IGNITION TRANSIENT IN AN ETHYLENE FUELED SCRAMJET ENGINE WITH AIR THROTTLING

A Dissertation in
Mechanical Engineering

by

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This research focuses on the modeling and simulation of ignition transient and subsequent combustion dynamics in an ethylene fueled supersonic combustion ramjet (scramjet) engine. The primary objectives are: 1) to establish an efficient and accurate numerical framework for the treatment of unsteady flow and flame dynamics in scramjet propulsion systems; and 2) to investigate the effects of transverse air throttling on flow development and fuel-air mixing, and to identify its positive influence on ignition and flameholding in a scramjet combustor; and 3) to construct a detailed study investigating ignition transient to identify underlying essential mechanisms by means of air throttling implementation technique.

A comprehensive numerical study of the combustion dynamics in a scramjet combustor is performed. The analysis treats the conservation equations in three dimensions and takes into account finite-rate chemical reactions and variable thermophysical properties for a multi-component reacting flow. Menter’s $k-\omega$ SST two-equation turbulence model is implemented, as it performs well for shear-layer flows and wall turbulence effects. The governing equations and the associated boundary conditions are solved using a density-based finite-volume approach and four-stage Runge-Kutta scheme to utilize explicit time marching. The code is parallelized using the domain decomposition technique and message passing interface (MPI). The theoretical formulation and numerical scheme is first validated with two test cases including turbulent flow over a flat plat and a two-dimensional oblique shock wave, and then validated with engine test data.
The analysis is first employed to a detailed investigation into the flow development and fuel-air mixing in the scramjet engine for non-reacting flow at Mach 5 flight condition. As the air throttling is implemented to increase the combustor pressure, a series of subsequent oblique shock waves following the fuel injectors is generated to separate the wall boundary layer, and lead to a dramatic increase in the fuel/air mixing. The detailed investigation reveals enhanced fuel-air mixing primarily results from elevated vorticity over combustor and cavity, as well as from increased residence time.

Effort is then expended to study the ignition and subsequent reacting flow in the modeled combustor. The ignition transient and flame development are comprehensively studied to investigate the influence of air throttling implementation on ignition and flameholding. The time history of combustion indicates that the engine model can hardly offer the ignition under the given flight condition in the absence of air throttling, as the ignition of ethylene fuel flow on the cowl surface fails to be initiated. Calculation is then employed to demonstrate the significant flow accommodation induced by air throttling implementation, including subsequent decrease in flow velocity and increases in temperature and pressure in the combustor. Autoignition occurs on the cowl surface due to extended residence time and higher initiate temperature, and results in an intense combustion zone with rapid flame spreading in combustor. Results indicate that the pre-combustion shock train is generated as a result of the combustion-induced pressure rise begins just upstream of the combustor entrance. The pre-combustion shock train at this condition forms a large region of low-momentum/separated flow near the combustor sidewalls. This proved to be an additional source for flameholding with the recessed
cavity as primary flameholding support. The predicted combustor performance and flow
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NOMENCLATURE

\( A, B, C \) \hspace{1cm} \text{Jacobian matrices of convective flux}

\( C_p, C_v \) \hspace{1cm} \text{Specific heat, } J\cdot K^{-1}\cdot kg^{-1}

\( C_R, C_I \) \hspace{1cm} \text{Empirical constants}

\( c \) \hspace{1cm} \text{Speed of sound, } m/s

\( E \) \hspace{1cm} \text{Specific total energy, } J\cdot kg^{-1}

\( \mathbf{E}, \mathbf{F}, \mathbf{G} \) \hspace{1cm} \text{Convective flux vector}

\( \mathbf{E}_*, \mathbf{F}_*, \mathbf{G}_* \) \hspace{1cm} \text{Diffusion flux vector}

\( S \) \hspace{1cm} \text{Source terms for the } k \text{- and } \omega \text{-equations}

\( h_{f,i}^0 \) \hspace{1cm} \text{Heat of formation of species } i \text{ at reference condition}

\( k \) \hspace{1cm} \text{Turbulent kinetic energy}

\( N \) \hspace{1cm} \text{Total number of species}

\( p \) \hspace{1cm} \text{Pressure}

\( P_r \) \hspace{1cm} \text{Prandtl number}

\( q \) \hspace{1cm} \text{Rate of heat release per unit volume}

\( R \) \hspace{1cm} \text{Gas constant}

\( S_y \) \hspace{1cm} \text{Strain-rate tensor}

\( \tau \) \hspace{1cm} \text{Viscous stress}

\( u_i \) \hspace{1cm} \text{Velocity, } m/s

\( u_* \) \hspace{1cm} \text{Friction velocity, } m/s

\( W_i \) \hspace{1cm} \text{Molecular weight of species } i

\( Y_i \) \hspace{1cm} \text{Mass fraction of species } I

\( H \) \hspace{1cm} \text{Isolator height}

\( W \) \hspace{1cm} \text{Width of combustor}

\( Y \) \hspace{1cm} \text{Mass fraction}

\( y^* \) \hspace{1cm} \text{Normalized distance from wall}
**Greek symbols**

- $\phi$: Equivalence ratio
- $\mu$: Dynamic viscosity, $kg/ms$
- $\tau_{ij}$: Viscous shear stress, $N/m^2$
- $\rho$: Density, $kg/m^3$
- $\eta$: Kolmogorov length scale, $m$
- $\eta_m$: Fuel-air mixing efficiency
- $\varepsilon_w$: Fuel-air mixing effectiveness
- $k$: Turbulent kinetic energy
- $\omega$: Specific turbulence dissipation rate
- $\gamma$: Ratio of specific heats
- $\omega$: Specific turbulence dissipation rate

**Subscripts**

- $i$: Property of species $i$
- $k$: Property for the $k$-equation
- $\omega$: Property for the $\omega$-equation
- $F$: Property of fuel
- $T$: Turbulent property
- $c$: Property of cavity
- $\xi, \eta, \zeta$: Each direction in body fitted coordinate system
- $\text{air}$: Property for mean air flow
- $\text{throttle}$: Property for air throttle activated
- $ST$: Stoichiometric proportion of the fuel-air composition

**Superscripts**

- $\bar{\cdot}$: Ensemble averaging
- $\sim$: Favre averaging
- $\cdot$: Mass flow rate
- $'$: Fluctuation
Complex variable
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Chapter 1

Introduction

1.1 Background and Motivation

1.1.1 History of Scramjet Engine Development

Supersonic combustion air-breathing engines have long been recognized as the well-suited for hypersonic propulsion in the flight Mach number 5 to 25 ranges. Designs for hypersonic engines have been developed since the early 1900’s. The first theoretical studies and patents of the ramjet principle were obtained in the 1920’s. In 1938, R. Leduc presented an aircraft with an integrated ramjet engine designed for subsonic flight in Paris. During the World War II, German developed supersonic air-intakes and realized some practical devices, including gun-lunched supersonic ramjets and ramjets for solid fuels and even ramjets for driving helicopter rotors. After the World War II, tremendous efforts had been put into study on high-speed jet-powered aircraft.

In recent years, significant progress has been made in the development of hypersonic technology, particularly in the field of scramjet engines. NASA believes hypersonic technology could help develop economical and reusable launch vehicles. The US Air Force is interested in a wide range of hypersonic systems, from air-launched cruise missiles to orbital space planes. The first well-known demonstration of a scramjet operating in an atmospheric test was the Australian HyShot project at the University of
Queensland that demonstrated scramjet combustion in 2002, as shown in Fig. 1-1. In the HyShot project the scramjet engine was accelerated to the necessary flight speed by means of a two-stage Orion-Terrier Mk70 rocket to achieve an altitude of 330 km along a parabolic trajectory. The craft dropped to a speed of Mach number 7.6 at the altitude between 35 km and 23 km as it re-entered the atmosphere. Meanwhile the scramjet engine started, and it flew at a Mach number of 7.6 for about 6 s. During the middle 1990s NASA worked with the Russian Central Institute of Aviation Motors (CIAM) to test a dual-mode scramjet engine. Four tests took place at flight speed of Mach 5.5, 5.3, 5.8 and 6.5, respectively. However it was not clear whether the combustion took place in the engine regarding to the test data.

Fig. 1-1: Hyshot first launch on 10/31/2001. Photo taken from [www.mech.uq.edu.au/ hyper/hyshot/](http://www.mech.uq.edu.au/hyper/hyshot/)
The most advanced hypersonic program in US is the NASA Hyper-X program, which involves flight tests through the X-43 vehicles. The X-43A is a scramjet-powered research vehicle with a length of 3.6 m. Three X-43A aircraft were developed for NASA, boosted by Pegasus rockets (Fig. 1-2). The rocket is dropped by a B-52 aircraft and launched to an altitude of about 33 km, where the X-43A aircraft is released and flown under its own power. The three vehicles have slightly different designs of air intake, as required by their test flight speeds. The first successful flight was undertaken on March 27, 2004, following the first attempt failed on June 2, 2001. This second flight made a new speed record over Mach 7, with the engine running for 11 s, whereas the third flight approached Mach number 9 on November 16, 2004.

![Fig. 1-2: A concept picture of NASA’s X-43. Photo taken from www.alliedaerospace.com](www.alliedaerospace.com)

Hypersonic development efforts are also in progress in other countries. Although the Australia is the first to demonstrate scramjet operating in an atmospheric test, successful scramjet flights have also been performed in USA and Russia. In addition, France, Japan and India have hypersonic programs in developing scramjet test vehicles. The France is considering their own scramjet test vehicle and is in discussions with the
Russians for boosters that would carry it to launch speeds. The approach is very similar to that used in the US NASA X-43A craft tests. The Japanese scramjet effort is motivated to build the world’s first true space plane – a civilian spaceliner. The research has been mainly conducted by Kakuda Propulsion Research Laboratory in Japan, but also involved researchers from the University of Queensland. The spacecraft is designed to collect oxygen from the atmosphere and mix the oxygen with fuel (liquid hydrogen), and burn the mixture in a combustor to generate thrust. The spacecraft may travel at hypersonic flight speed, but the inlet air flow has to be decelerated to subsonic to sustain combustion. Since a spacecraft would have to go for enough hypersonic that the air could no longer be decelerated sufficiently, the ramjet mode would become unpractical as the flight speed is beyond the Mach 6, thus the engine would have to operate as a scramjet.

1.1.2 Schematic and Significance of Scramjet Engine

The successful development of scramjet vehicles would depend on the development of an efficient propulsion system to a large extent, as shown in Fig. 1-3. Turbojets, as the most commonly used propulsion systems for subsonic and moderately supersonic flight, is only operated under flight Mach number 3 due to the high temperature and pressure in the airflow before the compressor. For rocket engines, they are criticized for their relatively low fuel economy and low safety. In the typical supersonic regime (Mach number 3 ~ 5) a ramjet looks attractive for the propulsion systems for flight. Beyond that into the hypersonic regime (Mach number 5 ~ 25) a
ramjet with supersonic combustion so called scramjet is used. When a ramjet flies at a supersonic speed, the internal airflow has to be slowed down to subsonic, to reach the high enough temperatures and pressures for the stable combustion. At a higher flight speed (Mach = 6 ~ 7), the deceleration of the internal airflow would cause a dramatic increase of the total pressure losses, and the static temperature could reach material limit at very high flight speed. Therefore the internal airflow has to be slow down to a typical level of the supersonic speed regime, as a scramjet would be resulted. If the internal airflow is too fast, the injected fuel only has a very short residence time (about 1 ms) in the combustion chamber, which would be difficult for the fuel mixing with the air and thus the completion of the reactions during this short period of time.

The fundamental differences between the ramjet and scramjet are highlighted in Fig. 1-4. The normal or strong shock system required in the operation of a ramjet with subsonic combustion located downstream of the inlet throat in stabilized by backpressure generated by choking the flow in the throat of the exhaust nozzle. The maximized ramjet

Fig. 1-3: Approximate performance levels of various classes of engines

The fundamental differences between the ramjet and scramjet are highlighted in Fig. 1-4. The normal or strong shock system required in the operation of a ramjet with subsonic combustion located downstream of the inlet throat in stabilized by backpressure generated by choking the flow in the throat of the exhaust nozzle. The maximized ramjet
performance, the Mach number at the beginning of the shock system must be at the range of mach 1.4 to 1.8 to minimize total pressure loss across the normal shock wave. This requires a relatively large inlet contraction ratio, and boundary layer bleed may also be needed to prevent inlet unstart and to stabilize the shock system. The net result is a larger inlet total pressure loss compared to that generated by the scramjet cycle, which avoids the normal shock and operates at a lower inlet contraction ratio. The major advantage of the ramjet cycle is comparatively small Rayleigh losses associated with the combustion process, whereas the scramjet incurs higher Rayleigh losses associated with combustion at supersonic speeds. This tradeoff between inlet pressure recovery and combustion pressure losses determines the relative fuel specific impulse of the ramjet and scramjet propulsion cycles. However, the internal static pressure is another discriminator that is directly related to installed engine weight. The ramjet duct pressure within the subsonic diffuser increases rapidly as a function of the Mach number, and additionally, accelerator vehicles tend to optimize at high flight-dynamic pressures typically on the order of 2000 psf or more, to dictate high values for the internal static pressure. Rather than degrading ramjet performance through reduced pressure recovery, a change in the mode of engine operation to the scramjet cycle would effectively reduce engine internal static pressure by maintaining supersonic flow throughout the engine. A dual mode engine, operating as a ramjet at low mach numbers and transitioning to a scramjet cycle as flight speed increases, would satisfy these general criteria. The unique combination of heat addition in a diverging area combustor and the absence of a nozzle throat permit fixed-geometry scramjet to operate effectively over a wider flight Mach number range than a conventional ramjet. At low flight Mach numbers (Mach 3–5) and high fuel-air
equivalence ratio, it operates as a subsonic combustion ramjet, that is, the combustion begins in a subsonic flow generated by the pre-combustion shock system, but accelerates through a thermal throat before exiting the combustor. At higher flight speeds or lower fuel–air equivalence ratio, the strength of the pre-combustion shock system decreases, and combustion takes place at entirely supersonic speeds. This is commonly referred to as dual-mode combustion and allows efficient operation from Mach 3 to Mach 8 with storable liquid fuels and theoretically up to orbital speeds (Mach 26) with gaseous diatomic fuels such as hydrogen (a more practical upper bound may be near Mach 20).

Fig. 1-4: Schematic of ramjet and scramjet. Photo taken from www.aviation-history.com

Fig. 1-5 presents the schematic of a scramjet engine. The hypersonic incoming air is diffused to a lower supersonic speed at the entrance of the combustor. Fuel is then injected to mix and burn with the air in a generally diverging area combustor. A shock train is usually generated upstream of the combustor by means of heat addition in the combustor. The strength of the shock wave series depends on the inlet exit Mach number, overall fuel-air equivalence ratio, and supersonic combustor area ratio, etc.
Since scramjet combustion experiments usually are extremely complicated, only a few operation facilities are available currently. Therefore, more and more computer simulations are used for their cost efficiency to investigate the propulsion system performance at the hypersonic flight regime. In the past twenty years, Computational Fluid Dynamics (CFD) has gradually played an extensive role in aerospace science development. CFD can approach the analysis of flow conditions which can not be readily obtained, in addition, it can largely reduce the time and cost of the design cycle.

1.2 Technique Challenges for Scramjet

The typical scramjet engine includes an inlet that compresses the free-stream air from a hypersonic Mach number to nearly one-third of the value, a combustor to allow fuel-air mixing and chemical reaction, and an exhaust nozzle that expands the hot combustion products to free stream pressure. The most commonly-used fuel is gaseous
hydrogen or hydrocarbon, and the mixing process of fuel and air, as well as the resultant combustion, would involve turbulent flow due to the typical scramjet length scales (1~2 m). The major drawback of a traditional ramjet is the dissociation caused by the high flow temperature, which usually increases along the deceleration of the inlet flow. To overcome these effects, attention has been focused on the combustion sustaining at supersonic speeds in a scramjet, where the inlet acts as a compressor. As the air passes through a system of shock waves produced by the inlet, the air velocity is reduced slightly to a lower supersonic speed, while the static pressure increases dramatically. Fuel injectors can be mounted on the surface of the combustor or on struts, to achieve higher penetration to the centerline of the combustor. The fuel-air mixture is then ignited and burned in this supersonic flow environment. After passing through the combustor, the hot gases flow downstream and are accelerated through exhaust nozzle out of the engine. The thrust of a scramjet is produced by the pressure and momentum difference of the air flow between the inlet and exhaust regions. Variations and improvements have been implemented in past years to enhance this general scramjet cycle.

1.2.1 Obstacles in Scramjet Combustion

Although the concept of scramjet appears to be simple, supersonic combustion is extremely complex. The chemical kinetics, flow temperature, pressure, velocity, equivalence ratio, and fuel-air mixing rate could have critical influences on the combustion process, thus the supersonic combustion is usually difficult to initiate and maintain. The ignition delay time of a fuel-air mixture is also the limiting factor for all
scramjet engine designs. Reducing the ignition delay time could mean a shorter combustor and higher flight speed. The ignition delay time of a fuel is basically determined by flow properties and the type of fuel. Increasing the temperature of the fuel or air stream may reduce the ignition delay time, however flow pressure plays a more complex role. Increasing the pressure may improve the combustion conditions, as the ignition delay time is usually reduced by increasing pressure. But for a critical condition of pressure, the ignition delay time increases substantially. Therefore it is not always advantageous to increase the pressure. The equivalence ratio may not strongly affect the ignition delay time, but as equivalence ratios drop to below 0.3, the ignition delay time might increase dramatically. Therefore, these effects need to be considered by the scramjet designers. The major problem associated with combustion is the mixing of the fuel and air. Fuel ignition would be difficult to be initiated without properly injecting and mixing with air, regardless of the pressure, temperature and equivalence ratio. One of the challenges in the fuel injection in a scramjet is that the airflow speed and pressure could be so high that fuel injection flow has a tendency to be pushed against the wall and rendered ineffective. Another concern is that very high temperatures may cause the reactants dissociated before combustion occurs, resulting in lower levels of heat release. In addition to the problems above, the ignition and combustion at these high velocities can be extremely difficult. To overcome these challenges, several solutions have been proposed, and hereafter we will briefly review some of them.
1.2.2 Proposed Solutions to Supersonic Combustion Difficulties

Improved schemes for injection patterns have been designed and studied to overcome the obstacles of inadequate fuel penetration and mixing. In addition, the problem of ignition and flameholding can be handled in several ways: injecting combustion enhancing radical by use of a plasma torch can reduce the induction time of the mixture; recirculation zones can be created using aerodynamic bodies such as cavities, ramps or wedges to slow down the flow and provide an environment where combustion can occur; or imposing air throttle at exhaust part of the combustor can modulate the flow field in the scramjet engine.

1.2.2.1 Fuel Injection and Mixing

Although physical bodies such as ramps and cavities have proven to be effective mixing devices, the method of fuel injection itself should also be considered carefully. For fuel injection, the simplest traditional transverse injection provides good penetration and mixing. However, transverse injection produces large separation regions both upstream and downstream of the injection orifice, translating into significant pressure losses. This deficiency can be quite significant at supersonic speeds. Therefore at high flight velocities, parallel or angled injections are presented in the injector ramps, to achieve optimum effect between the pressure loss and mixing augmentation process, and resulting in as increasing of combustion efficiency. Further designs of aero-ramps (Fig. 1-6), short for “aerodynamic ramps”, consist of an array of flush-walled fuel injectors arranged in such a way as to produce fuel-vortex interactions beneficial for
mixing, similar to those produced by a physical ramp. In essence, the fuel injected by the aero-ramp creates a zone, which appears to function as a physical ramp to the supersonic crossflow, but with fewer total pressure losses, as there is no actual physical obstruction. The injected fuel causes the crossflow to rise and spill over the sides of the interface formed by the fuel and crossflow. This in turn causes vortical motions useful for mixing, similar to those produced by physical ramps, but with no physical obstruction, as the jets are flush-wall.

![Image of aero-ramp injector in Mach 2.4 flow](Anderson and Schetz, 2005)

Fig. 1-6: Liquid aero-ramp injector in Mach 2.4 flow (Anderson and Schetz, 2005)

### 1.2.2.2 Recessed Cavity Flameholder

Because of the inherent difficulties associated with hydrocarbon combustion in a high speed flow (slow overall kinetic rates and very short combustor residence time), there is a need developing of more robust flameholding schemes for the use in these combustors. Cavity flameholders, an integrated fuel injection flame-holding approach, have been proposed as a new concept for flameholding and stabilization in supersonic...
combustors. The purpose of a recessed cavity is to sustain a pool of hot combustion products where flame can be anchored. In addition, the cavity usually induces self-excited resonance within the free shear layer over itself by means of acoustic excitation, producing flow oscillations and enhancing the mixing of fuel and air and mass exchange to the cavity. Either the ability of the cavity flameholding, or enhancement of mixing of fuel and air or both is a function of the depth and length of the cavity. In recent years, experiments have showed that the use of a cavity after the ramp injector significantly improves the hydrocarbon combustion efficiency in a supersonic flow. Fuel can be introduced into the cavity either by entrainment from the freestream or by direct injection. The cavity offers a relatively long residence time for mixing and chemical reactions to take place, and furthermore, the total temperature of the fuel-air mixture within the cavity is close to the total temperature of the freestream. Thus, sustained combustion is likely to exist within the flameholder under supersonic operating conditions.

1.2.2.3 Ignition Enhancement by Means of Throttling

Another important task of a scramjet using the cavity-based flameholder is to sustain stable combustion anchored on the cavity by achieving a pre-combustion shock train in the isolator sections, which forms by the pressure rise due to the heat-release in combustor. But generally, there is no sufficient backpressure rise imposed in the engine before the combustion is established in the chamber. Moreover, the supersonic air occupying the combustor decreases the residence time of the flow, which may aggravate the ignition of scramjet fuel and consequently cause the flame blow off. Thus, the major
concern regarding stable ignition is how a subsonic combustion environment should be established. One of the approaches is imposing throttling air at the exhaust part of the combustor to modulate the flow field in an engine. As backpressure increases in the test rig due to throttling at the exhaust part of the combustor, the shock train forms and propagates upstream as backpressure increases, reducing flow velocity and increasing pressure and temperature in the combustor. Furthermore, the boundary layer separates from side walls due to a reversed pressure gradient, leading to large recirculation regions in the corner between side walls and bottom surface in the combustor, and the pre-combustion shock and boundary-layer interaction enhances flow distortion and turbulent diffusion in the combustor, and thus promote fuel-air mixing.

1.3 Literature Review

The history of scramjets began in the early 1950s. The initial theoretical and experimental feasibility studies on combustion in a supersonic flow were not carried out until 1952 by Pinkel, Serafini and Gregg on a flat plate. They were followed by several theoretical studies on the utility of external burning on supersonic airfoils to reduce drag and/or produce thrust and an experimental demonstration of net positive thrust on a double wedge by Dugger and Billig (1959). Interests in scramjet engines as we know today have not been developed since late 1950s and early 1960s. Plethora of theoretical studies in the United States, Canada, Great Britain, France, Germany, and Russia were conducted during this period, demonstrating the potential for scramjet engines at flight speeds above Mach 5.
A large development of supersonic combustion engines in the United States was gained in 1960s. The research engines were designed to test various aspects of ducted scramjet engine design. Ground tests between Mach numbers 5 and 7 on a model scramjet engine incorporating a rearward facing step, produced the first demonstration of net positive thrust (Swithinbank, 1966 and Ferri, 1968). Subsequent developments provided insight that higher levels of thrust and efficiency could be produced by ducted scramjets. The Navy began supporting efforts for development of these ducted scramjets in the early 1960s, as known as the Supersonic Combustion Ramjet Missile (SCRAM) (Billig, 1965). The SCRAM program successfully demonstrated the feasibility of the ducted supersonic combustion engine, but was cancelled in late 1970s due to technical shortcomings. The Dual-Combustor Ramjet (DCR) succeeded the SCRAM project, and the concept developed throughout the 1970s into the 1980s (Waltrup et al. 1979, 1982 and 1987; Billig et al. 1979). The DCR contains all the features of a scramjet with the addition of a small subsonic combustor to act as a pilot flame and fuel cracker for the main engine (Fig. 1-7). The vision of hypersonic jet got a boost in the 1980s from President Ronald Reagan. In 1986, President Reagan even announced a major scramjet project, the National Aerospace Plane (Rockwell X-30), as he envisioned the scramjet replacing the space shuttle, military bombers and commercial aircraft. The program never got off the ground and was canceled in 1994 because of all of the barriers and problems the research had.
Since the scramjet engine concept was first introduced in the late 50s and early 60s in last century, various encouraging studies and investigations of supersonic combustion phenomena have created the impression that the scramjet engine could be developed using the structured and controlled approach appropriate to subsonic combustors, such as fuel injection, mixing, ignition, stabilization by pilot zones, flame propagation, etc. However, in the scramjet, the presence of various problems including supersonic flows with corresponding shock fields, coupled combustion/shock generation, and shock/boundary-layer interactions demonstrated that scramjet combustor development is extremely complex. Among them, ignition and flame holding are two important problems that have to be addressed in the design of a scramjet system.

1.3.1 Scramjet Ignition and Flameholding

Sung (1999) investigated the ignition mechanism in a supersonic Hydrogen-air combustor. Once ignition is established, the efficiency of combustion depends directly on the efficiency of the fuel/air mixing. For ignition to be accomplished in a flowing combustible mixture, it is necessary that four quantities have suitable values: static
temperature, static pressure, fuel/air mixture, and fuel residence time. The ignition is considered accomplished when sufficient free radicals are formed to initiate the reaction system, even though no appreciable heat has yet been released. The primary objective of a flame holder in supersonic combustion, therefore, is to reduce the ignition delay time and to provide a continuous source of radicals for the chemical reaction to be established in the shortest distance possible.

Ramps and wedges have also long been used as bluff body flameholders. The shock waves produced by their edges, and the rapid change of duct area just past the bluff body enhance mixing. Typically, a fuel injector is located just downstream of the bluff body to take full advantage of the turbulence produced. Shock-induced combustion behind a wedge and ramp has been studied extensively. Shock waves are unavoidable in a scramjet combustor, and can change the temperature, velocity and flame characteristics, affecting the combustion process. Fujimori et al. (1997) found that the recirculation behind a wedge in a supersonic air-stream was very sensitive to the fuel flow rate. With low fuel flow rates, most of the reaction occurred within the recirculation zone, but with higher flow rates, the reaction zone moved away from the wedge and extinguished. Sands et al. proved analytically and experimentally that flameholding was possible with a rectangular ramp. Although they have been proven adequate flame-holders, bluff bodies also incur large flow losses due to low back-pressure as their cross-sectional area increases.

