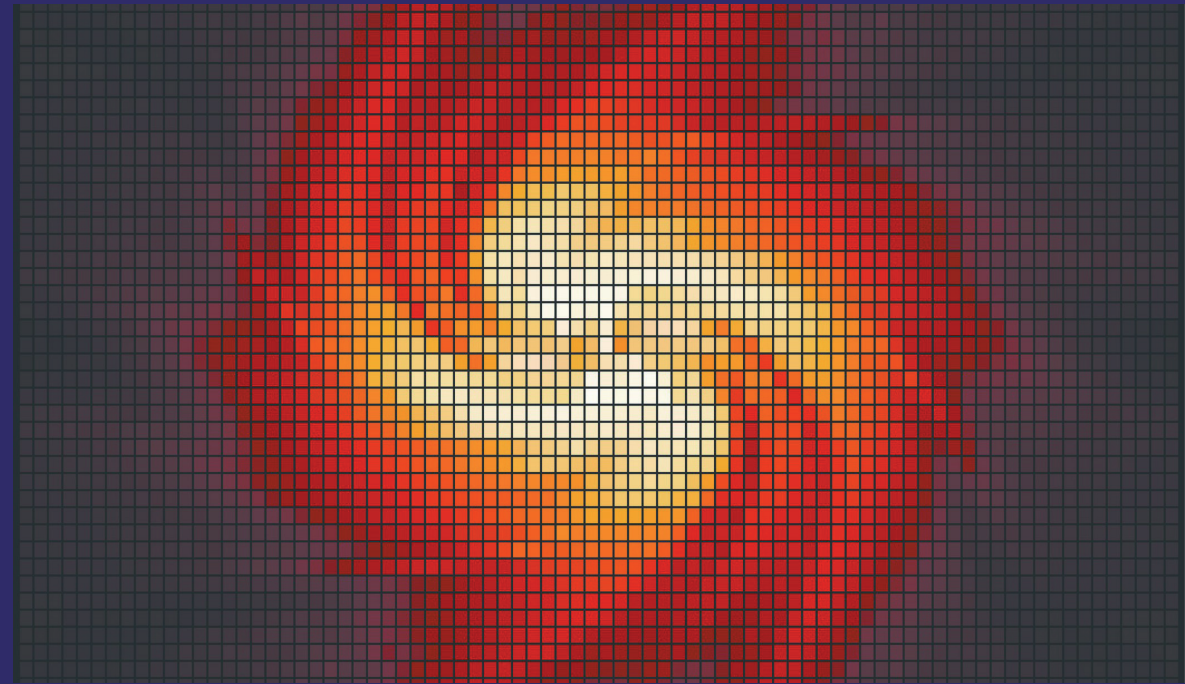


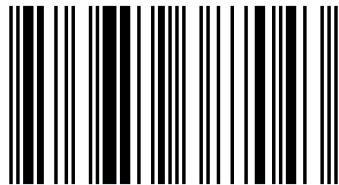


The design and off-design studies of the hypersonic air-breathing engines face many challenges, due to the complexity of their internal flows. The mixing and combustion processes in Supersonic-Combustion Ramjet (scramjet) engines involve complicated aerothermochemical features, such as: the interactions between shock-waves and boundary-layer, the shock induced-combustion and the recirculation zones. In this study, a numerical solver is developed and validated to be an efficient design tool capable of simulating these complicated flow features of the supersonic combustors. For the code validation, several test cases are considered to monitor the code ability to solve for the diffusive and turbulent fluxes, and the chemical source term. In addition, the code is validated by resolving the transverse sonic injection into supersonic air flow in the case of Helium injection from a flat plate, and in the case of Hydrogen injection in a single-strut scramjet engine. The effectiveness of this injection technique in mixing and flame-holding is demonstrated. The results show good agreement with the previous numerical and experimental investigations, and prove the simulator's accuracy.



