996 - Dec. 2002
- Mechanical Power Engineering Dept., Cairo University, Cairo, Egypt. Research and Teaching Assistant, Aug. 1988 - June 1994

HONORS AND AWARDS:

- Student Member, Virginia Academy of Science (5/1999 – Present).
- Student Member, American Society for Mechanical Engineers (ASME) (1/1999 – Present).
- Student Member, American Inst. for Aeronautics and Astronautics (AIAA) (12/1996 – Present).
- Member, Mechanical Engineering Branch, Engineers Syndicate, Cairo, Egypt (5/1988 – Present).
SCHOLARLY ACTIVITIES COMPLETED:

Refereed Journal Articles:


Selected Refereed Proceedings:


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