Plasma torches or plasma igniters have a wide range of applications in industry. However, plasma torches of interest to scramjet engines are those that are used for ignition and flame holding, and have been used by Sato et al. at flow Mach number 6.
Regardless of the design, the purpose of a plasma torch is to ionize and dissociate the feedstock gas in hot, reactive plasma. Typically, the power range of these devices is limited to a few kilowatts to consume only the smallest possible fraction of the total engine power. The feedstock is generally hydrogen, nitrogen or a mixture of these combined with argon. As the feedstock gas passes through an electric arc, it is ionized and in the case of more complex gases, it is also dissociated. This process produces combustion-enhancing radicals that reduce the reaction time for the combustion processes. This plasma is then injected into the fuel/air mixture stream where the combustion takes place.

1.3.2 Fuel Injection in Scramjet

Advanced fuel injector designs hold promise for solving mixing concerns. Numerous geometries have been tested to improve the mixing characteristics of fuel injection orifices. These include swept ramps, multiple aero-ramp injectors, inclined injection and circular and non-circular geometries.

Achasov et al. (1997) discovered that a jet recessed into a small cavity with incident jets focusing on the center of the cavity could produce a region of high energy density, which consequentially could lead to the onset of detonation. These jets enhanced the pressure and temperature within the volume of the cavity and produced a region of fast turbulent mixing.

The shape of the injection orifice is also important. Two recent improvements on the conventional circular orifice are the elliptical by Gruber et al. (1995) and diamond-
shaped orifices by Tomioka et al. (2000). Gruber et al. reported that elliptical jets could enhance the mixing rate of fuel into a supersonic air stream. Elliptical jets tested in a Mach number 2 cross flow demonstrated increased spinwise spreading of the shear layer and greater turbulence intensity when compared to a circular jet. Shadowgraphs revealed that structures of the elliptical jet produce a smaller separation region upstream of the jet and also produced a weaker bow shock. However, the elliptical jet also had reduced lateral penetration compared to the circular jet. Similarly, diamond-shaped injectors experienced greater spinwise spreading due to the production of streamwise vortices and greater penetration. In addition to the mixing benefits associated with the diamond shaped injector, Tomioka and his associates also noticed that the Mach disk was located closer to the injector orifice, reducing the total pressure losses through the disk.

Building upon the advances made with single-holed injectors, the next natural step would be to assume that injector jets could be arranged in such a way as to produce a synergistic effect between the jets, resulting in improved mixing over a single jet of the same effective diameter. Hollo et al. (1994) demonstrated that significant improvements in the initial mixing rate could be achieved over that of a single-hole injector, by using an array of jets. Cox (1994) supported these conclusions, and demonstrated that an injector array could be designed to generate vortical motions, similar to those produced by a physical ramp. This gave birth to the “aero-ramp,” a concept generally credited to Schetz et al. (1998). The design implementing the use of jet interaction, in which an aerodynamic ramp, rather than a physical one, is produced by means of nine differently-angled fuel orifices. These orifices were arranged to produce fuel-vortex interactions to enhance mixing in a supersonic cross flow. Experiments conducted with this aero-ramp
injectors showed that with increased jet momentum, penetration increased, while a comparable physical ramp showed no significant improvement. Also noteworthy was that the total pressure losses induced by the aero-ramp were less than those of the physical ramp.

Another method of fuel injection is to position the injectors on a strut. Huber et al. (1979) reported that autoignition of hydrogen occurred easier when injected from a strut than from a wall because of the smaller boundary layer and higher surface temperature of the strut. Masuya et al. (1995) later confirmed these findings, testing different strut designs in a Mach number 2.5 air stream. In some cases, struts are superior to other aerodynamic shapes, such as wedges and cavities, because they do not significantly disturb the flow and have fewer losses associated with them.

1.3.3 Recessed Cavity Flameholder

Another promising method of mixing and flameholding is recessed cavities. Ben-Yakar et al. (2001) investigated the flame holding capability of a transverse hydrogen injection of fuel from a wall orifice. As the fuel jet interacts with the supersonic cross flow, a bow shock is produced (Fig. 1-8). As a result, the upstream wall boundary layer separates, providing a region where the boundary layer and jet fluids mix subsonically upstream of the jet exit. This region is important in transverse injection flow field because of its flame-holding capability in combustion situations. However, this injection configuration has stagnation pressure losses due to the strong bow shock formed by the normal jet penetration, particularly at high flight velocities. Parker (1995) reported the
experimental investigations to achieve flame stabilization by means of a step followed by transverse injection. The step creates a larger recirculation area with the hot gases serving as a continuous ignition source. This approach can provide sustained combustion but, like the previously described method, has the disadvantage of stagnation pressure losses and increase in drag due to the low flow pressure base behind the step. Raggens (1995) studied the performance of angled injection to reduce the pressure losses associated with the injection process, so that the resulting bow shock is weaker. Additionally, jet axial momentum can also contribute to the net engine thrust.

Fig. 1-8: Transverse hydrogen injection of fuel from a wall orifice.

Different experimental and numerical investigations of cavity flame holders, an integrated fuel injection/flame-holding approach, have been reported (Vinagradov et al., 1995; Ortweth, et al., 1996; Owens, et al., 1998). They showed that the use of a cavity after the ramp injector significantly improved the hydrocarbon combustion efficiency in a supersonic flow. Their observations indicate the two main directions in which cavities have been considered as a tool for performance improvement in a supersonic combustor: 1) cavity-actuated mixing enhancement and 2) trapping a vortex within the cavity for flame-holding and stabilization of supersonic combustion.

Yu and Schadow (1994) reported using cavities to enhance the mixing of supersonic non-reacting and reacting jet, where the cavity was attached at the exit of the
jet circular nozzle. Sato (1997) also studied the effect of an acoustic wave, emitted from a cavity and impinging on the initial mixing layer. Their results revealed that the mixing was enhanced by the acoustic disturbance and the rate of the enhancement was controlled by the cavity shape while the total pressure losses were negligibly small.

Whereas an unstable cavity can provide enhancement in the turbulent mixing and combustion as discussed above, a stable cavity can be used for flame-holding applications. The main idea to stabilize and enhance supersonic combustion by the use of wall cavities is to create a recirculation region inside the cavity with a hot pool of radicals, which will reduce the induction time, and the cavity recirculation region has to be stable to provide a continuous ignition source for a stable combustion. Numerical studies (McClinto, 1996) of the integrated injection/cavity flame-holder approach showed that autoignition and flame holding within the cavity could be obtained at Mach number 6.5 flight, even without the spark ignition plugs. Owens et al. (1998) investigated the flame stability of kerosene injected upstream of a cavity flame holder with Mach 1.8 freestream conditions. Because of the low stagnation temperatures, ignition was provided by pilot hydrogen fuel injected into the cavity. Flame holding could be achieved only when large flow rates of hydrogen were used. They reported the enlargement of the recirculation region led to entrainment of additional quantities of fresh air contributing to the flame stability. Other experimental and numerical studies concentrated on characterization of cavity flameholders in gaseous supersonic combustors. Initial experimental efforts were performed by Yu et al. (1998, 1999). They analyzed flow stability and flame-holding characteristics of several wall cavities with various sizes and aspect ratios in a Mach number 2 air stream. Normalized flame intensity images suggested that short cavities
provided steady flame-holding. Longer cavity results in more compact, but intense flame structures. Finally, cavities with inclined downstream walls had poor flame holding capabilities. In general, cavities with small aspect ratios and vertical downstream walls appeared to be good flame-holders. Additional experiments conducted by Niioka et al. (1995) in Mach number 1.5 airflow showed that flame stability could be controlled by the cavity length, which controls the competition between the mass transfer rate and the chemical reaction rate. Wright–Patterson Air Force Research Laboratories (Mathur et al., 2001) have also investigated the effectiveness of cavities with upstream ethylene fuel injection in supersonic flows simulating flight Mach numbers between 4 and 6 (Fig. 1-9). Their reports indicated that the cavity geometry had an effect on mass entrainment rate and residence times. Further experimental studies of cavity-based flame-holder on a supersonic combustor, have been reported by Gruber et al. (2001), showing the residence time of the flow inside a cavity is a direct function of the mass exchange rate in and out of the cavity. Their observation indicated that in the open cavities, mass and momentum transfer mechanisms are controlled by the longitudinal oscillations and the vortex structure inside the cavity. The computational visualizations demonstrated the existence of one large vortex stationed near the trailing edge of the cavity and a secondary vortex near the upstream wall. The mass exchange of the cavity is controlled by the large trailing vortex, which interacts with the unstable shear layer.
1.3.4 Pre-combustion Shock Train in Scramjet

Another important task of a scramjet using the cavity-based flameholder is to sustain stable combustion anchored on the cavity by achieving pre-combustion shock train in the isolator sections, which forms by the pressure rise due to the heat-release in combustor. However, the supersonic air occupying the combustor decreases the residence time of the flow, which may aggravate the ignition of scramjet fuel and consequently cause the flame blown off. Moreover, for hydrocarbon fuels being the candidate fuels for supersonic flight below Mach 8, the cavity flameholder is required to achieve longer flow residence times inside the cavity because of the reduced total enthalpies and longer ignition delay times associated with fuel. Thus, one of the recent concerns regarding stable ignition is to impose sufficient backpressure rise in the engine chamber by imposing a throttle at exhaust part of the section to modulate the flow field in an engine. As backpressure increases in the test rig due to throttling at exhaust part of the combustor, the shock train forms and propagates upstream as backpressure increases, reducing flow velocity and increasing pressure and temperature in combustor.

Fig. 1-9: Cavity-based flame holder
The pressure profiles and length of pre-combustion shock trains have been studied by various researchers using constant-area ducts in cold flows. These studies can be briefly summarized in Tables 1-1.

Waltrup and Billig (1973) developed a correlation for the length of the shock train using axisymmetric ducts with downstream flow throttling to generate shock trains. Om and Childs (1985) performed an experiment of the shock train phenomena in a constant area circular duct. They reported that the subsonic flow, immediately behind the first shock, accelerates in the converging flow until the sonic state is reached, and then supersonic expansion takes place and terminated by the second shock, and the same process occurs to form the shock train. Carroll and Dutton (1990) also performed a detailed experiment on the characteristics of a multiple normal shock/boundary layer interaction for a rectangular duct flow at Mach 1.6. Their results indicated that the first
normal shock is bifurcated, and is followed by a series of symmetric weaker, nearly normal shock, and the spacing between the consecutive normal shocks increases respectively as confinement increases. Sullins and McLafferty (1992) also investigated the shock train behavior using a throttle valve to raise the back pressure. Based on the above fundamental studies, more quantitative investigations on Scramjet facilities flight test have been conducted thoroughly recently. Hsu et al. (2000) conducted an experiment to quantitatively investigate the fuel distribution around a cavity in a non-reacting Mach 2 flow. A mechanical throttle (Fig. 1-10) (i.e., butterfly valve) was mounted in the exhaust section of the combustor to increase the backpressure in the test section, simulating the pressure rise due to heat release in an actual combusting flow. Kanda and Tani also employed a mechanical throttle (i.e., throat) at the duct exit to induce a pseudo-shock in the ejector section (Fig. 1-11). The air-nitrogen flows were mixed through the pseudo-shock, decelerated, and choked at the throat by means of throttling. Lin et al. (2006) investigated the shock train structures inside constant-area isolators experimentally and numerically. A throttle valve was installed downstream of the isolator to create shock trains at various positions in the isolator by varying back pressures at the isolator exit.

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**Fig. 1-10:** Mechanical throttle in Scramjet engine facility
Some computational efforts have been conducted to the interaction physics in the simple internal flows with a constant area. These studies can be briefly summarized in Tables 1-2. Hataue (1989) computed the shock train phenomena in a constant area duct by using Harten-type second-order TVD scheme based on the two- and three-dimensional Navier Stokes equations and analyzed the mechanism of bifurcation of the first normal shock in the shock train and the transition process from the normal shock train to the oblique shock train. He also gained an insight into the effects of the upstream Mach number and the upstream boundary layer thickness on the shock/boundary layer interaction. Lin, Rao and O’Connor (1991) computed the compressible Reynolds-averaged Navier Stokes equations, employing the Baldwin-Lomax turbulence model for regions with no separation and a backflow turbulence model for regions with separation. Their computation contained the effects of boundary layer thickness and Mach number on the normal shock train, by placing the boundary layer profiles of various momentum thicknesses at the duct entrance and changing the incoming Mach number. Carroll, Lopez-Fernandez, and Dutton (1993) conducted numerical investigation for multiple shock wave/turbulent boundary layer interactions in the rectangular duct. The
computational results for Mach number 1.6, using MacCormack scheme, indicate the inadequacy of Baldwin-Lomax turbulence model for shock-induced boundary layer separation. Some improvement was made by applying the Wilcoxon-Rubesin two-equation turbulence model. However, numerical difficulty was still encountered for the case of higher Mach number flows. Also, Yamane et al. (1995) computed the Reynolds-averaged Navier Stokes equations with the Baldwin-Lomax turbulence mode and investigated the effects of upstream Mach number and upstream boundary layer on the structure of the shock train. However, great differences are still encountered in comparison with experimental results as will be shown in the next section. Although the computational results mentioned above provided much detailed information on the shock train phenomena, the data obtained by numerical calculations are not sufficient to fully grasp the flow physics with respect to the shock train phenomena. Further studies are needed to get better understanding on such complex flows.

<table>
<thead>
<tr>
<th>Reference</th>
<th>Fuel</th>
<th>Mach number</th>
<th>Stagnation pressure</th>
<th>Stagnation temperature</th>
<th>2D/3D</th>
<th>Turbulence model</th>
<th>Shock train</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hataue (1989)</td>
<td>N/A</td>
<td>1.5</td>
<td>0.4 atm</td>
<td>300 K</td>
<td>2D</td>
<td>Baldwin-Lomax</td>
<td>normal shock train</td>
</tr>
<tr>
<td>Lin, Rao and O’Connor (1991)</td>
<td>N/A</td>
<td>1.6</td>
<td>7.1 atm</td>
<td>283 K</td>
<td>2D</td>
<td>Baldwin-Lomax/Backflow</td>
<td>normal shock train</td>
</tr>
<tr>
<td>Yamane et al. (1995)</td>
<td>N/A</td>
<td>2.4</td>
<td>5.0 atm</td>
<td>900 K</td>
<td>2D</td>
<td>Baldwin-Lomax</td>
<td>normal shock train</td>
</tr>
</tbody>
</table>
Recent efforts have focused on enhancement effects on the ignition and flame stabilization in the Scramjet engine by installing throttling devices at the exit of the combustor section. A mechanism using a compressed air or variable duct flow area throttling attached to the exit of the combustor, was designed to throttle the flow gradually. These impressive studies are briefly summarized in Tables 1-3. Gruenig et al. (2000) conducted experimental investigations of the effects of a throttling wedge on the auto-ignition of the H\textsubscript{2} injected employing a set of the Transverse orifices and a pylon flameholder in the combustor. Mathur et al. (2000) conducted an experiment using air throttling to initiate combustion in a scramjet combustor. It was observed that once the air throttling was removed after the flame establishment, the shock train was retained leading to sustained combustion if sufficient heat release was produced in the combustor. Conversely, insufficient heat release may result in an unstable shock train and causes flame blowout. Donbar et al. (2001) later tested the operation sequence of ignition of ethylene in a supersonic reacting flow. Air throttling was engaged after stable fuel condition was reached. Once ignition occurred by activating spark igniters, the throttle was removed, after which sustained combustion proceeded. Gruber et al. (2001) conducted experimental investigations of ignition and flameholding in supersonic reacting flows, using an air throttle to supply modulated compressed air into the combustor to facilitate ignition (Fig. 1-12). Vinogradov et al. (2003) employed an air jet throttle device to initiate the scramjet combustor, throttling air to combustor duct flow aimed to increase local pressure and temperature in the ignition zone. It was observed that the fuel ignition, when the throttle air was supplied, did not guarantee combustion stabilization of the flame after the throttling was over. Goldfeld et al. (2004) also
explored the application of employing a plenum chamber to initiate the auto-ignition of
the hot kerosene injected from a set of the parallel orifices in the combustor. The latest
X43 flight test (2004) has successfully indicated the ignition and flameholding advantage
of the throttle in its flight operation.

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Fig. 1-12: Scramjet engine facility applied an air throttle to supply modulated compressed
compressed air into the combustor to facilitate ignition

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Tab. 1-3: Survey of experimental investigations of ignition and flame stabilization in
scramjet using throttle

<table>
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1.4 Research Objectives and Dissertation Outline

In spite of the encouraging results obtained so far to achieve reliable ignition using air throttling, quantitative understanding of the dynamic process from air throttling to flame establishment remains unavailable. In the present research, a comprehensive integrated three-dimensional numerical analysis has been established to investigate the detailed flow and flame dynamics, involved in the flame holding and spreading processes, in realistic engine environments in the Taitech/AFRL scramjet combustor operating under various conditions. The study of transient phenomena, such as the flow development, mixing of fuel and air, and ignition and flame dynamics at a given flight condition in scramjet engines, were investigated comprehensively in present work. The particular study on the responsibility of air throttling on combustor flow field, and the intricate interactions between the air throttling and mixing of fuel and air, as well as their ensuing influences on ignition transient and combustion dynamics in the chamber, were conducted and concluded thoroughly.

Hence, the purpose of the present work is to utilize contemporary numerical and analytical model techniques to conduct an analysis that allows for a complete treatment of the flow and flame dynamics, involved in the ignition of the fuel-air mixture, flame holding and spreading processes, in the Taitech/AFRL scramjet combustor operating under various conditions. Detailed analysis is employed to investigate the influence of air throttling on fuel-air mixing and ignition in a scramjet combustor, and to identify their underlying essential physics by means of air throttling implementation technique.
Chapter 2

Theoretical Formulation

2.1 Governing Equations

The theoretical formulation is based on the full conservation equations of mass, momentum, energy and species concentration in Cartesian coordinates:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \]  \hspace{1cm} (1)

\[ \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \]  \hspace{1cm} (2)

\[ \frac{\partial \rho E}{\partial t} + \frac{\partial \left[(\rho E + p)u_j\right]}{\partial x_j} = -\frac{\partial q_j}{\partial x_i} + \frac{\partial (u_i \tau_{ij})}{\partial x_j} \]  \hspace{1cm} (3)

\[ \frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho Y_k u_j}{\partial x_j} = \omega_k - \frac{\partial \rho Y_k U_{k,j}}{\partial x_j}, \quad k = 1, \ldots, N-1 \]  \hspace{1cm} (4)

where \( i, j, \) and \( k \) are the spatial coordinate index, the dummy index to spatial coordinate, and the species index, respectively. \( N \) is the total number of species. \( Y_k \) and \( U_{k,j} \) represent mass fraction and diffusion velocities of species \( k \), respectively. The viscous stress tensor \( \tau_{ij} \) for a Newtonian fluid (with Stokes assumption) and the heat flux vector \( q_j \) are defined as:

\[ \tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right) \]  \hspace{1cm} (5)

\[ q_j = -\lambda \frac{\partial T}{\partial x_j} + \rho \sum_{k=1}^{N} h_k Y_k U_{k,j} \]  \hspace{1cm} (6)
where $\mu$ and $\lambda$ are the coefficients of viscosity and heat conductivity, respectively. Within the thermodynamic regime of the present concern, viscosity coefficient $\mu$ and thermal conductivity $\lambda$ can be represented by polynomial functions of temperature. The specific total energy $E$ is given by:

$$E = e + \frac{u_i u_j}{2}$$  \hfill (7)

The governing equations are supplemented with the equation of state for an ideal gas. Then the specific internal energy, $e$, is obtained as:

$$e = h - \frac{p}{\rho}$$  \hfill (8)

The specific enthalpy of mixture, $h$, containing contributions from its constituent species, can be written as:

$$h = \sum_{k=1}^{N} Y_k h_k = \sum_{k=1}^{N} Y_k \left( \Delta h_{f,k} + \int_{T_{ref}}^{T} C_{p,k}(T') dT' \right)$$  \hfill (9)

The species specific heat at constant pressure, $C_{p,k}$, can be approximated by a polynomial function of temperature:

$$C_{p,k} = \sum_{p=1}^{M} a_{k,p} T^{p-1}$$  \hfill (10)

The formulation is closed by an equation of state for a perfect mixture:

$$p = \rho R_u T \sum_{k=1}^{N} \frac{Y_k}{W_k} = \rho RT$$  \hfill (11)

where $R_u$ is the universal gas constant and $W_k$ is the molecular weight of species $k$.

Variable transport and thermodynamic properties is fully taken into account in the present work. The viscosity and thermal conductivity for individual specie are
approximated by fourth-order polynomials of temperature. The coefficients of these polynomials for individual species are provided by McBride et al. (1993; 2002), where these coefficients are valid in the temperature range of 300 ~ 6000 K. The viscosity and thermal conductivity of the mixture are also obtained from Wilke’s method and Wassiljewa’s approach, respectively, as follows (Poling et al., 2000).

\[
\eta_{\text{mixture}} = \frac{\sum_{i=1}^{N} X_i \eta_i}{\sum_{i=1}^{N} X_i \phi_{ij}}
\]  

(12)

where \(X_i\) represents mole fraction of species \(i\) and the inter-collision parameter \(\phi_{ij}\) is given by,

\[
\phi_{ij} = \left[ 1 + \left( \frac{\eta_i}{\eta_j} \right)^{1/2} \left( \frac{W_i}{W_j} \right)^{1/4} \right] \left[ 8 \left( 1 + W_i / W_j \right) \right]^{1/2}
\]

(13)

The binary mass diffusivity \(D_{ij}\) between any two species \(i\) and \(j\) can be obtained through the Chapman-Enskog theory in conjunction with the Lennard-Jones intermolecular potential energy function (Poling et al., 2000),

\[
D_{ij} = 0.0018583 \left[ T^3 (1/W_i + 1/W_j) \right]^{1/2} \left[ 8 (1 + W_i / W_j) \right]^{1/2}
\]

(14)

The Lennard-Jones mixture length scale, \(\sigma_{ij}\), and the collision integral for diffusion, \(\Omega_{ij}\), are expressed as (Reid and Sherwood, 1966),

\[
\sigma_{ij} = \frac{1}{2} (\sigma_j + \sigma_i)
\]

(15)

\[
\Omega_{ij} = \frac{1}{T_D^{0.145}} + \frac{1}{(T_D + 0.5)^2}
\]

(16)
where $T_D$ is given by,

$$T_D = \frac{k}{\sqrt{\varepsilon_i \varepsilon_i}} \quad (17)$$

And $k$ is the Boltzmann constant. The constants $\sigma_i$ and $\varepsilon_i$ are defined by McBride et al. (1993; 2002). The effective diffusion coefficient $D_{im}$ in a multi-species mixture is related to the binary diffusion coefficient $D_{ij}$ through the following equation

$$D_{im} = (1 + X_i)/\sum_{i \neq j} X_i / D_{ij} \quad (18)$$

### 2.2 Favre-averaged Governing Equations

In his approach in 1894, Reynolds suggested that a fluctuating property $f$ can be split into an ensemble average and a fluctuation as following

$$f(x,t) = \bar{f}(x,t) + f'(x,t) \quad (19)$$

where the overbar denotes the ensemble average and $f'$ the fluctuation, respectively.

In variable density flows, the averaging procedure above is replaced by density weighted averaging, to avoid terms due to the density fluctuations. This method is introduced by Favre and given as

$$f(x,t) = \tilde{f}(x,t) + f''(x,t) \quad (20)$$

where

$$\tilde{f} = \frac{\rho f}{\bar{\rho}} \quad (21)$$
Applying the Favre-averaging concept to conservation equations above, the Favre averaged equations can then be written in a general vector form as

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial}{\partial x}(\mathbf{E} - \mathbf{E}_v) + \frac{\partial}{\partial y}(\mathbf{F} - \mathbf{F}_v) + \frac{\partial}{\partial z}(\mathbf{G} - \mathbf{G}_v) = \mathbf{H} \quad (22)$$

where the vector \( \mathbf{Q} \) contains dependent variables, and the convective flux vectors \( \mathbf{E} \), \( \mathbf{F} \), and \( \mathbf{G} \) in the \( x \), \( y \), and \( z \) directions, respectively, take the form

$$\mathbf{Q} = \begin{pmatrix} \bar{\rho} \\ \bar{\rho} \bar{u} \\ \bar{\rho} \bar{v} \\ \bar{\rho} \bar{w} \\ \bar{\rho} \bar{E} \\ \bar{\rho} \bar{Y}_i \end{pmatrix}, \quad \mathbf{E} = \begin{pmatrix} \bar{\rho} \bar{u} \\ \bar{\rho} \bar{u}^2 + \bar{p} \\ \bar{\rho} \bar{u} \bar{v} \\ \bar{\rho} \bar{u} \bar{w} \\ (\bar{\rho} \bar{E} + \bar{p}) \bar{u} \\ \bar{\rho} \bar{u} \bar{Y}_i \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \bar{\rho} \bar{v} \\ \bar{\rho} \bar{v}^2 + \bar{p} \\ \bar{\rho} \bar{v} \bar{u} \\ \bar{\rho} \bar{v} \bar{w} \\ (\bar{\rho} \bar{E} + \bar{p}) \bar{v} \\ \bar{\rho} \bar{v} \bar{Y}_i \end{pmatrix}, \quad \mathbf{G} = \begin{pmatrix} \bar{\rho} \bar{w} \\ \bar{\rho} \bar{w}^2 + \bar{p} \\ \bar{\rho} \bar{w} \bar{u} \\ \bar{\rho} \bar{w} \bar{v} \\ (\bar{\rho} \bar{E} + \bar{p}) \bar{w} \\ \bar{\rho} \bar{w} \bar{Y}_i \end{pmatrix} \quad (23)$$

The diffusive flux vectors \( \mathbf{E}_v \), \( \mathbf{F}_v \), and \( \mathbf{G}_v \) in the \( x \), \( y \), and \( z \) directions, and the source term \( \mathbf{H} \) respectively, are given as

$$\mathbf{E}_v = \begin{pmatrix} 0 \\ \tau_{xx} - \bar{\rho} \bar{u}' \bar{u}' \\ \tau_{xy} - \bar{\rho} \bar{u}' \bar{v}' \\ \tau_{xz} - \bar{\rho} \bar{u}' \bar{w}' \\ \bar{\rho} D_{lm} \frac{\partial \bar{Y}_i}{\partial x} - \bar{\rho} \bar{Y}_i \bar{u}' \\ \vdots \\ \bar{\rho} D_{N-l,m} \frac{\partial \bar{Y}_{N-1,i}}{\partial x} - \bar{\rho} \bar{Y}_{N-1,i} \bar{u}' \end{pmatrix}, \quad \mathbf{F}_v = \begin{pmatrix} 0 \\ \tau_{yx} - \bar{\rho} \bar{v}' \bar{u}' \\ \tau_{yy} - \bar{\rho} \bar{v}' \bar{v}' \\ \tau_{yz} - \bar{\rho} \bar{v}' \bar{w}' \\ \bar{\rho} D_{lm} \frac{\partial \bar{Y}_i}{\partial y} - \bar{\rho} \bar{Y}_i \bar{v}' \\ \vdots \\ \bar{\rho} D_{N-l,m} \frac{\partial \bar{Y}_{N-1,i}}{\partial y} - \bar{\rho} \bar{Y}_{N-1,i} \bar{v}' \end{pmatrix} \quad (24)$$
The additional terms appearing in these averaged equations are the Reynolds stresses arising from the fluctuating velocity field $\rho u'u''$ and the scalar fluxes of the species $\rho Y_i u''$ and energy $\rho E''w''$. These unclosed terms arise from the averaging procedure and lead to more unknowns than equations. Therefore turbulence model is required to give expressions for these Reynolds stresses and the scalar fluxes.