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Nomenclature

English Symbols

Symbol	Definition
$\mathcal{A}$	Arrhenius pre-exponential coefficient
A^+	Van Driest damping term constant
A_o	Intermediate function utilized in clustering transformation
$\mathbf{A}, \mathbf{B}$	Convective flux Jacobian in x and y directions
$\overline{\mathbf{A}}, \overline{\mathbf{B}}$	Convective flux Jacobian in ξ and η directions
b	Specific body force
c	Speed of sound in (x, y) domain
c_p	Specific heat coefficient at constant pressure
c_v	Specific heat coefficient at constant volume
c_v^*	Roe scheme's definition for c_v at the cell face
$c_{v_m}^*$	Roe scheme's definition for c_v for each species at the cell face
C_{cp}, C_{wk}, C_{Kelp}	Baldwin-Lomax closure coefficients
d_{mx}, d_{my}	Time-averaged mass fluxes in x and y directions
D	Mass diffusivity coefficient
e	Time-averaged specific internal energy
e_m	Time-averaged species specific internal energy
E_t	Time-averaged total specific internal energy
e_s	Time-averaged mixture sensible specific internal energy
E_{acu}	Activation energy
E, F, E_v, F_v	Convective and Diffusive fluxes in the x and y directions
$\mathcal{E}_R, \mathcal{E}_L$	Right and Left eigenvectors matrices

$\overline{E}, \overline{F}, \overline{E}_v, \overline{F}_v$	Convective and Diffusive fluxes in the ξ and η directions
$\vec{\mathbf{F}} f, f_1, f_2, f_3$	General flow variables
F/O	Fuel to oxygen ratio
F_{Klep}	Klebanoff's intermittency empirical function
$F(n)$	Intermediate function in the Turbulence Approach
F_{max}	Maximum value of $F(n)$
h	Time-averaged specific enthalpy
h_1, h_2, h_3	Transformation coefficients to a general orthogonal axes
H_t	Time-averaged total specific enthalpy
h_s	Time-averaged mixture sensible specific enthalpy
h_f^o	Enthalpy of formation at the energy reference level
H, H_v	Convective and Diffusive axisymmetric vector term
$\mathbf{H}$	Chemical source term Jacobian in the (x, y) domain
$\overline{\mathbf{H}}$	Chemical source term Jacobian in the (ξ, η) domain
$\mathbf{I}$	Identity matrix
J	Transformation Jacobian
$\vec{i}, \vec{j}$	Unit vectors in the x and y axes
$\vec{\mathbf{i}}, \vec{\mathbf{j}}$	Unit vectors in the ξ and η axes
$imax, jmax$	Number of the discrete nodes in ξ and η directions
k	Thermal conductivity coefficient
k_f, k_b	Forward and backward reaction rate
K_p	Reaction equilibrium constant
K	Baldwin-Lomax closure constant
Le	Lewis number
l_{mix}	Mixing length
$\mathbf{M}$	Mach number
M	Mass
$\mathcal{M}$	Molecular weight
N	Number of moles
$\mathcal{N}$	Arrhenius temperature exponent
n	Normal distance from the wall, or the jet centerline
$\hat{n}$	Unit vector normal to the boundaries towards the domain
$\hat{n}_w$	Normal unit vector out off the wall, or the jet centerline

$\hat{n}_S$	Normal unit vector out off the control volume surface
n_s, n_r	Number of species and reactions
n_{max}	The value of n at which $F(n) = F_{max}$
P	Pressure
P_{norm}	Normalized pressure
Pr	Prandtl number
Q	Conservative flow variables vector in the (x, y) domain
$\overline{Q}$	Conservative flow variables vector in the (ξ, η) domain
q_x, q_y	Heat fluxes in x and y directions
$\hat{\mathbf{q}}$	Roe-averaged velocity magnitude
$\vec{r}_{wp}, \vec{r}_p, \vec{r}_w$	Position vectors
$\mathcal{R}$	Universal gas constant
R	Gas constant
r	Flow variable slope at the cell face
$\mathbf{r}$	Geometric progression rate
R	Right hand side of the partial differential equation (Residual for steady-state problems)
R_I, R_V, R_C	Right hand sides of the invscid fluxes, the viscous fluxes and the chemical source term
$S, \overline{S}$	Source terms in the physical and computational domains
Sc	Schmidt number
$\mathbb{S}$	The total surface of the discrete control volume
T	Temperature
t	Time
Δt	The time step
u, v	Time-averaged velocity component in x and y direction
$\mathcal{U}, \mathcal{V}$	Contravariant velocities in the ξ and η directions
$\mathcal{U}', \mathcal{V}'$	Covariant velocities in $(\xi - \eta)$ domain
U_∞	Freestream velocity magnitude
V	Time-averaged velocity magnitude
$\vec{V}$	Velocity vector
u_τ	Wall friction velocity
u_{diff}	Difference between the maximum and minimum velocity