### 2.3 Turbulence Closure

Two equation models are the most wide-spread models used in averaged Navies-Stokes simulation. There are numerous concepts for two-equation models as the $k-\omega$ model and numerous variants of the $k-\varepsilon$ model. Among them, the Menter’s shear stress transport (SST) model (Menter, 1994) deserves particular attention, as it shows improved behavior for its treatment of the viscous near-wall region, and in processing the effects of streamwise pressure gradients in boundary-layer flow. Turbulence closure is achieved by means of SST model calibrated for high-speed compressible flows. The model
incorporates the standard $k$-$\varepsilon$ model that is suitable for shear-layer flows and the Wilcox $k$-$\omega$ model for wall turbulence effects. Derived from the $k$-$\varepsilon$ two-equation formulation, the SST model can be written in the following form

$$\frac{\partial \overline{\rho k}}{\partial t} + \frac{\partial \left( \overline{\rho u_j k} \right)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \mu_{k} \frac{\partial k}{\partial x_j} \right) + S_k$$  

(26)

$$\frac{\partial \overline{\rho \omega}}{\partial t} + \frac{\partial \left( \overline{\rho u_j \omega} \right)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \mu_{\omega} \frac{\partial \omega}{\partial x_j} \right) + S_\omega$$  

(27)

The viscosity terms are expressed as

$$\mu_k = \mu_i + \sigma_k \mu_i$$  

(28)

$$\mu_\omega = \mu_i + \sigma_\omega \mu_i$$  

(29)

and the source terms are

$$S_k = \tau_{ij} \frac{\partial \overline{u_i}}{\partial x_j} - \beta^* \overline{\rho \omega k}$$  

(30)

$$S_\omega = \frac{\nu}{\nu_t} \tau_{ij} \frac{\partial \overline{u_i}}{\partial x_j} - \beta^* \overline{\rho \omega} + 2(1-F_i)\sigma_\omega \overline{\rho \omega k} \frac{\partial \overline{\rho \omega k}}{\partial x_j}$$  

(31)

The model constants are obtained through the following blending relation:

$$\phi = F_i \phi_1 + (1-F_i) \phi_2$$  

(32)

where $\phi_1$, $\phi_2$, and $\phi$, respectively, represent any constant in the $k$-$\omega$ model ($\sigma_1$,···), the $k$-$\varepsilon$ model ($\sigma_2$,···), and the SST model ($\sigma_3$,···). The blending function, $F_i$, that controls the switch between the $k$-$\omega$ and $k$-$\varepsilon$ models takes the form

$$F_i = \tanh(\text{arg}_i^1)$$  

(33)

The argument is defined as
where $y$ is the distance to the wall and $CD_{k\omega}$ the positive portion of the cross-diffusion terms expressed as

$$CD_{k\omega} = \max \left( 2 \rho \sigma_{u\omega} \frac{\partial \tilde{\omega}}{\partial x_i} \frac{\partial \tilde{\omega}}{\partial x_j}, 10^{-20} \right)$$

(35)

The constants in the Wilcox $k-\omega$ model are

$$\sigma_{u1} = 0.85$$
$$\sigma_{u\omega} = 0.5$$
$$\beta_1 = 0.0750$$
$$\beta^* = 0.09$$
$$\kappa = 0.41$$
$$\gamma_1 = \frac{\beta_1}{\beta^* - \sigma_{u\omega} \kappa^2 / \sqrt{\beta^*}}$$

(36)

and the constants in the standard $k-\epsilon$ model are

$$\sigma_{e2} = 1.0$$
$$\sigma_{\epsilon\omega} = 0.856$$
$$\beta_2 = 0.0828$$
$$\beta^* = 0.09$$
$$\kappa = 0.41$$
$$\gamma_2 = \frac{\beta_2}{\beta^* - \sigma_{\epsilon\omega} \kappa^2 / \sqrt{\beta^*}}$$

(37)
2.4 Chemistry Model

The present work considers the ethylene/air systems. For ethylene/air systems, the two-step global kinetics scheme proposed by Westbrook and Dryer (1981) is adopted in light of its simplicity and reasonably accurate modeling of the burned gas containing incompletely oxidized species of hydrocarbon fuels. The scheme for ethylene oxidation involves the following two steps and five species:

\[ \text{C}_2\text{H}_4 + 2\text{O}_2 \rightarrow 2\text{CO} + 2\text{H}_2\text{O} \]  \hspace{1cm} (38)

\[ \text{CO} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}_2 \]  \hspace{1cm} (39)

The rate of the \( \text{C}_2\text{H}_4 \) oxidation per unit volume is expressed as

\[ \dot{\omega}_{f_1} = -A_1 \exp \left( \frac{-E_{a1}}{R T} \right) \left[ \chi_{\text{C}_2\text{H}_4} \right]^{0.1} \left[ \chi_{\text{O}_2} \right]^{0.65} \]  \hspace{1cm} (40)

The rate of the CO oxidation per unit volume is

\[ \dot{\omega}_{f_2} = -A_2 \exp \left( \frac{-E_{a2}}{R T} \right) \left[ \chi_{\text{CO}} \right]^{0.5} \left[ \chi_{\text{H}_2\text{O}} \right]^{0.25} \]  \hspace{1cm} (41)

In order to properly reproduce both the heat of reaction and pressure dependence of the [CO]/[CO\(_2\)] equilibrium, a reverse reaction is included for the second step,

\[ \dot{\omega}_2 = -B_2 \exp \left( \frac{-E_{r2}}{R T} \right) \left[ \chi_{\text{CO}_2} \right] \]  \hspace{1cm} (42)

In the above expressions, \( \left[ \chi_{\text{C}_2\text{H}_4} \right], \left[ \chi_{\text{O}_2} \right], \left[ \chi_{\text{CO}} \right], \left[ \chi_{\text{CO}_2} \right], \) and \( \left[ \chi_{\text{H}_2\text{O}} \right] \) represent the molar concentrations of species \( \text{C}_2\text{H}_4, \text{O}_2, \text{CO}, \text{CO}_2, \) and \( \text{H}_2\text{O}, \) respectively. The pre-exponential factors are taken as...
\[ A_1 = 1.12468 \times 10^{10} \text{ (kmol/m}^3\text{)}^{0.75}/s \]
\[ A_2 = 2.23872 \times 10^{12} \text{ (kmol/m}^3\text{)}^{0.75}/s \]
\[ B_2 = 5 \times 10^8 \text{ s}^{-1} \]

and the activation energies are given as
\[ E_{a1} = 125.52 \text{ kJ/mol} \]
\[ E_{a2} = 167.36 \text{ kJ/mol} \]

### 2.5 Turbulent Combustion Models

The interaction of turbulence and chemistry in supersonic conditions is an important issue. Recently, there were many attempts to address this issue using LES methods, PDF approaches, and other combustion models extended from subsonic combustion conditions. One of the simplest and yet most wide-spread models proposed by Magnussen (1981) is based on earlier work by Spalding (1970) for premixed turbulent flames and adopts the concept, that the turbulent mixing is the rate controlling parameter in nonpremixed combustion with fast chemistry. The effect of turbulent mixing on combustion is taken into account by means of the eddy-dissipation model (EDM) proposed by Magnussen (1981). In this model, the reaction rate associated with turbulence mixing, is given by the minimum of the following three rates:

\[
\dot{\omega}_r = -a[X_r](\varepsilon/k) \quad (43)
\]
\[
\dot{\omega}_o = -\frac{a}{v}[X_o](\varepsilon/k) \quad (44)
\]
\[
\dot{\omega}_p = -\frac{ab}{1+v}[X_p](\varepsilon/k) \quad (45)
\]
where \([\chi_f]\), \([\chi_o]\), and \([\chi_r]\) represent the molar concentrations of the fuel, oxygen, and product species, respectively, \(a\) and \(b\) are empirical constants taken to be 4.0 and 0.5, respectively, \(\epsilon/k\) the fluctuation frequency, and \(\nu\) the stoichiometric oxygen to fuel mass ratio. Combined, the actual reaction rate of a given species is determined by the smaller of that based on the finite rate chemical kinetics, and that based on the eddy-dissipation model.

### 2.6 Near-Wall Treatment

Special treatment is required in the near-wall region to save computational cost and expedite calculations. The wall-function concept proposed by Launder and Spalding (1972) is implemented in the numerical code, with the benefit for spatially resolving the boundary layer appropriately can be avoided. With the assumptions, that the viscosity-affected near-wall region does not need to be resolved; instead, an empirical wall function is used to determine the flow velocity. The variations in velocity, composition and temperature are only dependent on the wall-normal direction, the shear stress and velocity vectors are aligned parallel, the turbulence production balances dissipation and the variation of the turbulent length scale is linear. Therefore, a coarser grid can be used near the wall. The present work adopts the wall function used by Wilcox (1993) for the \(k-\omega\) model. The velocities can be computed from the following relation:
The effects of pressure gradients can not be neglected in the significant boundary layer separation regions, so $P^+$ is introduced to represent the dimensionless pressure-gradient parameter, which is defined as

$$P^+ = \frac{v}{\rho u'_i} \frac{dP}{dx}$$

Further details can be found in Wilcox (1993).
Chapter 3
Numerical Method

The original version of the numerical framework was developed in the late 1990’s in the Dr. Vigor Yang’s group at Penn State University. As several people have utilized and developed various version based on the original version of the numerical framework over time, it is constantly “under construction” with their contributions to code upgrades. The primary developers of the present numerical framework are Dr. S. Y. Hsieh, Dr. S. W. Wang and Dr. Y. Huang. The spatial and temporal discretization in the numerical approach is identical to that previously published by (Wang, 2002; Huang, 2003), except of the development and implementation of the source term treatment. The numerical approach is included in this chapter for the convenience of the reader to clarify the results reported in subsequent sections.

The numerical framework solves the time-dependent conservation law form of the Reynolds-averaged Navier-Stokes equations. The spatial discretization of the governing equations outlined above involves a finite-volume approach. The convective fluxes were formulated using Roe’s FDS (flux-differencing splitting) method derived for multi-species reactive flows along with the MUSCL (monotone upwind schemes for conservation laws) approach utilizing a differentiable limiter function. The spatial discretization employs a central difference strategy which satisfies the TVD (total variation diminishing) conditions for the convective and shear stress terms, as well as a high-resolution shock capturing capability. The discretized equations were temporally
integrated using a four-stage Runge-Kutta scheme, applying semi-implicit source term treatment to solve stiff chemistry source terms. Further efficiency was achieved with the implementation of the parallel computing technique based on the message-passing-interface (MPI) library.

3.1 Mathematical Equations

The formulation is based on the complete conservation equations in three dimensions. It also accommodates finite-rate chemical kinetics and variable thermophysical properties for a multi-component chemically reactive system. Turbulence closure is treated using an improved two-equation model calibrated for high-speed compressible flows. The coupled form of the species conservation, fluid dynamics, and turbulent transport equations can be summarized in a conservative vector form as follows.

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial}{\partial x}(\mathbf{E} - \mathbf{E}_s) + \frac{\partial}{\partial y}(\mathbf{F} - \mathbf{F}_s) + \frac{\partial}{\partial z}(\mathbf{G} - \mathbf{G}_s) = \mathbf{H}$$

(50)

where $x$, $y$, and $z$ represent the spatial coordinates. The conserved variable vector $\mathbf{Q}$, convective flux vectors $\mathbf{E}$, $\mathbf{F}$, and $\mathbf{G}$, diffusion-flux vectors $\mathbf{E}_s$, $\mathbf{F}_s$, and $\mathbf{G}_s$, and the source-term vector $\mathbf{H}$ are defined as
where subscript \( i \) stands for species \( i \), ranging from 1 to \( N-1 \). In the preceding equations, \( \rho \), \((u, v, w)\), \( e_i, Y_i \), and \( \tau \) represent the density, velocity components, specific total energy, mass fraction of species \( i \), and viscous stress, respectively. The thermal diffusion terms \( q_{e_x}, q_{e_y}, \) and \( q_{e_z} \) consist of contributions from heat conduction and mass diffusion processes. Fick’s law is used to approximate species diffusion terms \( q_{i_x}, q_{i_y}, \) and \( q_{i_z} \).
The source term \( \dot{\omega}_i \) is the mass production rate of species \( i \) due to chemical reactions.

The variables \( k \) and \( \omega \) represent the turbulent kinetic energy and turbulence frequency, respectively, \( \mu_k \) and \( \mu_\omega \) are the total dynamic viscosities for the \( k \)- and \( \omega \)-equations, respectively, and \( S_k \) and \( S_\omega \) the corresponding source terms. Each nomenclature is defined beforehand.

### 3.2 Spatial Discretization

#### 3.2.1 Finite Volume Approach

“The governing equations are solved numerically through a density-based finite volume approach. The numerical scheme exhibits excellent parallel efficiency and scalability attributes in the treatment of arbitrary geometry, and avoids problems of metric singularities, which are usually associated with the finite-difference approach. To utilize this approach, the governing equation is integrated over a control volume \( V \) enclosed by the surface \( S \) in the physical domain through the Gauss divergence theorem as:

\[
\int \int \int v \left( \frac{\partial Q}{\partial t} + \frac{\partial (E - E_v)}{\partial x} + \frac{\partial (F - F_v)}{\partial y} + \frac{\partial (G - G_v)}{\partial z} - H \right) dV = 0
\]

(54)

The integral conservation equation takes the following form

\[
\int_v \frac{\partial Q}{\partial t} dV + \int_S \vec{W} \cdot \vec{n} dS = \int_f H dV
\]

(55)
where vector $\mathbf{n}$ is the outward unit vector normal to each surface, and the flux tensor, $\mathbf{W}$, is expressed as:

$$\vec{W} = (E - F_y)\vec{i} + (F - F_x)\vec{j} + (G - G_y)\vec{k} \tag{56}$$

For the three dimensional cell with six surfaces as shown in Fig. 3-1, the governing equation can be written as follows:

$$\iiint \frac{\partial \mathbf{Q}}{\partial t} dV + \int_{S_x} \vec{W} \cdot \vec{n}_x dS_x + \int_{S_y} \vec{W} \cdot \vec{n}_y dS_y + \int_{S_z} \vec{W} \cdot \vec{n}_z dS_z = \iiint \mathbf{H} dV \tag{57}$$

Fig. 3-1: Schematic of three-dimensional adjacent cells

The subscripts $\xi$, $\eta$, and $\zeta$ represent quantities aligned with the axial, radial, and azimuthal directions, respectively, and $\vec{n}_\xi$, $\vec{n}_\eta$, and $\vec{n}_\zeta$ are unit vectors normal to the surface in the $\xi$-, $\eta$-, and $\zeta$-directions, respectively. The unit normal vectors are related to the cell surface areas $S_\xi$, $S_\eta$, and $S_\zeta$ as:
The cell surface areas are defined as:

\[ \vec{n}_x = \left( S_{x,x} \hat{i} + S_{x,y} \hat{j} + S_{x,z} \hat{k} \right) / \left| \vec{S}_x \right| \]
\[ \vec{n}_y = \left( S_{y,x} \hat{i} + S_{y,y} \hat{j} + S_{y,z} \hat{k} \right) / \left| \vec{S}_y \right| \]
\[ \vec{n}_z = \left( S_{z,x} \hat{i} + S_{z,y} \hat{j} + S_{z,z} \hat{k} \right) / \left| \vec{S}_z \right| \] (58)

The magnitude of each surface vector represents the corresponding cell interface area and can be obtained as:

\[ \vec{S}_x = \frac{1}{2} \left( \vec{r}_{x2} \times \vec{r}_{x6} \right) = \frac{1}{2} \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x_2 - x_1 & y_2 - y_1 & z_2 - z_1 \\ x_6 - x_3 & y_6 - y_3 & z_6 - z_3 \end{vmatrix} = S_{x,x} \hat{i} + S_{x,y} \hat{j} + S_{x,z} \hat{k} \]
\[ \vec{S}_y = \frac{1}{2} \left( \vec{r}_{y6} \times \vec{r}_{y5} \right) = \frac{1}{2} \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x_6 - x_3 & y_6 - y_3 & z_6 - z_3 \\ x_5 - x_7 & y_5 - y_7 & z_5 - z_7 \end{vmatrix} = S_{y,x} \hat{i} + S_{y,y} \hat{j} + S_{y,z} \hat{k} \] (59)
\[ \vec{S}_z = \frac{1}{2} \left( \vec{r}_{z4} \times \vec{r}_{z3} \right) = \frac{1}{2} \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x_4 - x_7 & y_4 - y_7 & z_4 - z_7 \\ x_3 - x_8 & y_3 - y_8 & z_3 - z_8 \end{vmatrix} = S_{z,x} \hat{i} + S_{z,y} \hat{j} + S_{z,z} \hat{k} \]

The magnitude of each surface vector represents the corresponding cell interface area and can be obtained as:

\[ \left| \vec{S}_x \right| = \left( S_{x,x}^2 + S_{x,y}^2 + S_{x,z}^2 \right)^{1/2} \]
\[ \left| \vec{S}_y \right| = \left( S_{y,x}^2 + S_{y,y}^2 + S_{y,z}^2 \right)^{1/2} \]
\[ \left| \vec{S}_z \right| = \left( S_{z,x}^2 + S_{z,y}^2 + S_{z,z}^2 \right)^{1/2} \] (60)

The cell volume \( \Delta V \) associated with each individual cell is evaluated using the formula provided by Kordulla and Vinokur (1983):

\[ \Delta V = \frac{1}{3} \vec{r}_1 \left( \vec{S}_x + \vec{S}_y + \vec{S}_z \right) \] (61)

The cell surface areas per cell volume are also defined as:

\[ \vec{\tilde{S}}_x = \vec{S}_x / \Delta V, \vec{\tilde{S}}_y = \vec{S}_y / \Delta V, \vec{\tilde{S}}_z = \vec{S}_z / \Delta V \] (62)
Substitution of Eqs. (7) and (9) in Eq. (8) gives,

\[
\int_{V} \frac{\partial Q}{\partial t} dV + \int_{S_x} \left[ S_{\phi} (E - E_{\phi}) + S_{\phi'} ((F - F_{\phi}) + S_{\phi} (G - G_{\phi}) \right] |S_{\phi}| dS_{\phi} \\
+ \int_{S_y} \left[ S_{\phi} (E - E_{\phi}) + S_{\phi'} ((F - F_{\phi}) + S_{\phi} (G - G_{\phi}) \right] |S_{\phi}| dS_{\phi} \\
+ \int_{S_z} \left[ S_{\phi} (E - E_{\phi}) + S_{\phi'} ((F - F_{\phi}) + S_{\phi} (G - G_{\phi}) \right] |S_{\phi}| dS_{\phi} = \int_{V} H dV 
\]

Assuming that the increments in the body-fitted coordinate system are unity, i.e., \( \Delta \xi = \Delta \eta = \Delta \zeta = 1 \), Eq. (63) yields the following governing equation in the general coordinates:

\[
\frac{\Delta Q}{\Delta t} + \left( E_{\xi} - E_{\xi+1/2} \right)_{i+1/2,j+1/2,k} + \left( F_{\eta} - F_{\eta+1/2} \right)_{i,j+1/2,k} + \left( G_{\zeta} - G_{\zeta+1/2} \right)_{i,j,k+1/2} = H 
\]

where the vectors \( E_{\xi}, F_{\eta}, G_{\zeta}, E_{\phi}, F_{\phi}, G_{\phi} \), and \( \Delta Q \) are defined as:

\[
\Delta Q = Q^{n+1} - Q^n \\
E_{\xi} = \left( \tilde{S}_{\xi} E + \tilde{S}_{\xi} F + \tilde{S}_{\xi} G \right), \quad E_{\eta} = \left( \tilde{S}_{\eta} E + \tilde{S}_{\eta} F + \tilde{S}_{\eta} G \right) \\
F_{\eta} = \left( \tilde{S}_{\eta} E + \tilde{S}_{\eta} F + \tilde{S}_{\eta} G \right), \quad F_{\phi} = \left( \tilde{S}_{\phi} E + \tilde{S}_{\phi} F + \tilde{S}_{\phi} G \right) \\
G_{\zeta} = \left( \tilde{S}_{\zeta} E + \tilde{S}_{\zeta} F + \tilde{S}_{\zeta} G \right), \quad G_{\phi} = \left( \tilde{S}_{\phi} E + \tilde{S}_{\phi} F + \tilde{S}_{\phi} G \right) 
\]

And the indices \( i \pm 1/2, j \pm 1/2 \) and \( k \pm 1/2 \) represent the each individual cell interfaces.

The quantities \( E_{\xi,j+1/2,k+1/2}, E_{\eta,j+1/2,k+1/2}, F_{\eta,j+1/2,k+1/2}, F_{\phi,j+1/2,k+1/2}, G_{\zeta,j+1/2,k+1/2}, G_{\phi,j+1/2,k+1/2} \) represent the numerical fluxes associated with each cell interface (as shown in Fig. 3-1).

\( \tilde{S} \) represents the cell surface area per cell volume. The above analysis describes the transformation of a quadrilateral cell with a volume \( \Delta V \) in the \( x-y-z \) coordinates to a cubic cell with unit volume in the general coordinate (i.e., \( \xi-\eta-\zeta \) coordinates). The maximum time increment \( \Delta t \) for each cell can be evaluated by:

\[
\Delta t = \frac{\Delta t_{\xi} \Delta t_{\eta} \Delta t_{\zeta}}{\Delta t_{\xi} + \Delta t_{\eta} + \Delta t_{\zeta}} 
\]
where

\[
\Delta t_\xi = \frac{CFL \cdot \Delta V}{\sqrt{\bar{u} S_\xi + \bar{v} S_\eta + \bar{w} S_\zeta + \left| \frac{\partial \bar{S}_\xi}{\partial \xi} \right| + c \left| \frac{\partial \bar{S}_\eta}{\partial \eta} \right|}},
\]

\[
\Delta t_\eta = \frac{CFL \cdot \Delta V}{\sqrt{\bar{u} S_\eta + \bar{v} S_\eta + \bar{w} S_\zeta + \left| \frac{\partial \bar{S}_\xi}{\partial \xi} \right| + c \left| \frac{\partial \bar{S}_\eta}{\partial \eta} \right|}},
\]

\[
\Delta t_\zeta = \frac{CFL \cdot \Delta V}{\sqrt{\bar{u} S_\xi + \bar{v} S_\eta + \bar{w} S_\zeta + \left| \frac{\partial \bar{S}_\xi}{\partial \xi} \right| + c \left| \frac{\partial \bar{S}_\eta}{\partial \eta} \right|}},
\]

where CFL is the Courant number and \( c = \sqrt{\gamma RT} \) is the local speed of sound.”

### 3.2.2 Evaluation of Inviscid Fluxes

“Different numerical approaches used for evaluating the numerical fluxes can lead to different schemes with disparate numerical characteristics. For example, for a central difference scheme, the convective flux at any cell face in the \( \xi \)-direction usually can be written as:

\[
\hat{E}_{\xi,j+1/2,f} = \frac{1}{2} \left[ E_{\xi,l}(Q^L) + E_{\xi,r}(Q^R) \right]
\]

(68)

where the left and right stencils are used to give desired accuracy. The above equation corresponds to the stencil illustrated in Fig. 3-2. The superscripts \( L \) and \( R \) represent the left and right cells. Depending on the manner in which these terms are evaluated, a wide variety of central and upwind schemes can be obtained. In the present work, the methodology proposed by Rai and Chakravarthy (1993) is used. Accordingly the numerical flux is calculated as:

\[
\hat{E}_{\xi,j+1/2,f,k} = \hat{E}_{\xi,j+1/2,f,k}^{(\xi)} - \varphi_{j+1/2,f} \left( \hat{E}_{\xi,j+3/2,f-k}^{(\xi)} - 2 \hat{E}_{\xi,j+1/2,f+k}^{(\xi)} + \hat{E}_{\xi,j+1/2,f-k}^{(\xi)} \right)
\]

(69)
where $\phi^{(4)}$ is the flux limiter. This term switches the truncation error associated with the flux-difference from fourth-order accuracy when $\phi^{(4)} = 1$, to second-order accuracy when $\phi^{(4)} = 0$. To approach at the desired accuracy in Eq. (68), the left and right state terms in Eq. (69) must be computed using the same or higher order accuracy. These terms are written as follows to facilitate easy switching and grand the numerical scheme with total variation diminishing (TVD) property.

\[
Q_{i+1/2,j,k}^L = Q_{i,j,k} + \phi_{i+1/2,j,k}^{(2)} \left( \frac{3VQ_{i+1,j,k} + \nabla Q_{i,j,k}}{8} \right) + \phi_{i+1/2,j,k}^{(4)} \left( \frac{-5VQ_{i+2,j,k} + 7VQ_{i+1,j,k} + \nabla Q_{i,j,k} - 3VQ_{i-1,j,k}}{128} \right)
\]

\[
Q_{i+1/2,j,k}^R = Q_{i,j,k} - \phi_{i+1/2,j,k}^{(2)} \left( \frac{\nabla Q_{i+2,j,k} + 3VQ_{i+1,j,k}}{8} \right) + \phi_{i+1/2,j,k}^{(4)} \left( \frac{3VQ_{i+3,j,k} - \nabla Q_{i+2,j,k} - 7VQ_{i+1,j,k} + 5VQ_{i,j,k}}{128} \right)
\]

\[
\nabla Q_{i,j} = Q_{i,j} - Q_{i-1,j}
\]

Fig. 3-2: Schematic diagram of the stencil used for evaluating inviscid fluxes in x-y plane
Furthermore, these stencils can be used to get fifth-order accuracy ($\phi^{(4)} = 1, \phi^{(2)} = 1$), third-order accuracy ($\phi^{(4)} = 0, \phi^{(2)} = 1$), and first-order accuracy ($\phi^{(4)} = 0, \phi^{(2)} = 0$), respectively. The present work utilizes second-order overall accuracy for the spatial discretization except in regions close to physical boundaries. At the cell near boundary region, the third-order accurate evaluation of the left and right states is thus employed, with the numerical fluxes in the $\eta$- and $\zeta$-directions computed following a similar procedure as above.”

### 3.2.3 Evaluation of Viscous Fluxes

“A central difference (CD) scheme is employed to evaluate the viscous flux terms. The procedure requires the calculations of the gradients of $u$, $v$, $w$, and $T$ at the cell interfaces. An example of auxiliary cell is shown schematically by the dash-dotted lines in Figure 3-3. Their centers are located at the midpoints of the primary cell interfaces with solid lines. The viscous fluxes need to be evaluated at the center of the cell faces, i.e., $i+1/2, j, k$ for the viscous flux in the axial direction. By applying the Gauss divergence theorem to an individual control volume $\Delta V$, a volume integral of vector $f$ can be transformed into a surface integral as following

$$\int_V \nabla \cdot \vec{f} dV = \int_S \vec{f} \cdot \vec{n} dS$$

(73)

The viscous fluxes can then be approximated as:

$$\nabla \cdot \vec{f} = \frac{1}{\Delta V} \int_S \vec{f} \cdot \vec{n} dS$$

(74)
Applying the above formulation to the auxiliary cell at \((i + 1/2, j, k)\) gives:

\[
\left( \frac{\partial f}{\partial x} \right)_{i+1/2,j,k} = \frac{1}{\Delta V_{i+1/2,j,k}} \left[ f \left[ S_{\varphi_x} \big|_{i+1/2,j-k} \right] - f \left[ S_{\varphi_x} \big|_{i,j,k} \right] + f \left[ S_{\varphi_x} \big|_{i+1/2,j,j} \right] - f \left[ S_{\varphi_x} \big|_{i+1/2,j,k} \right] \right] \quad (75)
\]

Similarly,

\[
\left( \frac{\partial f}{\partial y} \right)_{i+1/2,j,k} = \frac{1}{\Delta V_{i+1/2,j,k}} \left[ f \left[ S_{\varphi_y} \big|_{i+1/2,j-k} \right] - f \left[ S_{\varphi_y} \big|_{i,j,k} \right] + f \left[ S_{\varphi_y} \big|_{i+1/2,j,j} \right] - f \left[ S_{\varphi_y} \big|_{i+1/2,j,k} \right] \right] \quad (76)
\]

\[
\left( \frac{\partial f}{\partial z} \right)_{i+1/2,j,k} = \frac{1}{\Delta V_{i+1/2,j,k}} \left[ f \left[ S_{\varphi_z} \big|_{i+1/2,j-k} \right] - f \left[ S_{\varphi_z} \big|_{i,j,k} \right] + f \left[ S_{\varphi_z} \big|_{i+1/2,j,j} \right] - f \left[ S_{\varphi_z} \big|_{i+1/2,j,k} \right] \right] \quad (77)
\]

Where the quantities \(f\) in the above equations represent \(u\), \(v\), \(w\), and \(T\) at the cell interfaces as the elements of the viscous flux vectors \(E_{\varphi_x}, F_{\varphi_y}\), or \(G_{\varphi_z}\). Physical variables with one-half indices also need to be interpolated from the quantities at the neighboring cell centers and are given as

\[
f_{i+1/2,j+1/2,k} = \frac{1}{4} (f_{i,j,k} + f_{i+1,j,k} + f_{i+1,j+1,k} + f_{i,j+1,k})
\]

\[
f_{i+1/2,j,k+1/2} = \frac{1}{4} (f_{i,j,k} + f_{i+1,j,k} + f_{i+1,j,k+1} + f_{i,j,k+1})
\]

(78)
3.2.4 Evaluation of Artificial Dissipation

“Numerical dissipation turns out to be essential in central differencing schemes to avoid artificial oscillations in flow regions with discontinuity and steep density gradient, and thus to improve numerical stability and convergence. The expression of these artificial dissipation terms is determined by the order of accuracy of the numerical scheme, which must be higher-order accurate to limit its magnitude to the minimal. As shown previously, the numerical differentiation of the flux vectors in the present case can be second-order accurate in the core region of the computational domain. The corresponding artificial dissipation would have a forth-order accuracy. As the order of
accuracy of the numerical scheme decreases close to the physical boundary, the artificial
dissipation terms accordingly drop to a lower order. The form of numerical dissipation
employed in the present scheme is a combination of second- and fourth-order dissipation
terms. The second-order terms are used to prevent spurious oscillations near shock
waves and in flame zones, while the fourth-order terms play essential roles for stability
and convergence. The standard dissipation model can be written as:

\[ \text{Artificial Dissipation} = \mathbf{d}_{i+1/2,j,k} - \mathbf{d}_{i-1/2,j,k} \quad (79) \]

where

\[ d_{i1/2,j,k} = \frac{\varepsilon_2}{8} \frac{1}{\Delta \xi} \frac{\partial Q}{\partial \xi} \bigg|_{i1/2,j,k} - \frac{\varepsilon_4}{8} \frac{1}{\Delta \xi} \frac{\partial^3 Q}{\partial \xi^3} \bigg|_{i1/2,j,k} + \frac{\varepsilon_6}{8} \frac{1}{\Delta \xi} \frac{\partial^5 Q}{\partial \xi^5} \bigg|_{i1/2,j,k} \quad (80) \]

The quantities \( \varepsilon_2, \varepsilon_4, \varepsilon_6 \) correspond to the coefficients of the second-, fourth- and
sixth-order accurate artificial dissipation terms and the coefficients used in the present
study are \( \varepsilon_2 = 0.1, \ varepsilon_4 = 0.01, \ varepsilon_6 = 0.001 \), and \( \Delta \xi = 1 \).

Although the standard dissipation model has been shown to be reasonably
effective in various problems, application of the numerical dissipation should be cautious.
The standard model may also encounter difficulties in supersonic flows and reacting
flows due to the discontinuities near the flame fronts and shock waves as in the present
study. A matrix dissipation model has been developed by Swanson and Turkel (1992)
and Jorgenson and Turkel (1993) to overcome the above difficulties. In their model,

\[ d_{i1/2,j,k} = \varepsilon_{(2)}^{i+1/2,j,k} \left| \frac{\hat{\lambda}}{\Delta \xi} \right|_{i+1/2,j,k} \frac{\partial Q}{\partial \xi} \bigg|_{i1/2,j,k} - \varepsilon_{(4)}^{i+1/2,j,k} \left| \frac{\hat{\lambda}}{\Delta \xi} \right|_{i+1/2,j,k} \frac{\partial^3 Q}{\partial \xi^3} \bigg|_{i1/2,j,k} \quad (81) \]

with
The matrix dissipation model offers the central-difference scheme with the numerical features resemble to an upwind scheme near flow discontinuities, as well as the TVD property, which prevents the occurrence of spurious oscillations. The terms $M_{\xi}$ and $M_{\xi}^{-1}$ are the right and left eigenvectors matrices, which diagonalize $A$, where $A = \partial E_{\xi} / \partial Q$. The eigenvalues of the flux Jacobin matrix $A$ are:

$$\lambda_1 = \lambda_2 = \lambda_3 = \lambda_6 = U, \ \lambda_{4,5} = U \pm C$$

where $U = \bar{S}_{\xi} u + \bar{S}_{\xi} v + \bar{S}_{\xi} w$ and $C = \|\bar{E}_{\xi}\|$. The term $\tilde{\Lambda}_{\xi}$ above represents the modified diagonal matrix of eigenvalues $\tilde{\Lambda}_{\xi} = diag(\tilde{\lambda}_1, \tilde{\lambda}_2, \tilde{\lambda}_3, \tilde{\lambda}_4, \tilde{\lambda}_5, \tilde{\lambda}_6)$ to avoid zero eigenvalues, which can be expressed as:

$$\tilde{\lambda}_1 = \tilde{\lambda}_2 = \tilde{\lambda}_3 = \tilde{\lambda}_6 = \max(|\lambda_1|, Vf\sigma), \ \tilde{\lambda}_{4,5} = \max(|\lambda_{4,5}|, Vf\sigma)$$

where $\sigma$ is the spectral radius of the flux Jacobian matrix $A$. $V_f = 0.025$ and $V_a = 0.25$ are employed for the present study (Zingg et al, 2000). In present study, the Roe average is used to evaluate $[\tilde{\Lambda}] = M_{\xi} [\tilde{\Lambda}_{\xi}] M_{\xi}^{-1}$ due to the large density-gradient.
The matrix dissipation model has a simpler expression as a scalar dissipation model first introduced by Jameson, Schmidt and Turkel (1981). The scalar dissipation model gives the modified eigenvalues as

\[ \tilde{\lambda}_1 = \tilde{\lambda}_2 = \tilde{\lambda}_3 = \tilde{\lambda}_4 = \tilde{\lambda}_5 = \tilde{\lambda}_6 = \sigma \]  

(89)

Then Eq. (81) can be written in a similar expression as

\[
\begin{align*}
\mathbf{d}_{i+1/2,j,k}^{(2)} &= \epsilon^{(2)}_{i+1/2,j,k} \sigma^{i+1/2,j,k} \frac{\partial \mathbf{Q}}{\partial \xi} |_{i+1/2,j,k} \\
&\quad - \epsilon^{(4)}_{i+1/2,j,k} \sigma^{i+1/2,j,k} \frac{\partial^3 \mathbf{Q}}{\partial \xi^3} |_{i+1/2,j,k}
\end{align*}
\]

(90)

The matrix dissipation model is obviously more generalized and accurate than the scalar model, but the computation of these matrices at every grid-cell requires more computational time and memory.

The nonlinear second-difference dissipation term is given in Eq. (81) and Eq. (90), to introduce an entropy-like condition and to suppress oscillations near the flow discontinuities. This term is small in the smooth portion of the flow field. The switch \( \nu_{i,j,k} \) is crucial near the flow discontinuities due to the large pressure-gradients across them. In reacting flows, this term is adjusted to include temperature or density gradients instead of pressure gradient, as pressure may still be uniform across the flame. The linear fourth-order term affects the linear stability of the scheme, which is introduced to damp high-frequency modes and to allow the scheme to approach a steady state. This term reduces to zero near discontinuities.”
3.3 Temporal Integration

“A fourth-order Runge-Kutta (RK4) explicit scheme is used to solve the governing equations due to its higher temporal accuracy and relatively larger CFL number (i.e. $2\sqrt{2}$ for the Euler calculations using RK4). Thorough investigations on the RK4 scheme have been conducted in various turbulence flow cases (Hsieh and Yang, 1997; Apte and Yang, 2001) due to its creditability and accuracy. The governing equation in the general coordinates can be written as

\[
\Delta Q = H \cdot \Delta t - \Delta t[(E_{\xi} - E_{\xi+1/2,j,k})_{i-1/2,j,k} + (F_{\eta} - F_{\eta+1/2,j,k})_{i,j-1/2,k} + (G_{\varphi} - G_{\varphi+1/2,j,k})_{i,j,k+1/2}] \tag{91}
\]

Applying the four-stage Runge-Kutta scheme to the above, each temporal-integration is achieved through four consecutive intermediate steps,

\[
\begin{align*}
Q_0 & = Q^n \\
Q_1 & = Q_0 + \alpha_1 \Delta t \cdot R(Q_0) \\
Q_2 & = Q_0 + \alpha_2 \Delta t \cdot R(Q_1) \\
Q_3 & = Q_0 + \alpha_3 \Delta t \cdot R(Q_2) \\
Q^{n+1} & = Q_0 + \Delta t \cdot R(Q_3)
\end{align*}
\tag{92}
\]

where $R(Q)$ is written as

\[
R(Q) = H - [(E_{\xi} - E_{\xi+1/2,j,k})_{i-1/2,j,k} + (F_{\eta} - F_{\eta+1/2,j,k})_{i,j-1/2,k} + (G_{\varphi} - G_{\varphi+1/2,j,k})_{i,j,k+1/2}] \tag{93}
\]

Superscripts ‘$n$’ and ‘$(n+1)$’ stand for the solution at the ‘$n$th’ and ‘$(n+1)$th’ time steps, respectively. Evaluation of the $\Delta Q = Q^{n+1} - Q^n$ term in Eq. (91) is thus performed as explained above. The coefficients $\alpha_1$, $\alpha_2$, and $\alpha_3$ can be varied to obtain a variety of schemes with different stability properties. The standard four-stage scheme has the following values (Jameson, 1983):
In order to enhance numerical efficiency and minimize complexities arising from the irregular shape of the computational mesh, a curvilinear coordinate transformation of the governing equations is employed so that the grid spacing in the transformed domain is unity.

3.4 Source Term Treatment

The fourth-order Runge-Kutta algorithm has second-order time accuracy, which is convenient to program because there is no need to store intermediate solutions. However, one of the concerns in handling the chemical reacting terms is the stiffness of the equations, since chemical processes have a wide range of time scales which are much smaller than the flow ones. As a result, if explicit methods are used to integrate the stiff governing equations, the computations will become inefficient, because the time step sizes directed by the stability requirements are much smaller than those required by the accuracy considerations. The basic solution procedure for the dependent variable Q depends on whether the source term is treated explicitly or implicitly. In general, the explicit treatment is used for non-stiff source term while the implicit treatment is used for stiff source term.

The three-dimensional governing equation with chemical reaction source terms is expressed as:

\[
\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x} (E - E_x) + \frac{\partial}{\partial y} (F - F_y) + \frac{\partial}{\partial z} (G - G_z) = H \tag{95}
\]
where $Q$ is the dependent variable vector, $E$, $F$, and $G$ are convective flux vectors, $E_v$, $F_v$, and $G_v$ are diffusion-flux vectors, and $H$ is the source term vector. If the source term is treated explicitly, then the discretization of Eq. (95) yields

$$\Delta Q = Q^{n+1} - Q^n = R_s^n + \Delta t \cdot H^n$$  \hspace{1cm} (96)

where the Right-Hand-Side term $R_s$, take the formulation form by Eq. (93), defined as,

$$R_s = -\Delta t \cdot \left[ \left( E_{i,j-1/2,k} - E_{i,j+1/2,k} \right) + \left( F_{i,j-1/2,k} - F_{i,j+1/2,k} \right) + \left( G_{i,j-1/2,k} - G_{i,j+1/2,k} \right) \right]$$  \hspace{1cm} (97)

The marching in time for chemical source terms in $H$ can be either explicit or semi-implicit. To overcome the stiffness problem arising from chemical reactions, a semi-implicit treatment renders the numerical scheme more stable. In this technique, the dependent variable $Q$ is solved from

$$\Delta Q = Q^{n+1} - Q^n = \Delta t \cdot R_s + \Delta t \cdot H^{n+1}$$  \hspace{1cm} (98)

The source term $H$ can be expanded by means of the Jacobian matrix $D$ as

$$H^{n+1} = H^n + D^n \cdot \left( Q^{n+1} - Q^n \right)$$  \hspace{1cm} (99)

where the Jacobian matrix $D$ is treated explicitly as

$$D^n = \frac{\partial H^n}{\partial Q^n}$$  \hspace{1cm} (100)

Substitution of Eq. (99) into Eq. (98) gives

$$\Delta Q = \Delta t \cdot R_s + \Delta t \left[ H^n + D^n \cdot \left( Q^{n+1} - Q^n \right) \right]$$  \hspace{1cm} (101)

The Eq. (101) can be rewritten as

$$\left( I - \Delta t \cdot D^n \right) \Delta Q = \Delta t \cdot R_s + \Delta t \cdot H^n$$  \hspace{1cm} (102)
The above equation requires the calculation of the Jacobian matrix D. The approach to calculate the Jacobian matrix D for chemical source terms is elaborated in Appendix B.

3.5 Parallel Implementation

3.5.1 Parallel Architecture

The parallel computing architecture can be classified into the following four categories depending on whether there is one or several of instruction streams and data streams: Single Instruction Single Data stream (SISD), Multiple Instruction Single Data stream (MISD), Single Instruction Multiple Data stream (SIMD), Multiple Instruction Multiple Data stream (MIMD). The most widely used computing architecture is the MIMD system, which is indicated schematically in Fig. 3-4. In this configuration, each processor has its own data set and also a set of instructions to follow. These processors work independently of each other on these data sets and only communicate at some point during the computation where the data set and the results obtained are shared by two or more processors. MIMD-type computers include IBM SP-2, Cray T3E, CM5 and Beowulf Clustered computers.

For an SIMD or MIMD system, it is usually necessary to exchange data between processors. This can be done in two different ways: 1) Shared Memory systems, and 2) Distributed memory systems or Message Passing Interconnection (MPI) Network. The shared memory system consists of global address space, which is accessible by all the processors and thus the memory is shared among these processors. One processor can
communicate with other processors by writing into or reading from the global memory. This architecture inherently solves the inter-processor communication problem, but introduces bottleneck problems created from the simultaneous access of the memory by more than one processor. In the distributed memory systems, each processor has its own local (or private) memory and the global/shared memory is absent. The processors are connected externally to switches and network of wires to allow communications among them. The efficiency of these systems is based on the communication time required among these processors. The system has several advantages such as hardware compatibility, functionality, and performance. The only drawback of this architecture is the enormous responsibility placed on software programmers. The programmers must provide an efficient scheme to distribute the data and set of instructions, and also explicitly provide the instruction set for communications among the various CPUs. This requires reconstruction of the numerical algorithm and synchronization of the processors for efficient, parallel computing.

Fig. 3-4: Multiple Instruction Multiple Data (MIMD) architecture
3.5.2 Beowulf Cluster Parallel Computers

A Beowulf system is a multi-computer architecture, which is used for parallel computations. In a Beowulf system, one server computer and many other client computers are connected together via high-speed network. It is a distributed memory MIMD system built primarily using commodity hardware components, such as any PC capable of running a free operating system Linux, standard Ethernet adapters, and switches. The first Beowulf system was built by Donald Becker in 1994, which consists of 16 486DX4-100MHz machines each with 16 MB memory. The main advantage of a Beowulf system is its high compatibility. The changes in hardware, including node and network system, will not affect the programming model. A Beowulf system also uses commodity software, such as the Linux operating system, Message Passing Interface (MPI) and other available open-source software.

The present research work is performed on an in-house Beowulf system operated at Dr. Vigor Yang’s group, which consists of three Intel-based and one AMD-based Linux clusters. The parallel computing system presently includes 510 Pentium IV and 160 AMD Opteron processors, as shown in Fig. 3-5. These computers are connected with nine 100M Fast Ethernet switches and 4 Gbit switches in a tree topology to facilitate parallel processing. The cumulative internal memory is 210 GB, and the total disc storage is 5 TB. This system can sustain 1200 gigaflops total peak performance, providing substantial number-crunching capabilities for large-scale computations. Parallel operation is accomplished by implementing the MPI (Message Passing Interface) library.
Representative parallel performance of CFD algorithms on 120 Pentium processors with Fast Ethernet interconnection is about 80-85% efficient. In addition to those high-performance computing systems, two Pentium workstations with high-speed graphics cards are used to provide 3D visualization capabilities. This allows researchers to explore 3D flow structures obtained from numerical calculations in real time.

3.5.3 Domain Decomposition

The explicit time stepping numerical scheme (RK4) is applied in the current study, only the neighboring data instead of the data from the entire computational domain is required during the calculation of flow variables in each cell, which implies weak data dependence. The domain decomposition technique is best suitable for this kind of application, and is also commonly implemented for a distributed-memory parallel computer system. In the field of computational fluid dynamics (CFD), it is generally
referred to as mesh partitioning, based on the geometric substructure of the computational domain.

The basic idea of a domain-decomposition technique is to divide the physical domain into several sub-domains. Variables in each cell are updated to the next time step simultaneously. In order to calculate the spatial derivatives at the sub-domain boundaries, ghost cells or halo data around the computing cells are introduced. Figure 3-6 shows an example of a two dimensional sub-domain with ghost cells. Because the variables in the ghost cell are updated in another sub-domain, message passing is required to synchronize data between different sub-domains. Figure 3-7 shows an example of the inter-processor communication. Overlapped regions, where information must be obtained from neighboring processors, exist on each side of the local domain. Likewise, these processors would also need to send some data to their neighbors. Data at the eight corners of the overlapped regions are exchanged with that at the diagonally opposite corner to evaluate viscous fluxes at that corner. The communication overhead is directly proportional to the volume-to-surface ratio of the grid system in that sub-domain. Increasing the computation-to-communication ratio could lead to a higher parallel execution efficiency.
Fig. 3-6: Schematic of a two-dimensional sub-domain with ghost cells

Fig. 3-7: An example of the data communication with an east surface in three-dimensional simulation (second-order spatial accuracy)
3.6 Validation

The theoretical formulation and numerical scheme should usually be validated with several fundamental problems, to prove the reliability of the CFD simulations. Various aspects of the analysis are investigated and compared with the corresponding test results. In this section, two cases including turbulent flow over a flat plate and a two-dimensional oblique shock wave are presented to test various aspects of the numerical methods. These validation cases are chosen because of their relevance to the present topic of investigation.

3.6.1 Turbulent Flow over a Flat Plate

Since the accurate prediction of flows in scramjet engines is significantly dictated by the turbulence model that accounts for velocity fluctuations in the near-wall flow region, the accuracy of the turbulence model close to the surface should be carefully assessed.

To establish confidence in the turbulence modeling, the Menter’s SST model is first used to calculate near-wall flow properties for a flat-plate boundary layer. The modeled flow field is first reported by Wieghardt and Tillman (1952) and is included in the later work of Coles and Hirst (1969). The physical domain is 250 cm in length. To accelerate the convergence rate of these compressible flow solvers for this case, the freestream Mach number was set to 0.20, with the corresponding flow temperature and pressure as 298 K and 1 atm, respectively. The overall computational region consists of
144 x 51 x 4 grids. Calculations are made on a grid having \( y^+ \) values of 1 at the first point off the wall to capture the turbulent boundary-layer flow characteristics.

Figure 3-8 compares the calculated skin friction coefficient \( (C_f) \) with experimental data. Figures 3-9 and 3-10 show the variation of \( y^+ (= yu_{\tau}/v) \) versus \( u^+ (= u/u_{\tau}) \) at two axial locations, one is at near the front edge of the plat \( (x = 48.70 \text{cm}) \), another one close to the tailing edge \( (x = 228.70 \text{cm}) \). The calculations exhibit a reasonable agreement with the available experimental data, indicating the high fidelity of the current numerical model.

Fig. 3-8: Comparison of calculated skin-friction coefficient with experimental data
Fig. 3-9: Comparison of calculated velocity profile with experimental data (x = 0.4870 m)

Fig. 3-10: Comparison of calculated velocity profile with experimental data (x = 2.2870 m)
3.6.2 Oblique Shock Wave

The artificial dissipation implemented using the TVD feature enables the numerical scheme to capture such gradients or shock waves accurately. This verification case involves the computation of the supersonic flowfield over a wedge with a half angle of 10 degrees. The supersonic inlet flow pressure is set as 1Bar, temperature as 300 K and the freestream Mach number of 2.0162. An ideal gas is considered, with the ratio of heat capacity $\gamma$ as 1.4. Figure 3-11 shows the main features of the two-dimensional flowfield under investigation. As the supersonic inflow meets the leading edge of the wedge, an oblique shock is formed as the flow turns to become tangent with the wedge surface. The flow field past the shock is uniform.

![Fig. 3-11: Schematic diagram of two-dimensional oblique shock wave](image)

An analytic solution for this flow is well known (Anderson, 1982). The solution gives the change in properties across the oblique shock as a function of the freestream Mach number and shock angle. The shock angle is known as an implicit function of the freestream Mach number and wedge half-angle (theta-beta-Mach relation). The slip wall boundary condition is specified at the bottom plane. At the supersonic inlet chamber
pressure is set as 1Bar, temperature as 300 K and the Mach number is 2.0162. Other boundaries are all set as supersonic outlet conditions.

The snapshots of temperature and Mach number fields indicate the good capability to resolve an oblique shock of the present scheme, as shown in Fig. 3-12. The results calculated based on theoretical oblique shock relation and the numerical simulation are listed in Tab. 3-1. The agreement with the predictions from the oblique-shock relations is excellent, with a relative error of less than 1%.