	magnitudes
$\mathcal{W}$	Characteristic variable / Wave strength
X, Y	Mole and Mass fraction
x, y	Orthogonal axes in the physical domain
x_{norm}, y_{norm}	Normalized axial and transversal distances
$\mathbf{X}, \mathbf{Y}$	Intermediate coordinate system in the physical domain

Greek Symbols

Symbol	Definition
α	Logical switch between the planar two dimensional and the axisymmetric domains
$\alpha_y, \beta_y, \beta_x$	Grid lines clustering constants
γ	Specific heat ratio
Γ	Intermediate function utilized in clustering transformation
δ_{ij}	Kronecker delta function
δ_1	First and smallest spatial interval next to the wall surface
ε	Logical Switch between the first and the second order spatial accuracies
κ	Kármán constant
λ	Eigenvalue of the convective flux Jacobian
λ_ξ	Eigenvalue of the convective flux Jacobian in ξ -direction
λ_η	Eigenvalue of the convective flux Jacobian in η -direction
Λ	Eigenvalues matrix of the convective flux Jacobian
Λ_ξ	Eigenvalues matrix of the convective Jacobian in ξ -direction
Λ_η	Eigenvalues matrix of the convective Jacobian in η -direction
μ	Dynamic viscosity
ν	Kinematic viscosity
ν'	Stoichiometric coefficient of the reactants
ν''	Stoichiometric coefficient of the products
ξ, η	Generalized axes in computational domain
ξ_x, ξ_y	Derivatives of ξ with respective to x and y

η_x, η_y	Derivatives of η with respect to x and y
$\Delta\xi, \Delta\eta$	The spatial discretization step in the $(\xi - \eta)$ domain
ρ	Time-averaged density
σ	Courant-Friedrichs-Lewy (CFL) number
τ	Time-averaged shear stress
ϕ	Equivalence ratio
ψ	Slope limiter function
$\Theta_\xi, \Theta_\eta, \widehat{\psi}_m$	Energy terms in Roe's formulation of the convective fluxes
ω	Vorticity vector magnitude
$\dot{\omega}$	Time-averaged chemical source term

Indices, Subscripts and Superscripts

Subscripts

Symbol	Definition
F	Properties at the cell face
<i>max, min</i>	Maximum, and Minimum values
<i>mix</i>	Whole mixture property
<i>L</i>	Laminar flow property
<i>ref</i>	Test case reference value
<i>st</i>	Stoichiometric property
<i>T</i>	Turbulent flow property
<i>w</i>	Property at the wall
<i>in</i>	Given flow inlet condition
<i>out</i>	Given flow exit condition

Indices

Symbol	Definition
<i>i, j, k</i>	Spatial indices

m, q, p	Species indices
r	Reaction index
n	Time level index

Superscripts

Symbol	Definition
o	Energy reference level
L, R	Properties of the cell face, at the left and right sides

Other

Symbol	Definition
$+$	Sub-layer scaled value referred to properties at the wall
$\wedge$	Roe averaging at the cell interface
$\langle \ \rangle$	Averaging between the left and right sides of the cell face
$\llbracket \ \rrbracket$	Difference between the left and right sides of the cell face

Abbreviations

Symbol	Definition
1D	One-dimensional
2D	Two-dimensional
DNS	Direct Numerical Simulation
CFD	Computational Fluid Dynamics
CFL	Courant-Friedrichs-Lewy
LES	Large Eddy Simulation
MUSCL	Monotone Upstream-centered Schemes for Conservative Laws
PDF	Probability Density Function
RANS	Reynolds averaged Navier-Stocks
TVD	Total Variation Diminishing