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Fig. 3-12: Snapshots of flowfields of a 2D oblique shock (a) static temperature contour (b) Mach number contour
Tab. 3-1: Theory and numerical simulations on oblique shock wave for perfect gas

<table>
<thead>
<tr>
<th></th>
<th>M₁</th>
<th>M₂</th>
<th>Shock angle</th>
<th>p₂/p₁</th>
<th>T₂/T₁</th>
</tr>
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<tbody>
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<td>2.0162</td>
<td>1.6556</td>
<td>38.99°</td>
<td>1.711</td>
<td>1.171</td>
</tr>
<tr>
<td>numerical</td>
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<td>1.66</td>
<td>39°</td>
<td>1.72</td>
<td>1.173</td>
</tr>
</tbody>
</table>
4.1 Introduction

The scramjet engine is one of the candidates for a hypersonic flight propulsion system which is designed for the hypersonic flight regime of the range of flight Mach number 4 ~ 25. Many studies have been conducted from 90’s in last century to investigate preferred hydrogen-fueled concepts of scramjet engine, and it was indicated that the upper speed bound on flight Mach number lies in the Mach 12~16 range (Kimura, et al., 1981; Kim, 1995; Nishioka and Law, 1997; O’Brien, et al., 2001; Jacobsen, et al., 2003; Choi, et al., 2005). A number of studies were also conducted on hydrocarbon-fueled scramjets in which upper speed bound was established in Mach number 8~10 range (Yu and Schadow, 1994; Ju and Niioka, 1995; Fotache, Kreutz, and Law, 1997; Mathur, et al., 2001; Starkey and Lewis, 2003). For both hydrogen-fueled and hydrocarbon-fueled scramjets, the flow velocity at the entrance of the combustor can achieve at Mach number 2~5, although the most frequent experimental studies on the hydrocarbon-fueled scramjet combustor chamber have been performed at the entrance Mach number 1.5~2.5 (Yu and Schadow, 1994; Mathur, et al., 2001).

Hydrocarbon fuels are more attractive for the hypersonic flight regime than hydrogen fuels because of their higher volumetric energy content, lower cost and the relative simplicity of operational utilization, however their drawbacks are also obvious
due to the longer residence time required for vaporization, mixing of the fuel and air, and processing of their chemical reactions. Therefore numerous studies have been conducted in last twenty years to overcome these problems. For fuel injection to the supersonic crossflow, the traditional transverse injection provides good penetration and mixing, but at the expense of shock losses (Lavante, Zeitz, and Kallenberg, 2001; Lee and Mitani, 2003). Therefore in high-speed flow, parallel or angled injections were present in the injector ramps (Northam, et al., 1992; Ben-Yakar and Hanson, 2001; Mathur, et al., 2001), to achieve optimum effect between the total pressure loss and mixing augmentation process, and then increase of combustion efficiency. On the other hand, the relatively low reaction rate of hydrocarbon fuels can be enhanced by using a gaseous pilot flame (such as hydrogen or silane) (Kitagawa, et al., 2003). Fuel pre-heating can also be used to accelerate mixing and ignition of fuel-air mixture by enhancing the fuel vaporization.

In spite of these numerous efforts on improving the fuel ignition and flame stabilization, considering the complexity of the phenomenon, the methods mentioned above are of limited adaptability and do not always give satisfactory results. Unfortunately, ignition and flame stability have long been a serious concern in the development of hydrocarbon-fueled scramjet engines due to the difficulties to anchor flames in a high-speed environment. The situation becomes even more challenging during the engine start-up stage at which the low chamber pressure and unsettled fuel-air mixing tend to blow out the flame, even when a flame holding device such as a cavity is employed. To circumvent this difficulty, much effort was recently devoted to modulating the flowfield in the isolator and combustor by imposing blockage within the flow path.
The blockage can be established physically (a mechanical throttle such as a throat or a butterfly valve) (Hsu, et al., 2000; Kanda and Tani, 2005), aerodynamically (an air throttle) (Mathur, et al., 2000; Donbar, et al., 2001; Gruber, et al., 2001), or thermally (pyrophorics such as silane) downstream of the flame holder. The purpose was to slow the supersonic inlet flow and establish a proper pre-combustion shock train in the isolator, so that the resultant decrease in the local flow velocity and increase in the pressure in the combustor section can effectively enhance the ignition and flame stabilization.

In this chapter, the effects of transverse air throttling downstream of the combustor on flow development and fuel-air mixing phenomenon in a scramjet combustor, will be investigated numerically. Various fundamental processes, such as flow structure accommodation in combustor, fuel-air mixture expansion and filling in cavity, and mixing enhancement process, responsible for the air throttling transition in the combustor exhaust are carefully identified and quantified.

4.2 Physical Model and Boundary Conditions

4.2.1 Engine Configuration and Operating Conditions

The physical model of concern is shown in Fig. 4-1 as the direct-connect scramjet combustor test facility operated at the Air Force Research Laboratory. It includes a facility (inlet) nozzle, an isolator, a combustor equipped with a cavity flame holder, and an exhaust nozzle. The entire system measures 1789 mm in length. The isolator has a constant cross-sectional area with an entrance height of 38.1 mm. The combustor starts
with a short constant-area section, followed by a channel with a divergence angle of 2.6°. Gaseous ethylene is injected from aero-ramp fuel injectors with orifice diameter of 3.2 mm (I-1, I-2, I-3, I-4) flush mounted on both the top and bottom walls upstream of the cavity. The injection angle is 15° from the wall. Throttling air is discharged from a 3-section slit with a width of 3.2 mm and a length of 25.4 mm for each section (~76.2 mm for the entire 3-section slit). The slit is orientated normal to the main airflow and is located on the body-side surface at about 100 mm downstream of the cavity. The test rig is capable of simulating Mach 3.5-6 flight conditions at a dynamic pressure of 24-96 kPa (500-2000 psf).

Figure 4-2 shows a schematic of the operation sequence of the system. As a comparison, the situation without air throttling is also included. The operation starts with the delivery of the airflow through the entire system. Once a steady flow is established, the fuel injectors are turned on. After a short period, the air throttling is activated. Compressed air is introduced in a controlled manner through the air throttle to generate a pre-combustion shock train in the isolator. Ignition then occurs in the combustor, and the air throttling is terminated after the flame is stabilized. The heat release and associated pressure rise in the combustor retains the shock train required for sustaining combustion. Insufficient heat release leads to an unstable shock train and a premature removal of air throttling often results in flame blowout. It should be noted that the shock train interacts with the inlet flowfield; significant flow spillage or even inlet unstart may occur if the combustor is overpressurized. Thus, the interaction between the ignition transient dynamics and air throttling must be carefully studied and optimized.
4.2.2 Computational Grid and Boundary Conditions

The computational domain of concern includes the entire facility, spanning from the entrance of the inlet nozzle to the combustor exit. As a first approach, the entire computational domain was divided into 164 blocks to handle the irregular geometry and to facilitate parallel computation. The overall region consisted of (1654x95+361x85)x173 (32.5 million) grids, of which 361x85x173 grids were in the cavity. A total number of 164 processors were used in the present study.

At the inlet of the facility nozzle, the stagnation pressure and temperature corresponding to the experimental conditions are employed. A one-dimensional approximation to the axial momentum equation is then used to determine the pressure, along with the assumption of zero velocities in the vertical and spinwise directions. At the outlet where the flow is predominantly supersonic, the flow properties are extrapolated from the interior points. All the solid walls are assumed to be adiabatic, with the normal flow velocity and normal gradients of other flow variables set to zero, to be consistent with physical model coated with a layer of 0.5 mm thick thermal barrier coating (TBC) on interior surface of isolator to prolong the testing duration and to protect the metal wall from excessive heating. Heat loss from the flow may enhance the isolator performance by delaying boundary layer separation or even retarding flow choking, although the increase in shock train length for the high temperature flow comes mainly from flow properties, not from heat transfer (Lin et al. 2006). At the fuel injection ports and air throttling slits, the pressure, temperature, and velocity are specified in accordance with the injector geometry and local flow conditions.
Fig. 4-1: Schematic of a scramjet test rig. Integrated 3-D schematic of the injection block, cavity flameholder, and air throttle block on the body wall.

Fig. 4-2: Schematic of operation sequence of a scramjet combustion system with and without air throttling.
4.3 Results and Discussion

The theoretical and numerical framework is employed to study the unsteady flowfield in a scramjet facility shown schematically in Fig. 4-1. Numerical simulations were first carried out for non-reacting flow under a flight test condition specified in the experimental test conducted in AFRL, including a calculation of steady state baseline non-reacting flow, an injection of gaseous ethylene fuel at an equivalence ratio 0.6 after the steady baseline non-reacting flow is established. Once the stable fuel flow is established, air throttling at a mass flow rate of $\dot{m}_{\text{throttle}} = 20\% \dot{m}_{\text{air}}$ is introduced at the downstream of the combustor. The detailed flow field development driven by air throttling in the Scramjet engine is investigated, and the intricate interactions between the air throttling and mixing of fuel and air is systematically studied. The following sections will choose the representative cases to discuss the impact of air throttle on the flowfield and mixing process in the studied Scramjet engine. Calculations corresponds to 20~30 ms in physical time from the initial condition, which is enough for a supersonic flow stabilization and ignition process, but shorter than the typical test time of the ground based experiments (10~20 s).
4.3.1 Baseline Non-reacting Flow

Analyses are first conducted for non-reacting flows in the absence of fuel injection and air throttling. As a specific example, the total temperature and total pressure at the entrance of the facility nozzle are set to 1106.7 K (1992 R) and 3.51 atm (51.6 psia), respectively, simulating a flight Mach number of 5 and a dynamic pressure of 24 kPa (500 psf). The corresponding air mass flow rate is 0.757 kg/s. The airflow at the entrance of the isolator has a static temperature of 560 K, a static pressure of 0.328 atm, and an axial velocity of 1045 m/s. The corresponding inlet air flow Mach number at the entrance of the isolator is 2.2.

Figure 4-3 shows the distributions of the static wall pressure $p_w$ and flow Mach number along the centre line of the mean stream under a steady condition, the corresponding entire facility flowpath is demonstrated at the top of the figure. Supersonic air enters the constant cross-section area duct of the isolator. The air flow slows down due to the viscous boundary layers on the walls, and then accelerates from Mach number of 1.8 through the divergent duct to Mach number of 2.1 at the combustor exit. Owing to the flow expansion near the cavity front edge, a locally peak Mach number of 2.2 is achieved in the combustor, where the static wall pressure on the cowl surface drops. The pressure decreases along the cavity bottom wall to a locally minimum value at the rear ramp wall, where the shear layer experiences recompression and leads to higher pressures on the tailing edge. The comparison of the wall pressure distribution
between the numerical result and experimental data along the entire facility flowpath is also presented in Fig. 4-3. The overall agreement is quite promising.

Figure 4-4 presents the flow static pressure, Mach number and temperature distributions in the combustor on the x-y plane \((z/W = 1/2)\). Fig. 4-4a illustrates that the back wall of the cavity leads to the formation of an expansion wave at the leading edge that reduces the local pressure in the high speed flow stream. The free shear layer then deflects farther into the cavity, which results in a recompression on the inclined rear ramp of the cavity. Although the consequence pressure gorge over the cavity would increase the drag of the engine combustor, the shear layer impingement on the inclined rear ramp induces more entrainment of air into the cavity. The reattached shock wave at the cavity trailing edge reflects downstream between the body- and cowl-side walls, resulting in a series of shock/compression waves. Fig. 4-4b shows the flow Mach number distribution.

Fig. 4-3: Distributions of wall pressure and Mach number in the flowpath in the non-reacting flow case
on the x-y plane near the cavity. The main flow passage is predominantly supersonic. A free shear layer divides high momentum air stream from cavity. Inside the cavity the entrapped air is significantly decelerated to Mach 0.2 and lower, and consequence flow recirculation form in the cavity. Fig. 4-4c shows the flow static temperature distribution on the x-y plane near the cavity. The inlet flow at the isolator entrance has a static temperature of $T_0 = 560$ K. The flow temperature increases along the isolator due to the viscous boundary layers on side walls. It reaches a peak value of about 640 K at the entrance of the combustor, and decreases continuously through the expansion in the divergent combustor channel. In the contrast to the mean flow, the cavity withstands temperatures of over 800 K within itself due to the locally low-momentum flow condition.

The detailed supersonic flow structure with enormous density variations can be demonstrated in terms of shadowgraph images in Fig. 4-5 ~ Fig. 4-7. Fig. 4-5 shows a perspective shadowgraph through the facility flowpath, on the centre x-y plane ($z/W = 1/2$). The supersonic flow enters the constant cross-section area isolator and the viscous boundary layers develop with a series of compression waves as well on the side walls. The detailed illustrations of the flow structure in the isolator and combustor sections are presented in Fig. 4-6 and Fig. 4-7, respectively. Fig. 4-6 shows the perspective shadowgraph images inside the constant cross-section area isolator on the x-y ($z/W = 1/2$) and x-z ($y/H = 1/2$) planes. Weak compression waves sequence is obviously exhibited by the viscous boundary layers on the isolator walls, resultant increase of ambient flow pressure and reduction of flow momentum along the flow path have been indicted in Fig. 4-3. To illustrate the details of the oblique shock wave and viscous boundary layers formations, these planes are shifted out of the isolator. The gradually thickening viscous
boundary layers develop along the side walls, as the boundary layer-induced compression waves weaken and disappear before they reach the exit of isolator. Fig. 4-7 shows the close-up shadowgraph image in the combustor region on the center x-y plane (z/W = 1/2). The supersonic main flow accelerates in the 2.6°-angle divergent channel. A shear layer separates from boundary layer at the leading edge of cavity and comes to take a shape over the cavity due to the momentum gorge from the main stream, following by an expansion wave anchored at the leading edge of the cavity, and reattached by the rear ramp wall of the cavity.

Fig. 4-4: Close-up view of the pressure, Mach number and temperature contours on x-y plane (z/W = 1/2) in the combustor section for the non-reacting flow case
Fig. 4-5: Shadowgraph of the flowfield in the entire channel, \( z/W = 1/2 \).

Fig. 4-6: Shadowgraphs on x-y and x-z planes in the isolator section.

Fig. 4-7: Slice of shadowgraph on x-y plane in combustor section for the non-reacting flow case.
4.3.2 Fuel Injection and Air Throttling in Non-reacting Flow

As indicated in the operation sequence shown in Fig. 4-2, once a steady flow is established, ethylene fuel is injected into the chamber at an inclined angle of 15°, from aerodynamic ramp injectors on both the body- and cowl-side walls. The arrangement of these injection orifices is illustrated in Fig. 4-1. To evaluate the ignition and combustion characteristics, fueling locations and the fueling spit between the body and cowl walls are selected properly. In the present work, body-side only fueling from I-2 injectors and cowl-side fueling from I-4 injectors with a 60/40 fueling split (I-2/I-4 at 60/40) are chosen as the baseline fueling scheme. There are four orifices on the body side and three orifices on the cowl side. Each gaseous fuel injector features a flush-wall plain orifice upstream of the cavity at $x_{\text{inj}} = 1.11$ m. The total mass flow rates of the air and fuel are 0.757 and 0.052 kg/s, respectively, corresponding to an overall fuel-air equivalence ratio of 0.6. The momentum-flux ratio between the fuel jet and inlet air stream is 0.5.

4.3.2.1 Flow Field Development

After the stable fuel flow has been established in the combustor, air throttling is activated to increase the back pressure in the combustor. The sonic air injection at the throttling slit has a static temperature of 273 K and a static pressure of 1.92 atm, the resultant throttling air mass flow rate is 0.151 kg/s, which is equal to 20% of the inlet air mass flow rate ($m_{\text{air}} = 0.757$ kg/s). Figure 4-8 demonstrates the air-throttling transient and
time evolution of the flow structures inside the combustor section in the combustor in terms of the shadowgraph images. The throttle-induced boundary layers separation and derived shock/boundary layer interactions in the combustor are illustrated by the shadowgraph image on the x-y plane at z/W = 3/8, as shown in Fig. 4-8a. Throttled air is discharged at the beginning of the calculation (t = 0.0 ms), as the established fuel flow has been stable. Within a very short time after the throttle is activated (t = 0.044 ms), a bow shock wave is produced due to the throttling air penetration (Fig. 4-8a-1). The bow shock develops with the strengthening air throttling, and expands down to the cowl-side wall, as the back pressure rises at t = 0.089 ms (Fig. 4-8a-2). The further growing adverse pressure gradient obliges the boundary layer to separate from the body-side wall at t = 0.446 ms (Fig. 4-8a-3). The bow shock becomes an oblique shock at the front edge of the boundary separation and is pushed upstream as the separation region grows. At the time t = 1.478 ms (Fig. 4-8a-4), the oblique shock merges with the attached shock wave originating from the rear ramp of the cavity. The enhanced adverse pressure gradient downstream of the oblique shock then leads to the boundary-layer separation on the cowl-side wall. This backpressure-driven oblique shock wave continually propagates upstream over the trailing edge of the cavity, as shown in Fig. 4-8a-5 at t = 2.011 ms. Fig. 4-8a6 ~ Fig. 4-8a8 illustrate that the shear layer over the cavity is lifted from the cavity ramp due to the enhanced adverse back pressure gradient, and at the steady state, a series of oblique shocks form between the boundary layer and shear layer. The vertical sidewall effects on the flowfield are also presented on the x-y plane at z/W = 1/8 in Fig. 4-8b. The plane cut through one of the Ethylene fuel injectors (I-2) on the body surface, which is closest to the vertical sidewall among all injectors (I-2 and I-4). The flow
development suggests that the boundary-layer separation on both body and cowl surfaces between the cavity and throttle appear to be more extensive near the vertical sidewalls. The enhanced boundary layer separation should be explained as the results of the additional influence from the side walls and the corners.

The back pressure rise due to the downstream air throttling implementation significantly accommodates the flow structure in the combustor. Flow static wall pressures are probed at three different axial locations near the injectors ($P_1(t), x_1 = 1.11$ m), combustor ($P_2(t), x_2 = 1.20$ m), and throttle slit ($P_3(t), x_3 = 1.36$ m) respectively, and the time evolution of the pressure can be demonstrated in Fig. 4-9. Once the stable fuel flow has been established in the scramjet combustor, the throttle slit starts to discharge the compressed air at sonic speed with the mass flow rate $0.151$ kg/s, about $20\%$ of that of the inlet airflow ($\dot{m}_{\text{throttle}} = 20\% \dot{m}_{\text{air}}$). The air throttling drives the local static wall pressure $P_3$ to jump from $0.40$ atm to $0.74$ atm in a short time period of $2$ ms. The throttle-induced adverse pressure gradient separates the boundary layer from the upstream sidewalls, and obliges the shock waves to form and move upstream to match the backpressure rise. The resultant wall pressure increasing inside the cavity and the injectors upstream the cavity are demonstrated as $P_2$ and $P_3$ pressure evolutions. The pressure evolution on the probe $P_2$ in the cavity section presents obvious oscillating characters due to the instability from the shock/shear layer interaction. The shear layer above the cavity is reattached with the oblique shock wave originating from the rear ramp of the cavity. As the shock/shear layer reattachment point oscillates above the rear ramp of the cavity, periodic acoustic waves propagate into the cavity accompanied with some mass exchange at the cavity trailing edge.
Fig. 4-8: Time evolution of shadowgraph view on x-y planes (a. z/W = 3/8, b. z/W = 1/8) in the combustor section for the non-reacting flow case with air throttling ($\dot{m}_{throttle} = 20\% \dot{m}_{air}$).
Detailed discussions are conducted to explore the effects of air throttling on the non-reacting flow. Figure 4-10 shows the shadowgraph image on the center x-y plane (z/W = 1/2) under the steady state. A close-up view inside the combustor section is also presented below. Compared with the previous results without air throttling implemented, no visible change is observed in the boundary layers and flow structures in the isolator, indicating that the influence on the flow field by air throttling is limited within the combustor. The close-up shadowgraph image in the combustor illustrates the tremendous penetration of the throttling air into the supersonic cross-flow. Upstream of the air throttling, significant boundary layer separation spreads upstream to the cavity, as a result, the shear layer impingement on the rear edge of the cavity is eventually lifted into the

**4.3.2.2 Stable Flow Field**

Detailed discussions are conducted to explore the effects of air throttling on the non-reacting flow. Figure 4-10 shows the shadowgraph image on the center x-y plane (z/W = 1/2) under the steady state. A close-up view inside the combustor section is also presented below. Compared with the previous results without air throttling implemented, no visible change is observed in the boundary layers and flow structures in the isolator, indicating that the influence on the flow field by air throttling is limited within the combustor. The close-up shadowgraph image in the combustor illustrates the tremendous penetration of the throttling air into the supersonic cross-flow. Upstream of the air throttling, significant boundary layer separation spreads upstream to the cavity, as a result, the shear layer impingement on the rear edge of the cavity is eventually lifted into the
downstream separated boundary layer, inducing extensive oblique shock and compression wave sequence over the mean stream. As shock/shear layer interactions generate the shock/shear layer reattachment point oscillations above the rear ramp of the cavity, acoustic waves propagate inside the cavity, accompanied with enhanced mass exchange at the cavity trailing edge and fuel-air mixing in the cavity. Figure 4-11 presents the flow vorticity magnitude in the combustor under the steady-state condition and the typical streamlines over the cavity to demonstrate the significant recirculation zones. Large recirculation zones have formed inside the cavity, accompanied with significant vorticity magnitude. In addition, intense flow recirculation zone has been formed downstream of the cavity by means of the back pressure rise from the air throttling.
Fig. 4-10: Shadowgraph on x-y plane in the combustor section under a steady-state condition with air throttling ($\dot{m}_{\text{devail}} = 20\% \dot{m}_{\text{air}}$)
Figure 4-12 presents a three-dimensional perspective shadowgraph image of the steady-state flowfield in the combustor. Four horizontal planes are also extracted to demonstrate the detailed flow structures at vertical locations of $y = 0.6$, $1$, $2$, and $3$ cm, respectively. The perspective shadowgraph view clearly shows the bow shock structure as arrays on both sidewalls, induced by the compression of the high-speed mainstream to the inclined fuel injections. It is clearly visible on each horizontal plane that the induced shock waves have bow-shape structures circling the orifices, and cross with the neighbor shocks in the spinwise directions. The bow shock waves from both body and cowl side walls penetrate into the main flow stream, and cross through each other at the height $y = 20$ mm. At a short distance downstream of the orifices, the oblique shock waves reach and interact with the boundary layer on the side walls where they reflect back into the cross-flow. The propagation of these oblique shock waves make the flow field complicated while they reflect between sidewalls in the combustor.
Fig. 4-12: Perspective view of shadowgraph in the combustor section under a steady-state condition with air throttling ($m_{\text{thrott}} = 20\% m_{\text{air}}$).
4.3.3 Influence on Flow Field by Air Throttling

4.3.3.1 Throttle-Induced Flow Structure Accommodation

Detailed study of the influence on the combustor flow field by the throttle-induced shock/boundary layer interactions are conducted in this section. Figure 4-13 compares the calculated static wall pressure $p_w$ and flow Mach number distributions along the centre line of the flowpath under the conditions with and without air throttling. The penetration of air throttling downstream of the combustor mimics a stagnation point and causes intensive flow recompression and boundary separation on the body surface, with a resultant significant back pressure rise to about 0.7 atm. Meanwhile, the shear layer is lifted from the cavity as a result of the downstream boundary separation, resulting in the compression waves and pressure rise over the cavity, and the decreasing of center flow Mach number as well.

More comprehensive combustor flow field accommodations are demonstrated in Mach number contours in Figure 4-14. The effects of the compression and expansion waves in reducing and elevating the flow Mach number are clearly evident. As the penetration of air throttling partially shields the high-speed air flow, the resultant compression and diffusion of the throttling air certainly reduces the surrounding air flow Mach number, and reverses axial velocity gradient to induce the upstream boundary layer separation. The recirculation air flow in separation zone has low Mach numbers below 0.2, resulting a longer residence time for a better mixing performance, as measured and
discussed in the following sections. On the other hand, the low-momentum boundary separation zone expands to corners by means of sidewall effects from vertical sidewalls, and becomes an important reason of mixing enhancement of the fuel-air mixture.

The throttling-induced flow separations and consequence flow field accommodations considerably enhance the flow distortions and fuel residence ability in the cavity. Figure 4-15 outlines the schematic of a horizontal plane at a typical height in the bulk of the cavity ($\Delta y/H_c = 1/3$). Accommodations of the flow field as pressure, velocity, vorticity magnitude and fuel-air equivalence ratio distributions by means of air throttling on this horizontal plane inside the cavity are studied. The contributions of air throttling on the pressure field in the cavity are clearly illustrated in Figure 4-16. The ambient static pressure inside the cavity has been noticeably increased in the presence of the downstream air throttling, ranging between the pressure of 61 and 66 kPa, while its baseline flow counterparts in the absence of air throttling are only averaged at a value of about 46 kPa, as the latter has a relatively uniform pressure field. Obvious variant pressure spots are found in the cavity flow region, in terms of strong flow distortions as results of the shock/shear layer interactions over the cavity.
Fig. 4-13: Wall pressure and Mach number in the flowpath in the non-reacting flow with and without air throttling.

Fig. 4-14: Mach number contours in combustor section under conditions with and without air throttling.
Figure 4-17 presents the accommodations of axial flow velocity inside the cavity by means of air throttling. With the reduction of the flow momentum in the presence of air throttling, the flow streams in the cavity appear to become chaos and disordered. The flow recirculation is established in a length scale of entire cavity and well enhanced, indicating stronger air entrainment and mass exchange into the cavity as a matter of fact. Subsequent data supports to the point are given in terms of the vorticity magnitude and fuel-air equivalence ratio distributions in Figures 4-18 and 4-19.

Figure 4-18 presents the corresponding flow vorticity magnitude distributions in the cavity under conditions with and without air throttling downstream of the cavity. Instability of the shear layer impingement on the rear ramp of the cavity induces flow distortions and shedding-vortices, spreading either downstream of the combustor or upstream into the subsonic cavity flow region. The upper image shows the vorticity magnitude decays into the deeper upstream portion of the cavity flow field. In the presence of the air throttling, as the lower image presents, the vorticity magnitude is largely strengthened in the entire cavity chamber, because the shock wave/shear layer
interactions over the cavity significantly enhance the flow distortion and turbulence diffusion into the cavity.

The enhanced fuel-air mixing and mass entrainment into the cavity by means of the air throttling are then present in terms of fuel-air equivalence ratio in Fig. 4-19. The fuel lean mixture composition in the cavity has an averaged value of 0.5 ~ 0.6 in the absence of air throttling in the Scramjet engine. On the other hand, fuel entrainment into the cavity is largely enhanced by means of air throttling, as the fuel-air equivalent ratio achieves over 0.7 over the cavity region. The enhanced fuel-air mixing and mass entrainment into the cavity are gratefully appreciated, as closer to unit stoichiometric ratio, more beneficial for the combustion.
Fig. 4-16: Pressure contours in the cavity ($\Delta y/H_c = 1/3$) under conditions with and without air throttling.

Fig. 4-17: Velocity contours in the cavity ($\Delta y/H_c = 1/3$) under conditions with and without air throttling.
Fig. 4-18: Vorticity contours in the cavity ($\Delta y/H_c = 1/3$) under conditions with and without air throttling.

Fig. 4-19: Fuel-air equivalence ratio contours in the cavity ($\Delta y/H_c = 1/3$) under conditions with and without air throttling.
4.3.3.2 Fuel-air Mixing Enhancement by Means of Air Throttling

Figure 4-20 presents the accommodations of the fuel concentration distributions by means of air throttling, in terms of iso-surfaces of ethylene fuel mass fraction in the flow field, with the throttling air stream demonstrated by iso-surfaces of temperature as well. For the fuel mass concentration, semi-transparent iso-surfaces are colored at the corresponding concentration scales so that the images are biased to regions of locally significant fuel distribution. Although the penetrations of the fuel injection to the main flow show the similar plume stream, the fuel entrainment into the cavity differ significantly as fuel concentrations inside the cavity indicate. The bottom image presents stronger fuel concentration in the presence of the air throttling, than the baseline flow counterpart shown in top image. The latter flow field has typical ethylene mass fraction about 2.0% ~ 2.5% in the cavity, while the former reaches over 5.0% in fuel mass fraction if the air throttling is present. The fuel entrainment into the cavity has been largely enhanced because throttle-induced shock waves strongly interact with the shear layer over the cavity, and significantly enhance the flow distortion and turbulence diffusion into the cavity, which induces stronger fuel-air mixing and mass exchange to the cavity.
The more detailed data analyses have led to the conclusion that the air throttling indeed improvises the fuel entrainment into the cavity to facilitate the ignition and flame holding processes. Figure 4-21 presents the comparison of the spatial fuel concentration in the combustor under conditions with and without air throttling, with the fuel mass fraction distributions illustrated on vertical planes and the aerodynamic ramp injectors present on both body- and cowl-side walls. The baseline flow in the absence of air throttling in the top image has clearly visible fuel injection plumes, with each individual fuel plume remaining largely intact with neighboring plumes, and expanding laterally by turbulent diffusion and vortex motion downstream. The lower image presents the significantly different fuel concentration distributions from their counterparts in the baseline flow, offering an insight into the influence on fuel-air mixing by the air throttling.
throttling. The air throttling effects the ethylene concentration distributions from the cavity entrance. The extensive expansion of the fuel jet plumes occurs consequently downstream, where each individual fuel plume interacts with their neighboring plumes over the cavity. The simulation results indicate that the shock-induced boundary layer separations on the sidewalls largely enhance the flow distortions and therefore the fuel lateral spreading toward the sidewalls and corners, as a results, distinctive extent of the fuel jet plumes occupies about one-third of the downstream cross-sectional area before they reach air throttling (x/H = 35.5).

The throttling-induced boundary layer separations and the flow distortions indeed improve the fuel-air entrainment and mixing substantially inside the cavity, as illustrated by the ethylene concentration distributions in Figure 4-22. The images in left column show the cross-sectional fuel mass fraction distributions in the baseline flow field, while the corresponding cross-sectional fuel mass fraction distributions in the presence of the air throttling are shown in the right column. The former flow field indicates a small transportation of the ethylene fuel into the cavity through the air entrainment, but the majority of each fuel jet flow bypasses the cavity and remains individual plume downstream. In the contrast, the air throttling has imposed distinctly change to the fuel penetration and diffusion in the combustor flow field. At the entrance of the cavity, the ethylene fuel starts expanding laterally into the cavity with strong flow convections. The large transportation of the ethylene fuel trapped in the cavity, as shown in the image (x/H = 32), clearly imply the different controlling physics of the mass exchange and fuel-air mixing from the ordinary influence of cavitations. The flow separations on the sidewalls dramatically lift the shear layer from the cavity, which interacts with the shock waves to
induce large vortex and flow distortion into the cavity, delivering more fuel-air mixture as a result. Therefore the total ethylene fuel mass concentration in the cavity has largely increased by means of the air throttling implementation. In addition, the flow distortions and inner cavity recirculation significantly enhance the fuel diffusion inside of the cavity. On the other hand, the fuel jet plumes penetrate deeper into the main flow under the influence of the shock-induced flow separations.

Fig. 4-21: Comparison of ethylene mass-fraction contours on cross flow planes under conditions with and without air throttling.
Fig. 4-22: Distributions of ethylene mass fraction at various axial locations under conditions with and without air throttling.
Streamwise vorticity characterizes the contribution of convection to fuel-air mixing by increasing the interfacial area between the fuel and air flows. The mass-weighted averaged streamwise vorticity is calculated at the axial direction. Figure 4-23 shows the spatial distribution of the mass-weighted averaged streamwise vorticity for the non-reacting flow under conditions with and without air throttling. The spatial distribution of the streamwise vorticity in the baseline flow has a substantial increase at the entrance of the cavity, due to the additional contribution of the vorticity inside the cavity. The shear layer impinges on the cavity ramp and interacts with the reattached shock wave, to induce more vortices into the flow. In the presence of air throttling, the streamwise vorticity contribution in the cavity is significantly higher than its counterpart in the baseline flow. The measured stronger streamwise vorticity is triggered by two major factors. On one hand, the vorticity in the cavity is remarkably enhanced by means of the downstream air throttling. On the other hand, the enhanced oblique shock waves interact with the shear layer over the cavity, resulting in more vorticity in the wall shear flow. Downstream of the cavity, the flow separations caused by air throttling obviously induce the higher vorticity level than the counterpart in the baseline flow. A vorticity spike is clearly observed at the axial location x = 1.36, caused by the throttling air penetration and compression to the main flow field at the throttle slit.
Then the quantitative evaluations of the fuel-air mixing processes are investigated by means of two measures of mixing. The mixing efficiency, \( \eta_m \), is first employed which is defined as the ratio of fuel that would react if the fuel-air mixture is brought to complete reaction to the total fuel present. The mixing efficiency can be determined as follows

\[
\eta_m = \frac{m_{F,\text{mix}}}{m_F} = \frac{\int \rho Y_{\text{air}} (\vec{v} \cdot \vec{n}) dA}{\int \rho Y_F (\vec{v} \cdot \vec{n}) dA}
\]

where

\[
Y_{\text{air}} = \begin{cases} Y_F, & \text{if } Y_F \leq Y_T \\ Y_T, & \text{if } Y_F > Y_T \end{cases}
\]

and

\[
Y_T = Y_\text{str} \left( \frac{Y_F}{Y_\text{str}} \right)
\]
where the subscript $ST$ stands for the stoichiometric proportion of the fuel-air composition. In the preceding equations, $\rho$, $A$, $Y_F$ and $Y_A$ represent the density, duct cross section area, and mass fractions of ethylene fuel and air, respectively. Another measurement quantity is called as the mixing effectiveness, $\varepsilon_m$. It is expressed as the ratio of fuel that would react if the fuel-air mixture is brought to complete reaction to the maximum amount of fuel that could burn given the mass of air (the stoichiometric amount of fuel).

$$\varepsilon_m = \frac{\dot{m}_{F,\text{mix}}}{\dot{m}_{F,ST}} = \frac{\int \rho Y_F \left( \hat{V} \cdot \hat{n} \right) dA}{\int \rho Y_T \left( \hat{V} \cdot \hat{n} \right) dA}$$

(106)

Fig. 4-24 presents the spatial distributions of both the mixing efficiency and mixing effectiveness for the flowfield under conditions with and without air throttling. A schematic of the combustor section is also illustrated on the top of the figure to show the corresponding distance from the fuel injectors where the cross-sectional mixing parameters are measured. Compared to baseline flow, a substantial increase in fuel-air mixing efficiency occurs downstream of the injectors in the combustor with the presence of air throttling. The mixing has been slightly enhanced though the separated boundary layer upstream of the cavity. Significant increase of the mixing occurs over the cavity as seen in the Fig. 4-19, it is because the low-momentum flow zone inside the cavity has been increased in terms of the shear layer stream lift if the air throttling is present. More ethylene fuel has been entrained into the cavity and mixed with air in a longer residence time. Downstream of the cavity, the enhanced mixing is primarily due to the stronger flow distortion and increased residence time along the boundary layers on the side walls.
The enhancement effects on the fuel-air mixing by means of the air throttling are clearly illustrated in terms of the mixing efficiency and mixing effectiveness.

Fig. 4-24: Comparison of fuel-air mixing effectiveness in the combustor section for steady state non-reacting flow with and without air throttling (\(\dot{m}_{\text{throttle}} = 20\% \dot{m}_{\text{air}}\)).
4.4 Summary

A comprehensive theoretical and numerical framework has been established to study the influence of the air throttling on the fuel-air mixing characteristics of a supersonic combustor employing an aerodynamic ramp fuel injector and a cavity flameholder. The analysis treated the complete conservation equations in three dimensions and accommodates finite-rate chemical kinetics and variable thermophysical properties for a multi-component chemically reactive system. Turbulence closure was achieved by means of Menter’s shear-stress transport (SST) model calibrated for high-speed compressible flows. The predicted wall static pressure of the non-reacting flow was validated by engine test data. The influence of the air throttling on the fuel distribution in the combustor and cavity regions was investigated in detail. For the start-up stage, represented by the baseline case in present work, fuel injection flow has transported the fuel ‘fairly’ effectively into the cavity. As the air throttling was established to increase the combustor pressure, a series of resultant extensive oblique shock waves was generated at the entrance of the combustor. The shock waves separated the side wall boundary layer to modify the fuel entrainment into the cavity, and to cause a dramatic enhancement in the fuel-air mixing. The enhanced mixing resulted primarily from elevated vorticity over the combustor, as well as from increased residence time.
Chapter 5
Ignition and Flame Development

5.1 Problem Description

The experimental studies have been conducted to explore the impact of air throttling on ignition transient processes in the AFRL Scramjet engine facility, where a series of ignition experiments were conducted under various flight conditions and fuel equivalence ratios. During the facility tests, air throttling was implemented to explore the ignition enhancement. Based on the current operations, air throttle flows are required to be no more than 20 percents of main intake air flow rate. Primary numerical studies have been performed in the Chapter 4 at non-reacting flow conditions that closely matched those used in experimental tests of a similar combustor configuration in AFRL. The initial calculations include the steady baseline cold flow, and the steady baseline cold flow with gaseous ethylene injection at an overall equivalence ratio 0.6. The sequent transient study of cold flow with air throttling activated at an experiment-consistent mass flow rate of 20 percent of inlet air flow rate once the stable fuel flow is established. Following these pretest studies, the present chapter investigates the detailed ignition transient and flame dynamics, and the positive influence on ignition and flameholding by air throttling.

The theoretical and numerical framework was employed to study the unsteady reacting flow in the scramjet combustor facility shown schematically in Fig. 4-1. The
present chapter reproduces two different ignition and combustion modes consistent with the experiment configurations, in which the reacting flow development has demonstrated the ignition enhancement effect by implementing air throttling. In the present chapter, results from reacting flow calculations for both chosen representative ignition and combustion flow cases are discussed and compared. Both the cases were run for 10~15 ms starting from the initial condition, which is enough for a supersonic flow stabilization and ignition process, but is less than the typical test time of the ground based experiments (10~20 s), which is usually determined by the device operation time.

5.2 Combustion Blown-off in Baseline Reacting Flow

5.2.1 History of Combustion

Calculations were first conducted for the baseline flow case in the absence of air throttling implementation. The chemistry is initiated after a stable fuel flow field has been established in the previous non-reacting flow study. Typical flow conditions at the isolator entrance are listed in Table. 5-1. The table describes inlet flow velocity, static inlet pressure, static inlet temperature, and fuel equivalence ratio. The inlet condition corresponds to a flight Mach number $M_f = 5$, and the estimated residence time of air in the engine facility is about 1.7 ms.

| Tab. 5-1: Flow conditions and air throttling parameter for the test flow |
|-----------------|-------|-------|-------|-------|-------|-------|
| Case | $M_{in}$ | $U_{in}$ | $p_{in}$ | $T_{in}$ | $\phi$ | $\dot{m}_{air}$ | $\dot{m}_{throttle}$ |
| 1    | 2.2   | 1045   | 0.328  | 560    | 0.6   | 0.757          | 0.0                 |
| 2    | 2.2   | 1045   | 0.328  | 560    | 0.6   | 0.757          | 0.151               |
Figures 5-1 shows the spreading of flame in the modeled combustor, with the flame position illustrated in terms of iso-surfaces of temperature between $T = 2400 \sim 2800$ K. A hot-spot igniter at the cavity ceiling is activated to initiate combustion from beginning of simulation. Fig. 5-1a indicates that ignition of the fuel-air mixture occurs at 1.180 ms near the igniter, as the iso-surfaces of temperature outline the region of hot combustion products. The flame propagates to the cavity ramp in a short time ($t = 1.487$ ms), as seen in Fig. 5-1b. Fig. 5-1c and Fig. 5-2d show the expansion of the flame out of the tailing edge of the cavity downstream by the time $t = 1.941$ ms. It is believed that this flame extension and propagation are strongly facilitated by the flow convection in the boundary layer. In addition, the extensive expansion of the combustion is largely confined in the premixed flame propagation in the near-wall low-momentum region. The reacting flow only lasts a very short time after the flame takes into shape over the cavity, as shown at $t = 3.563$ ms in Fig. 5-2e. The high-speed main stream blows off most of newborn flame attached on the cavity and wall surface downstream of it, only a small portion of the flame is anchored in the cavity, and gradually disappears as the initial premixed fuel-air mixture is consumed up inside the cavity. At the end of the calculation ($t = 12.550$ ms) as shown in Fig. 5-2f, the flame has almost completely disappeared in the cavity. Given this picture, the ignition of modeled engine fails under the test flight condition as the reacting flow can not be anchored in the combustor.
Fig. 5-1: Evolution of the temperature field in the cavity region during the ignition transient without air throttling.
Fig. 5-2: Evolution of the temperature field in the cavity region during the ignition transient without air throttling.
5.2.2 Ignition Transient and Flameholding Study

The failures of ignition and flameholding of the fuel-air mixture in the modeled combustor arise from the so-called flame uncoupling on the combustor cowl surface, while the details of the failures in ignition and flameholding are explored in present section. Calculated static wall pressure $p_w$ and flow Mach number distributions along the centre line of the main stream at $t = 3.563$ ms are presented Figure 5-3, with the corresponding facility flowpath drawn on the top. The heat release from the combustion clearly raises the static wall pressure to a value of 0.7 atm at the cavity rear ramp, inducing a drop of the mean flow Mach number to a value of 1.72. The spatial variation of reacting flow field can be demonstrated in terms of the axial flow velocity and temperature distributions, as the axial contours shown in Figure 5. The top and bottom images present the cross-section contours of axial flow velocity and temperature, respectively. At right downstream of the fuel injection, the mean stream speed is about 1000 m/s. The flow velocity decreases a half to about 500 m/s through the boundary layer, with a corresponding flow temperature at about 800 K. Therefore the flame anchored at the cavity can hardly propagate upstream to the injectors along the boundary layer. As the strip region in the cavity across which the axial velocity changes from 100 m/s to above 400 m/s is approximately recognized as the shear layer over the cavity, this region is filled with reacting gases mixture as shown in the temperature contours. The combustion is confined in the small plumes near the body surface and essentially ends somewhere downstream of the cavity.
Figure 5-4 reveals that the combustion can only survive in the low-momentum flow field as the high-speed flow produces poor residence time and easily blows off the flame. As a result, the ignition in the fuel-air mixture within the boundary layer near the cowl surface fails, because of the local high flow momentum and low temperature. Neither the cavity-anchored flame can spread downward through the supersonic main stream, nor the autoignition initiated by the low flow temperature less than 800 K.

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**Fig. 5-3:** Comparisons of measured and calculated wall static pressure $p_w$ and Mach number distribution at $t = 3.563$ ms.
Figure 5-5 presents the corresponding fuel concentration distributions in terms of iso-surfaces of ethylene fuel equivalence ratio distributions in the combustor. Semi-transparent iso-surfaces are colored at the corresponding equivalence ratio scales of 0.1, 0.3 and 1.0 so that the images are biased to regions of locally significant fuel distribution. The three-dimensional perspective image clearly shows the penetrations of the inclined fuel injection into the cross flow, as well as the fuel entrainment into the cavity during the combustion. The premixed ethylene fuel-air mixture in the cavity region apparently has been rapidly consumed, as the local fuel equivalence ratio drops under 0.1, and the
reaction of the lean fuel-air mixture is hardly able to sustain. The calculation reveals that the capability of air entrainment of the cavity and the resultant poor fuel supplying to the reaction could be one of the reasons for the failure of the flameholding at the cavity.

Further exploration into the combustion flow field in the modeled combustor provides the insight to the imbalance between the entrainment of the fuel-air mixture into the cavity and the reaction consumption. Figure 5-6 extracts the corresponding shadowgraph images of the flow field at spinwise locations of $z/W = 1/8$ and $1/2$, respectively. The top plane includes one of the I-2 injectors near the sidewall, while the bottom one splits the flowpath at middle. The shadowgraph images clearly demonstrate the flame and shock waves in terms of density gradient, the former is anchored over the cavity, and the latter are attached along the shear layer. As pointed out in Fig. 5-3, the
pressure at the cavity rises to 0.7 atm from the heat release of the combustion gas, whereas the subsequent boundary separation is not intensely enhanced by the back pressure rise, and the consequently combustion-induced upstream shock train has not formed. The corresponding vorticity magnitude distributions shown in Fig. 5-7 have indicated that the inactivated shock/boundary layer interactions on the sidewalls only slightly enhance the generation of the streamwise vorticity into downstream convection, and therefore is responsible to the fragile mass exchange into the cavity during the combustion, as vorticity is well recognized to have a significant influence on the mixing rate and thus on the burning process in turbulent flow.
Fig. 5-6: Shadowgraph in the combustor section at $t = 3.563$ ms during the ignition transient without air throttling.

Fig. 5-7: Vorticity in the combustor section at $t = 3.563$ ms during the ignition transient without air throttling.
5.3 Ignition and Flameholding in Presence of Air Throttling

5.3.1 History of Combustion

Calculations are then conducted for the ignition in the modeled combustor, based on the simulated stable ethylene injection and air throttling flow field established previously, in which the inlet conditions and air throttling mass flow rate are provided in Tab. 5-1. The ignition of the premixed ethylene/air mixture in the cavity is initiated at the beginning of the calculation by a hot-spot igniter at the cavity ceiling. Figure 5-8 shows the ignition transient and combustion development in the combustor, where isosurfaces of temperature at $T = 2400 \sim 2800$ K illustrate the flame position. As a stable air throttling has been introduced at axial location $x = 1.36$ m downstream of the cavity on the body surface of the combustor, a hot-spot igniter is activated to initiate the combustion of the fuel-air mixture in the cavity at the time 0.0 ms. Fig. 5-8a indicates that combustion first occurs surrounding the hot-spot igniter at $t = 1.121$ ms, as the isosurfaces of temperature outline the region of flame. The initiated flame spreads out of the cavity rear ramp in a short time ($t = 1.501$ ms), as seen in Fig. 5-8b. The flame propagation to downstream is largely dominated by the streamwise flow convection near the wall. Fig. 5-8c shows that the flame front reaches the air throttle slits at time $t = 1.930$ ms under a velocity of about 300 m/s through the boundary layer. Benefited from the significant reduction of boundary velocity, the reacting flow could spread upstream cross the cavity to reach and sustained at the fuel injection on the body surface. In Figure 5-9 the observing angle is lifted to describe the spontaneous ignition and combustion development of the fuel-air mixture on the cowl-side wall in the combustor.
Fig. 5-9a presents that the reacting flow begins as individual flame plumes near the fuel injectors on the body-side wall, and interacts and merges with each other together over the cavity region. Noticeable reacting gases spread into the corner regions, meanwhile on the cowl-side wall, ignition of the fuel-air mixture flow is first initiated near the corner at $t = 2.126$ ms. The flame propagates upstream and downstream along the fuel-air mixture flow within the low-momentum boundary layer, as Fig. 5-9b shows that another sequential ignition at the center region occurs following the spatial flame spreading downstream at $t = 3.015$ ms. Fig. 5-9c demonstrates that the established reacting flow at the end of the calculation ($t = 9.595$ ms). At an early moment the air throttle is turned off right after the flame is anchored near the ethylene injectors on the cowl-side wall, allowing the reacting flow to fully develop through the combustor nozzle. Stable combustion is sustained successfully in the modeled combustor at the time.
Fig. 5-8: Evolution of the temperature field in the cavity region during the ignition transient on the body-side wall with air throttling ($\dot{m}_{\text{throttle}} = 20\% \dot{m}_{\text{av}}$).
Fig. 5-9: Evolution of the temperature field in the cavity region during the ignition transient on the body-side wall with air throttling ($\dot{m}_{\text{throttle}} = 20\% \dot{m}_{\text{air}}$).
5.3.2 Pre-combustion Shock Train Formation

5.3.2.1 Flow Structure Evolution

It is important and essential to provide an insight into the details of the throttling-induced accommodation to the reacting flow field and the subsequent influences on the ignition enhancement and flameholding in the modeled combustor. Figure 5-10 presents the ignition transient and the time evolution of the flow structures in the combustor in terms of the shadowgraph images. The fuel-air mixture in the cavity is ignited by the hot-spot igniter at 1.121 ms later after its activation, and the initiated flame is clearly illustrated by the shadowgraph image on the x-y plane (z/W = 3/8), as shown in Fig. 5-10a. The reacting flow arises rapidly and develops over the cavity in the combustor in a short time, as the shadowgraph image in Fig. 5-10b shows the flame is anchored at the cavity and spreads downstream along the low-momentum shear flow and boundary layer. Heat release of the combustion induces local pressure rise and the resultant boundary layer separation forms upstream oblique shock waves spontaneously. Fig. 5-10c presents that at time 4.511 ms, the fuel-air mixture on the cowl surface has been ignited, and the reacting flow starts to develop intensively in the modeled combustor. As a result of the combustor pressure rise, the flow separation moves to upstream, subsequently the shock waves are pushed into the constant cross-sectional area isolator. The backpressure drives the shock waves extensively into the isolator at time t = 5.963 ms, when the air throttling is turned off as the reacting flow has been sustained in the combustor as seen in Fig. 5-
Fig. 5-10e presents that a fully developed reacting flow is sustained in the combustor at $t = 9.557$ ms. A steady pre-combustion shock train is established in the flow field in the constant cross-section area isolator.

**Fig. 5-10:** Evolution of the shadowgraph during the ignition transient with air throttle on ($\dot{m}_{\text{throttle}} = 20\% \dot{m}_{\text{air}}$).
5.3.2.2 Formation of Pre-combustion Shock Train

The primitive form of the pre-combustion shock train is shaped in the isolator and is demonstrated by the flow field at $t = 4.811$ ms. Corresponding shadowgraph image, flow static temperature, axial velocity and vorticity magnitude are presented respectively as following. Figure 5-11 extracts the combustor flow field in shadowgraph images ($z/W = 1/8, 1/2$). The top image indicates that upstream of the cavity, the boundary layer separation in the corner is significantly enhanced by the adverse pressure gradient. Although the separation zone is clearly anchored in the isolator corner, wedging into the air flow at the axial location $x = 0.91$ m, its spinwise extension is compressed by the mean flow near the centre region as seen in bottom image, where the shock/boundary layer interaction dominates the flow field and produces extensive oblique shock waves in the isolator.

The corresponding flow static temperature, axial velocity and vorticity magnitude distributions near the corner have offered more insight into the pre-combustion shock train formation and the subsequent influence to the ignition transient, as shown in Figure 5-12. The top image of the temperature contours illustrates the reacting flows has been anchored on both body- and cowl-side walls at time 4.811 ms. The combustion-induced back pressure rise causes the upstream boundary layer separations on the sidewalls, as demonstrated in terms of the reversed axial velocity gradient in the middle image. The bottom image shows that the enhanced upstream boundary layer separations generate the extensive vorticity and radical vortices into the combustor.
The significant boundary layer separations at the corners eventually lead to the primitive formation of the pre-combustion shock train waves in the main flow of the isolator. Away from the corners, shock/boundary layer interactions become more extensive in the center region. The top image of Figure 5-13 presents the flames are anchored at the cavity and cowl surface in terms of the temperature contours on the center plane. The middle image of the axial velocity contours shows that axial velocity gradient is clearly reversed where the shock wave attaches the boundary layer, due to the combustor pressure rise from the heat release. The shock/boundary layer interactions then generate large amounts of streamwise vorticity and disturbance to downstream as shown in the bottom image, resulting in the higher mixing rate of fuel-air mixture and then enhancing the combustion.

Figure 5-14 presents the distributions of corresponding static wall pressure $p_w$ and flow Mach number along the centre line of the mean stream at $t = 4.811$ ms, the corresponding entire facility flowpath is demonstrated at the top of the figure. The presence of the combustion of the fuel-air mixture flow on the cowl surface remarkably increases the heat release in the combustor, resulting in a pressure rise to about 0.9 atm at the cavity, and a reduction of the mean flow speed is to Mach 1.4. Compared with the pressure rise during the ignition transient of the baseline reacting flow in the absence of air throttling, the calculation results clearly illustrate that the coupled reacting flows in the combustor have made significant contributions to the pressure rise and momentum reduction of the mean flow through the cavity, and then further extend the residence time of the fuel-air mixture in the modeled combustor.
Fig. 5-11: Shadowgraph in the combustor section at $t = 4.811$ ms during the ignition transient.

Fig. 5-12: Temperature, velocity and vorticity magnitude contours near to combustor sidewalls at $t = 4.811$ ms during the ignition transient.
Fig. 5-13: Temperature, velocity and vorticity magnitude contours at combustor center at $t = 4.811$ ms during the ignition transient.

Fig. 5-14: Calculated wall static pressure $p_{w}$ at $t = 4.811$ ms for reacting flows.
5.3.2.3 Pre-Combustion Shock Train in Stable Flow Field

The air throttling as an efficient ignition enhancement aid is turned off immediately once the stable reacting flow has been established in the combustor. Figure 5-15 extracts the combustor flow field in shadowgraph images (z/W = 1/8, 1/2). At the end of calculation at time t = 9.557 ms, a steady reacting flow is sustained in the modeled combustor, upstream of which a pre-combustion shock train is well established in the isolator as shown in Fig. 5-15. In the isolator, a sequence of oblique shock waves in line forms the pre-combustion shock train, accompanied with the extensive interactions between the shock waves and the boundary layers. The subsequent deceleration of supersonic mean flow through the shock train is demonstrated by the corresponding axial velocity contours present in Figure 5-16. In addition to the momentum reduction of the mean flow, the shock/boundary interactions extensively separate the flow boundary layer at the foot of the shock. The pre-combustion shock train and its interactions with the boundary layer extensively distort the flow field in downstream and then considerably influence the fuel-air mixing. As shown in the corresponding vorticity magnitude distributions in Figure 5-17, the vorticity downstream of the pre-combustion shock train is largely enhanced and then migrates into the mean flow. The shock/boundary interactions induce more vertical structures to convect into the combustor, significantly increasing the vorticity field in it. The instability also affects the free shear layer over the cavity, causing more flow unsteadiness and consequent enhancement of the fuel-air mixing.
Fig. 5-15: Shadowgraph view of pre-combustion shock train in isolator in stable combustion ($\dot{m}_{\text{throttle}} = 20\% \dot{m}_{\text{air}}$).

Fig. 5-16: Axial velocity distributions in isolator in stable combustion ($\dot{m}_{\text{throttle}} = 20\% \dot{m}_{\text{air}}$).
The calculation results clearly indicate that the shock train forms in a sequence of oblique shock waves, as Lin et al. (1991) reported that the normal shock sequence becomes an oblique shock train under high flow Mach number (>1.6) and significant shock/boundary interactions, therefore the point of bifurcation of the shock moves away from the wall and reaches the centerline of the duct to form an oblique shock. The shadowgraph images in Fig. 5-15 capture the sequence of shock waves in the shock train, along which the space between two successive shocks decreases. Lin et al. (1991) pointed out that as the flow Mach number increases, the number of shock waves, the space between two consecutive shocks, and the length of shock train increase. The location and structure of the pre-combustion shock train are mainly influenced by the flow conditions and the shock/boundary layer interaction, and in turn, the pre-combustion shock train can largely affect the flow properties entering the combustor module for fuel-air mixing and the operability of a scramjet engine. The pressure profiles and lengths of pre-combustion shock trains have been studied by various researchers using constant-area...
ducts with rectangular and round configurations. Waltrup and Billig (1973) first developed a correlation for the length of the shock train using axisymmetric ducts with downstream flow throttling to generate shock trains. In their study, boundary layer momentum thickness and flow Mach number just before the shock train are identified as the dominant parameters and are utilized to develop the following correlation:

\[
\frac{x\left(M_1^2 - 1\right) \text{Re}_{\theta}^{1/5}}{H^{1/2} \theta^{1/2}} = 50 \left(\frac{p_f}{p_a} - 1\right) + 170 \left(\frac{p_f}{p_a} - 1\right)^2
\]

(107)

where \(x\) is the distance downstream from the beginning of the pressure rise, \(M_1\) is the Mach number of approach flow, \(\theta\) is the boundary layer momentum thickness for undisturbed flow, \(H\) is the duct height, \(\text{Re}_{\theta}\) is the Reynolds number based on boundary layer momentum thickness, and \(p_f/p_a\) is the ratio of the local wall pressure to the static pressure at the beginning of the pressure rise.

The present work compares the measured length of the computed static wall pressure rise with the pressure distributions predicted by Eq. (107) mentioned above. The data parameters are taken into considerations in the condition of the Mach number \(M_1\) and boundary layer momentum thickness \(\theta\) just upstream of the pre-combustion shock train as 1.9 and 9 mm, respectively, and the duct height \(H\) as 38 cm. The Reynolds number based upon boundary layer momentum thickness is calculated by the parameters mentioned above as \(\text{Re}_{\theta} = 8750\). The local wall pressure after the pressure rise \(p_f\) and at the beginning of the pressure rise \(p_a\) are 1.4 atm and 0.4 atm, respectively. The computation result indicates a reasonable agreement with the prediction from Eq. (107), that the measured length of the computed static wall pressure rise is 32 cm, while
predicted value by Eq. (107) is 27.5 cm. The difference of the prediction for the length of the shock train may be resulted from the insufficient vertical and axial grid resolutions near the centre region in the isolator section. The simulations might be explained as the failure to capture small subsonic flow following the centre portion of the shock waves, the over-prediction of the space between the shocks and the length of the shock train. Nevertheless, the calculation predicts well the global structure of the pre-combustion shock train in the isolator.

5.3.3 Flame Coupling and Autoignition

The experimental exploration on the ignition and flame holding in the modeled engine combustor is conducted by Lin, et al. (2006). In their experiments, the fuel-air mixture along the body-side wall is ignited first inside the cavity. The combustion of the fuel-air mixture occurs subsequently on the cowl-side wall. Unfortunately the cause of the latter remains unclear. The mechanism of the ignition on both the body- and the cowl-side walls in the combustor, is called flame coupling, which refers to the situation where the top wall combustion significantly influences the motion of the bottom wall combustion and vice versa. Lin’s study demonstrates that the flame coupling plays an important role in the engine ignition and start. Experimental engine tests show that the ignition on the cowl-side wall strongly depends on the flight conditions and throttling parameters. The present work comprehensively explores the flame coupling in the engine start by the numerical approach of ignition and combustion dynamics.
5.3.3.1 Autoignition near Cowl-Side Wall

The flame structures in the modeled combustor capture the autoignition of the fuel-air mixture on the cowl surface at time \( t = 2.098 \) ms, as shown in Figure 5-18. The flame is established at the cavity and spreads into the combustor, as the temperature contours outline. As the pressure rise in the cavity enhances the vertical flow convection and pushes the combustion production gas down to the combustor cowl surface, a resultant hot gas zone then forms along the sidewall and is anchored at the corners, near which autoignition of the fuel-air mixture occurs at an axial location \( x = 1.14 \) m downstream of the injectors. The flame of reacting gases is confined to a region just behind an oblique shock wave, which meets the boundary layer and raises the pressure and temperature, as evidenced in Fig. 5-10.

The corresponding cross-sectional temperature and velocity contours at an axial location \( x = 1.14 \) m in the combustor provide an insight to the autoignition process, as shown in Fig. 5-19. The top image presents the temperature contours of the reacting flow field. On the body-side, the flame plumes expand and merge together to a certain extent in the total duct area. However the mean flow region is still dominated by the cold air, as the flow temperature at the center cone region is as low as 700 K. Since the corresponding flow speed reaches 900 m/s as shown in the middle image of axial velocity contours, the reacting flow on the body surface can hardly spread over the center cone region down to the cowl surface, without being blown off by the high-speed main flow. The bottom image shows the corresponding low-momentum flow recirculation at corner regions in terms of the velocity vector, indicating the significant fuel-air mixture
entrainment to the corner for the flame expansion and sustaining in these regions. The autoignition is the mechanism most likely to cause the autoignition in the low-momentum region on the cowl-side wall, as the hot gas zone at the corners and sidewalls has the temperature over 1100 K, which can initiate autoignition of the fuel-air mixture on the cowl surface. In addition, the presented axial velocity contours show that the flow momentum is significantly reduced at the corners and sidewalls, with the typical axial velocity no more than 350 m/s, and the corresponding Mach number below 0.7. The resultant enlarged residence time of the fuel-air mixture and the higher temperature can help the flame surviving from being blown off by the main flow.

Fig. 5-18: Snapshot of the temperature field during the ignition transient with air throttle on ($m_{throttle} = 20\% \dot{m}_{air}$).
Fig. 5-19: Vertical images of the temperature, velocity and Mach number contours in the combustor section at $t = 2.098$ ms during the ignition transient with air throttling on ($m_{throttle} = 20\% m_{air}$).
5.3.3.2 Flame Propagation in Combustor

Figure 5-20 shows snapshots of the temperature field in the modeled combustor at time $t = 3.015$ ms. As the autoignited flame on the cowl surface propagates downstream and spreads laterally, the flame reaches and ignites the center fuel jet flow near the axial location $x = 1.20$ m in the combustor. The detailed explorations are conducted by means of the corresponding cross-sectional temperature and axial velocity contours as shown in Figure 5-21. The top image presents the reacting flow into separate combustion zones as demonstrated by the high temperature product gases regions ($T > 2400$K). The upper combustion zone is anchored at the cavity and body-side wall, as reacting flow sustains in the extensive recirculation zone in the cavity as well as in the low-momentum flow regions near wall surface and the corners ($U < 200$ m/s), as shown in the bottom image in Fig. 5-21. Intense combustion also occurs along the fuel-air mixture flow near the cowl-side wall. Flame plumes outline the reacting flow self-ignited upstream and induce the subsequent ignition of the fuel-air mixture along the center line.
Fig. 5-20: Snapshot of the ignition temperature field during the ignition transient with air throttle on ($\dot{m}_{\text{throttle}} = 20\% \dot{m}_{\text{air}}$).

Fig. 5-21: Vertical images of the temperature and axial velocity contours in the combustor section at $t = 3.015$ ms during the ignition transient with air throttling on ($\dot{m}_{\text{throttle}} = 20\% \dot{m}_{\text{air}}$).
5.4 Stable Reacting Flow

5.4.1 Comparison of Calculated Wall Pressure Distribution and Experimental Data

The ignition is successfully initiated in the fuel-air mixture flows near both body- and cowl-side walls in the presence of the air throttling. Robust combustion is sustained in the modeled combustor after the air throttling is turned down, and the reacting flow becomes steady at the end of the calculation ($t = 9.595$ ms). Calculated static wall pressure distribution $p_w$ is present in Fig. 5-22, as well as experimental measurement along the entire facility flow path. In isolator the wall static pressure prediction is in well consistency with the experimental data, as the substantial pressure rise through the pre-combustion shock train is clearly captured by the present calculation and agrees well with the measured pressure profile. The predicted pressure rise in the present calculation is under-estimated over the cavity where peak pressure from the heat release of the combustion is found to be about 0.1 atm lower than the measurement. The present numerical framework employs the simplified two-step finite-rate chemistry model on account of the availability of EBU model to predict the reaction rate of the ethylene combustion in the turbulent flow. The chemistry model apparently has an under-estimated reaction rate in the combustion flow field, which results in less heat release than the experiments. More detailed chemistry kinetics and an advanced turbulence-combustion model would improve the prediction in the future study. The pressure profile downstream in the combustor reasonably matches with the measurement as the exhaust
reacting flow is chemically frozen. The location of the shock train and the overall trend of pressure rise by the present calculation agree with the experimental data consistently.

5.4.2 Flame Structure under Stable Reacting Flow

Figure 5-23 presents the corresponding flame structure in the steady reacting flow field in terms of the temperature contours. The fully developed reacting flow includes two major combustion zones. First intensive combustion zone is attached on the cavity flameholder and the body surface, as the reacting flow sustains in the extensive recirculation zone in the cavity as well as in the low-momentum flow regions near wall surface and the corners. Second combustion zone is located on the lower cowl surface. The upstream shock train and the intensive combustion distinctly raise the flow pressure and temperature in the combustor, and largely reduce the local flow speed thus the unburned fuel-air mixture gains longer residence time to mix and react in the combustor.

Fig. 5-22: Comparison of measured and calculated wall static pressure $p_w$ for reacting flows.
Figure 5-24 presents the temperature distributions in the modeled combustor. The image presents the anchored flame on the body and cowl surfaces. The recessed cavity acts as a main flameholder while the combustion is established within the cavity in the presence of a steady pre-combustion shock train in the isolator, since the heat release from the combustion forces the shock train to sustain in the isolator, the shock train in return increases the downstream flow temperature and residence time of the fuel-air mixture into the combustor entrance, and as a result, to enhance the flameholding robustness in the combustor.

Figure 5-25 investigates the flameholding characteristics of the modeled combustor in terms of shadowgraph image and corresponding vorticity magnitude contours in the combustor, respectively. Fig. 5-25a illustrates the contribution of the pre-combustion shock train to the reacting flow field in the combustor. The shock waves interact with the boundary layer to induce the pressure oscillation waves, and thus the new vertical structures form and convect downstream with a large amount of fluctuation of velocity into the combustor. Meanwhile, the shear flow subsequently flows into the
cavity and rapidly rolls up into large-scale vortices. The resultant vorticity field enhancement cross the cavity is presented in the Fig. 5-25b. The cavity introduces disturbances into the vortices to generate small-scale turbulent eddies and to enhance their activities, as the initial vortex size is usually determined by the cavity size (height and width). While the separated boundary layer lifts the shear layer above the cavity enclosure, the resultant larger cavity height and flow recirculation contribute to the generation of the larger-scale vortices, and thus enhance the turbulence activity. Therefore the mixing of fuel-air flow is distinctly enhanced due to the increased area contact between low- and high-momentum flow streams.

The pre-combustion shock train significantly separates the boundary flows near the sidewalls and the corners. Recirculation zones are then generated and further enhanced by the shock/boundary layer interactions, which turn out to be the instinctive aids in anchoring the flame as additional flameholding support, with the recessed cavity as the primary source of flameholding support. The pronounced influence of this corner distortion on mixing can be clearly seen.
Fig. 5-24: Temperature distribution in the x-y plane (z/W = 3/8) in the cavity section at $t = 9.557$ ms in stable combustion.

Fig. 5-25: Shadowgraph and vorticity magnitude images in the x-y plane (z/W = 3/8) in the cavity section at $t = 9.557$ ms in stable combustion.
The perspective ethylene fuel concentration in the combustor is demonstrated in terms of iso-surfaces in Figure 5-26. At downstream of the pre-combustion shock train, a large amount of vortices is induced by the significantly enhanced shock/boundary layer interactions near the isolator sidewalls. As a result, the radically inward/outward airflow to the flame is strongly enhanced as well as the turbulence activity within the vortices. Therefore the entrainment and the mixing of the fuel-air mixture are significantly enhanced in the cavity. In addition of the cavity, the reacting flow is able to be anchored near the corners and sidewalls in the combustor. This secondary flameholding source has the contributions from the improved fuel-air mixing and contribution from the extensive combustion in the combustor.

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Fig. 5-26: Perspective ethylene fuel concentration under the stable combustion condition
5.5 Summary

A comprehensive theoretical and numerical framework has been employed to investigate the ignition transient and flameholding in an ethylene-fueled scramjet combustor employing an aerodynamic ramp fuel injector and a cavity flameholder. Various processes involved in the ignition transient and flame development were studied in detail under flow conditions with and without air throttling. A reacting flow of flame coupling in the modeled combustor facility, which was previously proposed by the co-authors (Lin et al. 2006), was validated by the present simulations. Ignition and combustion were achieved in the calculation under the Mach 5 flight condition by means of air throttling implementation at downstream of the combustor, where the air throttle was required as an external ignition aid. The predicted flow wall static pressure distribution agreed well experimental measurement.

The time history of the baseline reacting flow showed that the modeled engine could hardly start under the test flight Mach 5 condition. The results indicated that the fuel-air mixture flow on the cowl-side wall could be neither ignited by the body-side anchored flame nor self-initiated. On the other hand, the initiated combustion in the cavity apparently failed to provide sufficient heat release to generate and sustain strong shock waves upstream, thus residence time of fuel-air mixture in the boundary layer is severe for the ignition and flameholding in the combustor. Therefore in the absence of the cowl-side fuel combustion, the reacting flow was easily detached from the cavity.
when the most of the premixed fuel-air mixture inside the cavity has been consumed, and finally blown off by the main flow.

Ignition and modeled engine start are achieved in the presence of air throttling downstream of the combustor. As an external ignition aid, the air throttle is implemented to accommodate the upstream high-speed flow field. The resultant decrease in the flow velocity and increases in the temperature and pressure in the combustor can effectively enhance the ignition characteristics and flame stabilization near the cowl-side wall. The calculation results show that the autoignition of the fuel-air mixture takes advantage of the hot zone at corners to occur on the cowl surface and form an intense combustion flow. Furthermore, ignition and combustion produce a pre-combustion shock train, resulting in significant low-momentum/separated flow near the sidewalls and corners. These regions turn become an additional source for flameholding with the recessed cavity as a primary flameholding support. The predicted combustor performance and flow distributions agree well experimental measurements.
Chapter 6
Conclusions and Future Work

6.1 Conclusions

The present work has addressed a wide variety of basic and practical issues related to the modeling and analysis of non-reacting and reacting flows in a supersonic combustion ramjet (Scramjet) engine. The comprehensive investigation was conducted into the ignition transient mechanisms and flame-coupling response in a scramjet engine by means of air throttling, on which very little has been studied numerically to date. This investigation focused on the numerical study of ignition transient and combustion dynamics in the modeled combustor. The analysis treated the complete conservation equations in three dimensions and accommodates finite-rate chemical kinetics and variable thermophysical properties for a multi-component chemically reactive system. Turbulence closure was achieved by means of Menter’s shear-stress transport (SST) model calibrated for high-speed compressible flows.

The influence of the air throttling on the fuel distribution in the combustor and cavity regions was studied comprehensively. The air throttling mimicked a stagnation point to cause intensive flow recompression and boundary separation upstream. The subsequent back pressure rise effectively lifted the shear layer from the cavity, resulting in the compression waves and the momentum decrease in the main flow.
The flow compression and diffusion caused by the throttling air certainly reduced the surrounding air flow Mach number, and reversed axial velocity gradient to induce the upstream boundary layer separation. The recirculation air flow in separation zone had low Mach numbers below 0.2, resulting a longer residence time for a better mixing performance. Meanwhile, the low-momentum boundary separation zone expanded to corners by means of sidewall effects, and became an important reason of mixing enhancement of the fuel-air mixture. The fuel entrainment into the cavity has also been largely enhanced because of the intense interaction between the throttle-induced shock waves and the shear layer over the cavity, which significantly enhanced the flow distortion and turbulence diffusion, and then induced stronger fuel-air mass exchange into the cavity.

The calculation revealed that the streamwise vorticity distribution in the modeled combustor was significantly higher in the presence of air throttling, which was triggered by two major factors. On one hand, the vorticity in the cavity is remarkably enhanced due to the enhanced flow distortion and turbulence diffusion. On the other hand, the shock/boundary layer interaction and induced flow separations introduced more vorticity downstream in the wall shear flow.

The quantitative evaluations of the fuel-air mixing processes were investigated in terms of two measures of mixing, mixing efficiency $\eta_m$ and mixing effectiveness $\varepsilon_m$. Substantial increase in fuel-air mixing efficiency (more than 30%) occurred over the cavity and downstream in the combustor in the presence of air throttling. The mixing efficiency was enhanced by the stronger flow distortion and turbulence diffusion through the separated boundary layer and the low-momentum flow inside the cavity. The
enhanced mixing effectiveness is primarily caused by improved ethylene fuel entrainment into the cavity and increased residence time along the boundary layers.

The comprehensive analysis was further extended to study influence of the air throttling implementation on the ignition and flameholding in the modeled combustor at the Mach 5 flight condition. The time history of the baseline reacting flow showed that the modeled engine could hardly start under the test flight Mach 5 condition. The results indicated that the initiated combustion in the cavity apparently failed to provide sufficient heat release to generate and sustain strong shock waves upstream, thus residence time and temperature of fuel-air mixture in the boundary layer was severe for the ignition of the fuel-air mixture flow on the cowl-side wall in the combustor. Therefore in the absence of the cowl-side fuel combustion, the reacting flow was easily detached from the cavity when the most of the premixed fuel-air mixture inside the cavity has been consumed, and finally blown off by the main flow.

Ignition and modeled engine start are achieved in the presence of air throttling downstream of the combustor. As an external ignition aid, the air throttle is implemented to accommodate the upstream high-speed flow field. The resultant decrease in the flow velocity and increases in the temperature and pressure in the combustor could effectively enhance the ignition characteristics and flame stabilization near the cowl-side wall. The subsequent autoignition of the fuel-air mixture on the cowl surface took advantage of the hot zone at corners to occur and initiated intense combustion flows.

Combustion produced a pre-combustion shock train in the isolator. The prediction of the length of the shock train indicated a reasonable agreement (about 16% higher) with the correlation developed by Waltrup and Billig (1973). The difference of the prediction
for the length of the shock train may result from the insufficient vertical and axial grid resolutions near the centre region in the isolator section. The simulations might be explained as the failure to capture small subsonic flow following the centre portion of the shock waves, the over-prediction of the space between the shocks and the length of the shock train. Nevertheless, the calculation predicts well the global structure of the pre-combustion shock train in the isolator.

The pre-combustion shock train induced significant low-momentum/separated flow downstream near the sidewalls and corners. Recirculation zones were then generated and further enhanced by the shock/boundary layer interactions, which turn out to be the instinctive aids in anchoring the flame at the corners as additional flameholding support, due to the pronounced influence of the corner distortion on mixing. The predicted combustor performance and flow distributions agree well experimental measurements.

6.2 Recommendation for Future Work

Turbulent Effect on Combustion: It was reported that the combustion stability under supersonic conditions is largely influenced by the interaction between the chemical kinetics and the turbulence transports. However, in present work, the Eddy-Dissipation Model (EDM) can be used only for premixed combustion. Research work would benefit from an improved turbulent combustion model that can be used to properly treat partially premixed flame and diffusion combustion. This advanced turbulent combustion model is expected to be able to take care of diffusion flame near the injector orifices as well as the
almost premixed combustion in the cavity region. Further developments in boundary conditions are also needed.

**Optimization of Shock Train Dynamics:** In experiments, compressed air was introduced in a controlled manner through ports in the combustor to generate a pre-combustion shock train in the isolator. The resultant increases in the temperature and pressure of the air stream in the combustor, along with the decrease in the flow velocity, lead to smooth and reliable ignition. Furthermore, the shock train gives rise to low-momentum regions and separated flows adjacent to the combustor side-walls, in which the fuel/air mixing process is considerably more efficient due to the shock-induced flow distortion and larger residence time. In general, air throttling is activated prior to fuel injection, and then terminated once the flame is stabilized. Sufficient heat release should be produced in the combustor to preserve the shock train required for sustaining combustion. Insufficient heat release leads to an unstable shock train and a premature removal of air throttling often results in flame blowout. It should be noted that the shock train interacts with the inlet flow field, significant flow spillage or even inlet unstart could result if the combustor is overpressurized. Therefore, a dynamic optimization of the shock train needs to be processed.

**Combustion Oscillations:** Combustion instability may present an important obstacle in the development of scramjet engines, since acoustic waves can propagate upstream in various subsonic flow regions in an engine, such as boundary layers and recirculation zones in flame-holding cavities. Furthermore, fuel injection in a supersonic cross flow and associated shock-wave/shear-layer interactions are intrinsically unsteady. For a dual-mode scramjet (Waltrup et al., 2002) operating at a relatively lower flight
Mach number, combustion often takes place in a subsonic regime downstream of the pre-combustion shock wave. The flow then accelerates to become supersonic in the downstream section of a divergent combustor. Under such condition, longitudinal thermoacoustic instability may exist in the subsonic region between the shock train and flame zone. Recent experiments at the Air Force Research Laboratory (AFRL) have demonstrated oscillations of this kind with frequencies of 100-160 Hz for liquid JP-7 fuel and 300-360 Hz for gaseous ethylene fuel. Therefore, this research is going to conduct a unified theoretical/numerical analysis to study the underlying mechanism responsible for driving and sustaining the observed flow oscillations in the AFRL scramjet test rig.
Bibliography


Appendix A

Menter’s Shear Stress Transport Model

The turbulence kinetic energy $k$-equation can be derived to incorporate space and time correlation effects in the eddy viscosity. For an incompressible flow, the momentum conservation equation is written as

$$\frac{\partial u_i}{\partial t} + \rho u_i \frac{\partial u_i}{\partial x_k} + \frac{\partial p}{\partial x_i} - \mu \frac{\partial^2 u_i}{\partial x_k \partial x_k} = 0$$  \hspace{1cm} (108)

if a Navier-Stokes equation operator is defined as $N(u_i)$

$$N(u_i) = \rho \frac{\partial u_i}{\partial t} + \rho u_k \frac{\partial u_i}{\partial x_k} + \frac{\partial p}{\partial x_i} - \mu \frac{\partial^2 u_i}{\partial x_k \partial x_k}$$  \hspace{1cm} (109)

then the Navier-Stokes equation can be re-written as

$$N(u_i) = 0$$  \hspace{1cm} (110)

The instantaneous velocity $u_i$ can be decomposed into an average quantity $U_i$ and a fluctuating quantity $u'_i$

$$u_i = U_i + u'_i$$  \hspace{1cm} (111)

Multiply Eq. (110) by a fluctuating quantity $u'_i$, then the following time averaged equation is formed

$$\overline{u'_i N(u_j)} + u'_i N(u_i) = 0$$  \hspace{1cm} (112)
Substitute Eq. (109) into Eq. (112), and arrange the left hand side terms of the Eq. (112) to give

\[
\rho u_i \frac{\partial u_j}{\partial t} + \rho u_k \frac{\partial u_j}{\partial x_k} + \frac{\partial p}{\partial x_j} - \mu \left( \frac{\partial^2 u_j}{\partial x_k \partial x_k} \right) + u'_i \rho \frac{\partial u_i}{\partial x_j} + \rho u'_k \frac{\partial u_i}{\partial x_k} + \frac{\partial p}{\partial x_j} - \mu \frac{\partial^2 u_i}{\partial x_k \partial x_k} = 0
\]  

(113)

\[
\begin{align*}
\text{unsteady term} & \quad \text{convective term} & \quad \text{pressure gradient} \\
\left( u'_i \rho \frac{\partial u_j}{\partial t} + u'_j \rho \frac{\partial u_i}{\partial t} \right) & \quad \left( \rho u'_j \frac{\partial u_i}{\partial x_j} + \rho u'_k \frac{\partial u_i}{\partial x_k} \right) & \quad \left( u'_i \frac{\partial p}{\partial x_j} + u'_j \frac{\partial p}{\partial x_i} \right) \\
\end{align*}
\]

(114)

Follow the tensor notation for derivatives throughout the time average process

\[
(u_i)_t = -\frac{\partial u_i}{\partial t}
\]  

(115)

The first unsteady term in Eq. (113) is expressed as

\[
\begin{align*}
u'_i (\rho u_j)_t & + u'_j (\rho u_i)_t = \rho u'_i (U_j + u'_j)_t + \rho u'_j (U_i + u_i)_t, \\
& = \rho (u'_i u'_j)_t, \\
& = -\frac{\partial \tau_{ij}}{\partial t}
\end{align*}
\]

(116)

The second convective term in Eq. (113) is derived as

\[
\begin{align*}ho u'_i u'_k u_{j,k} + \rho u'_k u'_i u_{j,k} = U_k (\rho u'_i u'_j)_k + U_j (\rho u'_i u'_k)_j + U_{j,k} \rho u'_i u'_k + \rho u'_j (u'_i u'_j)_k \\
& = -U_k \frac{\partial \tau_{ij}}{\partial x_k} - \tau_{ik} U_{j,k} - \tau_{jk} U_{i,k} + \frac{\partial}{\partial x_k} \left( \rho u'_i u'_j \right)
\end{align*}
\]

(117)

to approach Eq. (116), condition \( \frac{\partial u'_i}{\partial x_k} = 0 \) must be used.

The third pressure gradient term in Eq. (113) is given as
Finally, the fourth viscous term in Eq. (113) is

$$u_i'p_j + u_j'p_i = u_i'(P + p')_j + u_j'(P + p')_j$$

$$= u_i' \frac{\partial p'}{\partial x_j} + u_j' \frac{\partial p'}{\partial x_i}$$

(118)

Collecting terms in Eq. (115) ~ Eq. (118), we arrive at the equation for the Reynolds stress tensor

$$\mu \left( u_i' u_{j,k} + u_j' u_{i,k} \right) = \mu \left( u_i' \left( U_j + u'_j \right)_{,k} + u_j' \left( U_i + u'_i \right)_{,k} \right)$$

$$= \mu \left( u_j' \right)_{,k} - 2\mu \left( u_{i,k} + u_{j,k} \right)$$

$$= -\nu \frac{\partial^2 \tau_{ij}}{\partial x_i \partial x_j} - 2\mu \frac{\partial u_i'}{\partial x_i} \frac{\partial u_j'}{\partial x_j}$$

(119)

Collecting terms in Eq. (115) ~ Eq. (118), we arrive at the equation for the Reynolds stress tensor

$$\frac{\partial \tau_{ij}}{\partial t} + U_k \frac{\partial \tau_{ij}}{\partial x_k} = -\tau_{ik} \frac{\partial U_j}{\partial x_k} - \tau_{jk} \frac{\partial U_i}{\partial x_k} + 2\mu \frac{\partial u_i'}{\partial x_i} \frac{\partial u_j'}{\partial x_j} + u_i' \frac{\partial p'}{\partial x_i} + u_j' \frac{\partial p'}{\partial x_j}$$

$$+ \frac{\partial}{\partial x_k} \left[ \nu \frac{\partial \tau_{ij}}{\partial x_k} + \rho u_i' u_j' \right]$$

(120)

then the Reynolds stress tensor Eq. (119) leads to the transport equation for the turbulence kinetic energy

$$\frac{\partial \tau_{ii}}{\partial t} + U_k \frac{\partial \tau_{ii}}{\partial x_k} = -\tau_{ik} \frac{\partial U_i}{\partial x_k} - \tau_{ik} \frac{\partial U_k}{\partial x_i} + 2\mu \left( \frac{\partial u_i'}{\partial x_i} \right)^2 - 2p' \frac{\partial u_i'}{\partial x_i}$$

$$+ \frac{\partial}{\partial x_k} \left[ \nu \frac{\partial \tau_{ii}}{\partial x_k} + \rho \left( u_i' \right)^2 + 2p' u_k' \right]$$

(121)

Since the kinetic energy per unit mass of the turbulent fluctuations $k$ is defined as

$$k = \frac{-\tau_{ii}}{2\rho} = \frac{1}{2} u_i' u_i'$$

(122)

and the dissipation per unit mass $\varepsilon$ is defined by the following correlation
we apply equations Eq. (122) and Eq. (123) into Eq. (121) to give the following transport equation for the turbulence kinetic energy

$$\varepsilon = \nu \frac{\partial u'_i \partial u'_j}{\partial x_k \partial x_k}$$

we apply equations Eq. (122) and Eq. (123) into Eq. (121) to give the following transport equation for the turbulence kinetic energy

$$\rho \frac{\partial k}{\partial t} + \rho U_j \frac{\partial k}{\partial x_j} = -\tau_{ij} \frac{\partial U_i}{\partial x_j} - \rho \varepsilon + \frac{\partial}{\partial x_j} \left[ \mu \frac{\partial k}{\partial x_j} - \frac{1}{2} \rho (u'_i)^2 u'_j - p'u'_j \right]$$

The various terms in Eq. (124) represent typical physical processes in the turbulence flow. The terms on the left hand side, as the unsteady term and the convection term, give the rate of change of turbulence kinetic energy following a fluid particle. The first term on the right hand side is a production term, representing the transportation rate of the kinetic energy between the mean flow and the turbulence. The second term is the dissipation term, which is the rate at which turbulence kinetic energy is converted into thermal internal energy. The molecular diffusion term involving $\mu \frac{\partial k}{\partial x_j}$ represents the diffusion of turbulence energy caused by the fluid’s natural molecular transport process. The last two terms are called the turbulent transport term and the pressure diffusion term, respectively. The former term represents the rate at which turbulence energy is transported through the fluid by turbulent fluctuations, and the latter one is the turbulent transport resulting from correlation of pressure and velocity fluctuations. The unsteady term, convection and molecular diffusion are exact while production, dissipation, turbulent transport and pressure diffusion involve unknown correlations. To close the Eq. (124), Reynolds stress term, dissipation, turbulent transport and pressure diffusion must be specified. The pressure diffusion term has generally been grouped with the
turbulent transport term, and the sum assumed to behave as a gradient-transport process. Mansour (1988) indicated the term is quite small for simple flows, then assumed

\[ \frac{1}{2} \rho \left( u'_i \right)^2 u'_j + p'u'_j = -\frac{\mu_k}{\sigma_k} \frac{\partial k}{\partial x_j} \]  

where \( \sigma_k \) is a constant closure coefficient. Therefore the transport equation for the turbulence kinetic energy assumes the following form

\[ \rho \frac{\partial k}{\partial t} + \rho U_k \frac{\partial k}{\partial x_k} = -\tau_{ij} \frac{\partial U_j}{\partial x_j} - \rho \varepsilon + \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] \]  

where the Reynolds stress tensor is given from the Boussinesq approximation as

\[ \tau_{ij} = 2\mu U_{ik} S_{kj} - \frac{2}{3} \rho k \delta_{ij} \]  

where \( S_{ij} \) is the mean strain-rate tensor.

To complete the turbulent model equation system, we need to formulate the exact equation for the dissipation per unit mass \( \varepsilon \), which is defined by Eq. (123). The equation can be derived from the Navier-Stokes equation

\[ 2\nu \frac{\partial u'_i}{\partial x_j} \frac{\partial}{\partial x_j} [N(u_i)] = 0 \]  

after an algebra process, the following \( \varepsilon \) equation is given

\[ \rho \frac{\partial \varepsilon}{\partial t} + \rho U_j \frac{\partial \varepsilon}{\partial x_j} = -2\mu \left[ u'_{i,k} u'_{j,k} + u'_{k,i} u'_{j,k} \right] \frac{\partial U_j}{\partial x_j} - 2\mu u'_{i,j} \frac{\partial^2 U_i}{\partial x_i \partial x_j} - 2\mu u'_{i,i} u'_{j,m} u'_{k,m} - 2\mu u'_{i,i} u'_{j,m} - 2\nu \frac{\partial^2 u'_{i,j}}{\partial x_j} \]  

\[ + \frac{\partial}{\partial x_j} \left[ \mu \frac{\partial \varepsilon}{\partial x_j} - \mu \frac{\partial u'_{i,j}}{\partial x_j} - 2\nu \frac{\partial^2 u'_{i,j}}{\partial x_j} \right] \]
Eq. (129) is far more complicated than the turbulence kinetic energy equation and involves several new unknown correlations of fluctuating velocity, pressure and velocity gradients. Therefore rather than being based on the exact equation, the standard model equation for $\varepsilon$ is actually an empirical equation for the rate of energy transfer from the large eddies

$$\frac{D\rho\varepsilon}{Dt} = C_{e1}\frac{\varepsilon}{k} \frac{\partial u_i}{\partial x_j} - C_{e2}\frac{\varepsilon^2}{k} + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_{e2}\mu_t) \frac{\partial \varepsilon}{\partial x_j} \right]$$  \hspace{1cm} (130)

The specific dissipation rate $\omega$ is defined as

$$\omega = \frac{\varepsilon}{k}$$  \hspace{1cm} (131)

then the original $\varepsilon$ equation can be derived to the $\omega$ equation applying Eq. (131), and hence the following transformed $k-\varepsilon$ model is given

$$\frac{D\rho k}{Dt} = \tau_{ij} \frac{\partial u_j}{\partial x_j} - \beta^* \rho \omega k + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_{e2}\mu_t) \frac{\partial k}{\partial x_j} \right]$$  \hspace{1cm} (132)

$$\frac{D\rho\omega}{Dt} = \rho \tau_{ij} \frac{\partial u_j}{\partial x_j} - \beta^* \rho \omega^2 + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_{e2}\mu_t) \frac{\partial \omega}{\partial x_j} \right] + 2\rho \sigma_{e2} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}$$  \hspace{1cm} (133)

The $k-\varepsilon$ model is the simplest complete two-equation turbulence model, and hence it has been applied to a diverse range of problems in heat transfer, combustion, and multi-phase flows. However, the inaccuracies stem from the $\varepsilon$ equation and the turbulent-viscosity hypothesis occur in the near-wall treatments, and hence modifications to the standard $k-\varepsilon$ model are required in order to apply it to the viscous near-wall region. The second most widely used two-equation model is Wilcox’s $k-\omega$ model, differing from the standard $k-\varepsilon$ model for $\omega$ equation rather than $\varepsilon$ equation.

Wilcox’s $k-\omega$ model is expressed as
As described in detail by Wilcox (1993), the $k-\omega$ model is suitable for boundary-layer flow both in its treatment of the viscous near-wall region, and in processing the effects of streamwise pressure gradients. However, the treatment of free stream boundary is problematic as a non-zero boundary condition on $\omega$ is required, and the calculated flow is sensitive to the value specified.

Menter proposed a shear stress transport (SST) two-equation $k-\omega$ model (Menter, 1994) designed to yield the best behavior of the standard $k-\varepsilon$ model and the Wilcox $k-\omega$ model (Wilcox, 1993). It is written as a $k-\omega$ model, with the final term multiplied by a ‘blending function’. Close to walls the ‘blending function’ is unity, leading to the Wilcox $k-\omega$ model that is suitable for wall turbulence effects, whereas remote from walls the ‘blending function’ is zero, corresponding to the standard $k-\varepsilon$ model that is suitable for shear layer problems.

The SST two-equation $k-\omega$ model is given as following

\[
\frac{D\rho k}{Dt} = \tau_{ij} \frac{\partial u_i}{\partial x_j} - \beta^* \rho \omega k + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_{\omega} \mu_t) \frac{\partial k}{\partial x_j} \right] \tag{134}
\]

\[
\frac{D\rho \omega}{Dt} = \frac{r_{ij}}{\nu_t} \tau_{ij} \frac{\partial u_i}{\partial x_j} - \beta_\rho \rho \omega^2 + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_{\omega} \mu_t) \frac{\partial \omega}{\partial x_j} \right] \tag{135}
\]

As described in detail by Wilcox (1993), the $k-\omega$ model is suitable for boundary-layer flow both in its treatment of the viscous near-wall region, and in processing the effects of streamwise pressure gradients. However, the treatment of free stream boundary is problematic as a non-zero boundary condition on $\omega$ is required, and the calculated flow is sensitive to the value specified.

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The SST two-equation $k-\omega$ model is given as following

\[
\frac{D\rho k}{Dt} = \frac{\partial}{\partial x_j} \left( \mu_k \frac{\partial k}{\partial x_j} \right) + S_k \tag{136}
\]

\[
\frac{D\rho \omega}{Dt} = \frac{\partial}{\partial x_j} \left( \mu_\omega \frac{\partial \omega}{\partial x_j} \right) + S_\omega \tag{137}
\]

where the viscosity terms are expressed as
\[\mu_i = \mu_i + \sigma_k \mu_i \quad (138)\]
\[\mu_\omega = \mu_i + \sigma_\omega \mu_i \quad (139)\]

and the source terms in Menter’s SST \(k-\omega\) equations are

\[S_k = \tau_{ij}^* \frac{\partial u_i}{\partial x_j} - \beta^* \rho \omega \quad (140)\]
\[S_\omega = \frac{\gamma}{\nu} \tau_{ij}^* \frac{\partial u_i}{\partial x_j} - \beta \rho \omega^2 + 2(1 - F_i) \sigma_{w^2} \frac{\rho}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} \quad (141)\]

let \(\phi_1\) represent any constant in the \(k-\omega\) model \((\sigma_{k_1}, \cdots)\), \(\phi_2\) any constant in the \(k-\varepsilon\) model \((\sigma_{k_2}, \cdots)\), and \(\phi\) the corresponding constant of the new model \((\sigma_k, \cdots)\), then the relation between them is

\[\phi = F_i \phi_1 + (1 - F_i) \phi_2 \quad (142)\]

and the ‘blending function’ \(F_i\) is represented as

\[F_i = \tanh(\text{arg}_i^4) \quad (143)\]

the argument of ‘blending function’ \(F_i\) is given as

\[\text{arg}_i = \min \left[ \max \left( \frac{\sqrt{k}}{0.09 \omega y} ; \frac{500 \nu}{y^2 \omega} \right) ; \frac{4 \rho \sigma_{w^2} k}{CD_{woo} y^2} \right] \quad (144)\]

where \(y\) is the distance to the next surface and \(CD_{woo}\) is the positive portion of the cross-diffusion terms expressed as

\[CD_{woo} = \max \left( 2 \rho \sigma_{w^2} \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} , 10^{-20} \right) \quad (145)\]

and the constants \(\phi_1\) in the Wilcox \(k-\omega\) model are
\( \sigma_{k_1} = 0.85 \), \( \sigma_{\omega_1} = 0.5 \), \( \beta_1 = 0.0750 \)

\( \beta^* = 0.09 \), \( \kappa = 0.41 \)
\( \gamma_1 = \beta_1 / \beta^* - \sigma_{\omega_1} \kappa^2 / \sqrt{\beta^*} \)  

(146)

the constants \( \phi_2 \) in the standard \( k - \varepsilon \) model are

\( \sigma_{k_2} = 1.0 \), \( \sigma_{\omega_2} = 0.856 \), \( \beta_2 = 0.0828 \)

\( \beta^* = 0.09 \), \( \kappa = 0.41 \)
\( \gamma_2 = \beta_2 / \beta^* - \sigma_{\omega_2} \kappa^2 / \sqrt{\beta^*} \)  

(147)
Appendix B

Jacobian Matrices for Chemical Source Terms

The approach to calculate the Jacobian matrix for chemical source terms is elaborated here. In the present case, the number of species treated are \( N = 8 \) for non-metallized and \( N = 9 \) for metallized propellants. Out of all the species considered, only \( \text{H}_2\text{O}, \text{CO}_2, \text{CO}, \text{and H}_2 \) participate in the reversible water-gas shift reaction in the gas phase. Consider the forward water-gas shift reaction represented by

\[
\text{C}_2\text{H}_4 + 2\text{O}_2 \rightarrow 2\text{CO} + 2\text{H}_2\text{O} \tag{148}
\]

\[
\text{CO} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}_2 \tag{149}
\]

The rate of the \( \text{C}_2\text{H}_4 \) oxidation per unit volume is expressed as

\[
\dot{\omega}_1 = -A_1 \exp\left(\frac{-E_{\text{a1}}}{R_T}\right) \left[ \chi_{\text{C}_2\text{H}_4} \right]^{0.1} \left[ \chi_{\text{O}_2} \right]^{0.65} \tag{150}
\]

The rate of the \( \text{CO} \) oxidation per unit volume is

\[
\dot{\omega}_2 = -A_2 \exp\left(\frac{-E_{\text{a2}}}{R_T}\right) \left[ \chi_{\text{CO}} \right] \left[ \chi_{\text{H}_2\text{O}} \right]^{0.5} \left[ \chi_{\text{O}_2} \right]^{0.25} \tag{151}
\]

In order to reproduce properly both the heat of reaction and pressure dependence of the \([\text{CO}]/[\text{CO}_2]\) equilibrium, a reverse reaction is included for the second step Eq. (151),

\[
\dot{\omega}_2 = -B_2 \exp\left(\frac{-E_{\text{r2}}}{R_T}\right) \left[ \chi_{\text{CO}_2} \right] \tag{152}
\]
According to the kinetics rate law, the rate of production of the five species \( \text{C}_2\text{H}_4, \text{O}_2, \text{CO}, \text{CO}_2, \) and \( \text{H}_2\text{O} \) are given by \( \dot{\omega}_1, \dot{\omega}_2, \dot{\omega}_3, \dot{\omega}_4, \) and \( \dot{\omega}_5 \), respectively.

\[
\begin{align*}
\dot{\omega}_1 &= -M_1 \dot{\omega}_1 \\
\dot{\omega}_2 &= -2M_z \dot{\omega}_1 - 2M_\rho \dot{\omega}_2 - \frac{1}{2} M_z \dot{\omega}_3 \\
\dot{\omega}_3 &= 2M_\rho \dot{\omega}_1 - M_\rho \dot{\omega}_2 + M_z \dot{\omega}_3
\end{align*}
\]

The Jacobian matrix is represented by

\[
D = \frac{\partial H}{\partial Q} = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{\partial \dot{\omega}_1}{\partial \rho} & \frac{\partial \dot{\omega}_1}{\partial \mu} & \frac{\partial \dot{\omega}_1}{\partial v} & \frac{\partial \dot{\omega}_1}{\partial w} & \frac{\partial \dot{\omega}_1}{\partial e} & \frac{\partial \dot{\omega}_1}{\partial Y_1} & \frac{\partial \dot{\omega}_1}{\partial Y_2} & \frac{\partial \dot{\omega}_1}{\partial Y_3} & \frac{\partial \dot{\omega}_1}{\partial Y_4} \\
\frac{\partial \dot{\omega}_2}{\partial \rho} & \frac{\partial \dot{\omega}_2}{\partial \mu} & \frac{\partial \dot{\omega}_2}{\partial v} & \frac{\partial \dot{\omega}_2}{\partial w} & \frac{\partial \dot{\omega}_2}{\partial e} & \frac{\partial \dot{\omega}_2}{\partial Y_1} & \frac{\partial \dot{\omega}_2}{\partial Y_2} & \frac{\partial \dot{\omega}_2}{\partial Y_3} & \frac{\partial \dot{\omega}_2}{\partial Y_4} \\
\frac{\partial \dot{\omega}_3}{\partial \rho} & \frac{\partial \dot{\omega}_3}{\partial \mu} & \frac{\partial \dot{\omega}_3}{\partial v} & \frac{\partial \dot{\omega}_3}{\partial w} & \frac{\partial \dot{\omega}_3}{\partial e} & \frac{\partial \dot{\omega}_3}{\partial Y_1} & \frac{\partial \dot{\omega}_3}{\partial Y_2} & \frac{\partial \dot{\omega}_3}{\partial Y_3} & \frac{\partial \dot{\omega}_3}{\partial Y_4} \\
\frac{\partial \dot{\omega}_4}{\partial \rho} & \frac{\partial \dot{\omega}_4}{\partial \mu} & \frac{\partial \dot{\omega}_4}{\partial v} & \frac{\partial \dot{\omega}_4}{\partial w} & \frac{\partial \dot{\omega}_4}{\partial e} & \frac{\partial \dot{\omega}_4}{\partial Y_1} & \frac{\partial \dot{\omega}_4}{\partial Y_2} & \frac{\partial \dot{\omega}_4}{\partial Y_3} & \frac{\partial \dot{\omega}_4}{\partial Y_4} \\
\frac{\partial \dot{\omega}_5}{\partial \rho} & \frac{\partial \dot{\omega}_5}{\partial \mu} & \frac{\partial \dot{\omega}_5}{\partial v} & \frac{\partial \dot{\omega}_5}{\partial w} & \frac{\partial \dot{\omega}_5}{\partial e} & \frac{\partial \dot{\omega}_5}{\partial Y_1} & \frac{\partial \dot{\omega}_5}{\partial Y_2} & \frac{\partial \dot{\omega}_5}{\partial Y_3} & \frac{\partial \dot{\omega}_5}{\partial Y_4}
\end{pmatrix}
\]

A given derivative example in the above matrix, with respect to any particular primary variable of \( Q \), is obtained by assuming all other primary variables as constants. For instance, \( \frac{\partial \dot{\omega}_1}{\partial \rho} \) is obtained by assuming \( \rho u, \rho v, \rho w, \rho e, \rho Y_1, \ldots, \) and \( \rho Y_5 \) as constants. The approach to derive the elements of the above matrix is shown below.

Eq. (153) can be rewritten as

\[
\log \dot{\omega}_1 = \log(A) - \frac{E}{R T} + 0.1 \log(\frac{\rho Y_1}{M_1}) + 1.65 \log(\frac{\rho Y_2}{M_2})
\]

The derivative of Eq. (157) is given as
\[ \frac{\partial \log \omega_{j1}}{\partial \rho} = \frac{1}{\omega_{j1}} \frac{\partial \omega_{j1}}{\partial \rho} = \frac{E_{d1}}{R T^2} \frac{\partial T}{\partial \rho} \]  \hspace{1cm} (158)

Since \( \rho u, \rho v, \rho w, \rho e, \rho Y_1, \ldots, \) and \( \rho Y_5 \) are constants. Then further simplification yields,

\[ \frac{\partial \omega_{j1}}{\partial \rho} = \hat{\omega}_{j1} \frac{E_{d1}}{R T^2} \frac{\partial T}{\partial \rho} \]  \hspace{1cm} (159)

Similarly, other derivatives can be written as

\[ \frac{\partial \hat{\omega}_{j1}}{\partial \rho u} = \hat{\omega}_{j1} \frac{E_{d1}}{R T^2} \frac{\partial T}{\partial \rho u} \]  \hspace{1cm} (160)

\[ \frac{\partial \hat{\omega}_{f1}}{\partial \rho v} = \hat{\omega}_{f1} \frac{E_{d1}}{R T^2} \frac{\partial T}{\partial \rho v} \]  \hspace{1cm} (161)

\[ \frac{\partial \hat{\omega}_{f1}}{\partial \rho w} = \hat{\omega}_{f1} \frac{E_{d1}}{R T^2} \frac{\partial T}{\partial \rho w} \]  \hspace{1cm} (162)

\[ \frac{\partial \hat{\omega}_{f1}}{\partial \rho e} = \hat{\omega}_{f1} \frac{E_{d1}}{R T^2} \frac{\partial T}{\partial \rho e} \]  \hspace{1cm} (163)

\[ \frac{\partial \hat{\omega}_{f1}}{\partial \rho Y_1} = \hat{\omega}_{f1} \left[ \frac{E_{d1}}{R u T^2} \frac{\partial T}{\partial \rho Y_1} + \frac{0.1}{\rho Y_1} \right] \]  \hspace{1cm} (164)

\[ \frac{\partial \hat{\omega}_{f1}}{\partial \rho Y_2} = \hat{\omega}_{f1} \left[ \frac{E_{d1}}{R u T^2} \frac{\partial T}{\partial \rho Y_2} + \frac{1.65}{\rho Y_2} \right] \]  \hspace{1cm} (165)

\[ \frac{\partial \hat{\omega}_{f1}}{\partial \rho Y_3} = \hat{\omega}_{f1} \left[ \frac{E_{d1}}{R u T^2} \frac{\partial T}{\partial \rho Y_3} \right] \]  \hspace{1cm} (166)

\[ \frac{\partial \hat{\omega}_{f1}}{\partial \rho Y_4} = \hat{\omega}_{f1} \left[ \frac{E_{d1}}{R u T^2} \frac{\partial T}{\partial \rho Y_4} \right] \]  \hspace{1cm} (167)

\[ \frac{\partial \hat{\omega}_{f1}}{\partial \rho Y_5} = \hat{\omega}_{f1} \left[ \frac{E_{d1}}{R u T^2} \frac{\partial T}{\partial \rho Y_5} \right] \]  \hspace{1cm} (168)

From energy equation,

\[ e = \sum_{i=1}^{\Phi} \rho_i h - \frac{P}{\rho} + \frac{1}{2} (u^2 + v^2 + w^2) \]  \hspace{1cm} (169)

The expression can be given as
For the specific heat at constant volume,

\[ \rho e = \sum_{i=1}^{n} \rho Y_i \left[ (h_i - h_N) - (R_i - R_N)T \right] + \rho (h_N - R_N T) + \frac{1}{2} \rho \left( (\rho u)^2 + (\rho v)^2 + (\rho w)^2 \right) \]  \hspace{1cm} (170)

For the specific heat at constant volume,

\[ \frac{\partial (\rho e)}{\partial T} = \rho C_{v,mix} \]  \hspace{1cm} (171)

then

\[ \frac{\partial T}{\partial \rho e} = \frac{1}{\rho C_{v,mix}} \]  \hspace{1cm} (172)

now the following derivatives are obtained as

\[ \frac{\partial T}{\partial \rho} = \frac{-1}{\rho C_{v,mix}} \left[ (h_N - R_N T) - \frac{1}{2} \left( u^2 + v^2 + w^2 \right) \right] \]  \hspace{1cm} (173)

\[ \frac{\partial T}{\partial \rho u} = -u \] \hspace{1cm} (174)

\[ \frac{\partial T}{\partial \rho v} = -v \] \hspace{1cm} (175)

\[ \frac{\partial T}{\partial \rho w} = -w \] \hspace{1cm} (176)

\[ \frac{\partial T}{\partial \rho e} = \frac{1}{\rho C_{v,mix}} \] \hspace{1cm} (177)

\[ \frac{\partial T}{\partial \rho Y_i} = \frac{-1}{\rho C_{v,mix}} \left[ (h_i - R_i T) - (R_i - R_N T) \right] \] \hspace{1cm} (178)

All the elements of Jacobian matrix \( \mathbf{D} \) can thus be computed.
VITA

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Jian Li was born in Xi’an, Shanxi Province, China. He received his Bachelor’s degree in July 2000 in Engineering Thermophysics from University of Science and Technology of China (USTC). In July 2003, he received his M.S. degree in Engineering Thermophysics from USTC. He joined the Mechanical Engineering Department at the Pennsylvania State University in Fall 2003 to conduct research in the areas of numerical/theoretical analysis of flow and combustion dynamics in scramjet engine.