Chemical Symbols

Symbol	Definition
H ₂	Hydrogen molecule
H ₂ O	Water molecule
O ₂	Oxygen molecule
OH	Hydroxyl group
N ₂	Nitrogen molecule
He	Helium molecule

Preface

The design and off-design studies of hypersonic air-breathing engines face many challenges because of the complexity of their internal flows. Mixing and combustion processes in Supersonic-Combustion Ramjet (scramjet) engines involve complicated aerothermochemical features such as interactions between shock-waves and boundary-layer, shock induced-combustion and recirculation zones. In this study, a numerical solver is developed and validated to be an efficient design tool capable of simulating these complicated flow features of supersonic combustors. The flow is solved based on the Reynolds Averaged Navier-Stocks equations (RANS), beside a chemical kinetics model for the computation the reactions finite rates. Finite-volume scheme is used where the convective fluxes are discretized by Roe's scheme using MUSCL approach. And, the diffusive fluxes are centrally discretized. Point-implicit Runge-Kutta method is applied for time integration. For the code validation, several test cases are to monitor the code ability to solve for the different diffusive and turbulent fluxes, and the chemical source term. In addition, the code is validated by resolving the transverse sonic injection into supersonic air flow in case of Helium injection from a flat plate, and the case of Hydrogen injection in single-strut scramjet engine. The effect of this injection technique in mixing and flame-holding is demonstrated. The results show good agreement with the previous numerical and experimental investigations. And, the numerical simulator proves its accuracy and robustness.

Chapter 1

Introduction

1.1 Historical Background of Hypersonic Vehicles

Air-breathing hypersonic vehicle is one of the most ambitious and challenging design concepts for the future aerospace plane, which is hoped to carry out orbital missions in atmospheric regions, or to assist in space access. The conceptual design of their operation can be simplified in: considering the breathed air as the main source of oxidizer, and the dependence on the ram-effect in raising the incoming air static pressure. As a result, this type of hypersonic air-vehicles can be so competitive to the rocket-powered missiles, in the previously mentioned missions, for the same flight speeds, as they are much lighter. That is because there is neither oxidizer storage tanks, nor turbo-machines used in air-compression. Consequently, there is a rising attention about developing air-breathing engines of satisfactory performance and efficiency at hypersonic regimes.

This concept was first seriously examined by U.S. Air Force in the early 1960's, and a combination of air-breathing and rocket propulsion was intended to power the vehicle. Work on the early aerospace plane was canceled in October 1963 due mainly to the design requirements exceeding the experimental and computational facilities at that

time. [63],[64]

This idea has been resurrected in the mid-1980's by both NASA and the Department of Defense, as well as by European aerospace companies. These aerospace planes will rely primarily on air-breathing propulsion provided by supersonic combustion ramjet engine (scramjet), which are preferred that ramjet engines in hypersonic regimes. That is because the conventional ramjets always decelerate the incoming air to a subsonic velocity within the combustor, by a system of strong shocks, which become more intense at higher flight speeds, and so stronger and *heavier* engine structure is required. On the other hand, as combustion takes place mainly at supersonic speeds in scramjet engines, the stagnation pressure recovered from the freestream is greatly raised, and as a result, the net thrust is improved.

In that regard, it is important to mention an aspect that distinguishes the hypersonic aerospace plane concepts from conventional subsonic and supersonic airplane design, whose components can be treated as separate aerodynamic bodies with only a moderate interactions. On the other hand, hypersonic aerodynamic design is exactly the opposite. Figure (1.1) illustrates an example of scramjet-powered hypersonic air vehicle, where the *waverider* airframe is fully integrated with the propulsive system, wherein the entire undersurface of the vehicle is part of the scramjet engine. Initial compression of the air takes place through the bow shock from the nose of the aircraft; further compression and supersonic combustion take place inside a series of modules near the rear of the aircraft, and then expansion of the burned gases is partially taking place through nozzles in the engine modules, but mainly over bottom rear surface of the aircraft, which is sculptured to a nozzle-like shape. Moreover, most of the lift is produced by high pressure behind the bow shock wave and exerted on the vehicle undersurface. So, the propulsion mechanism and airframe are intimately incorporated.

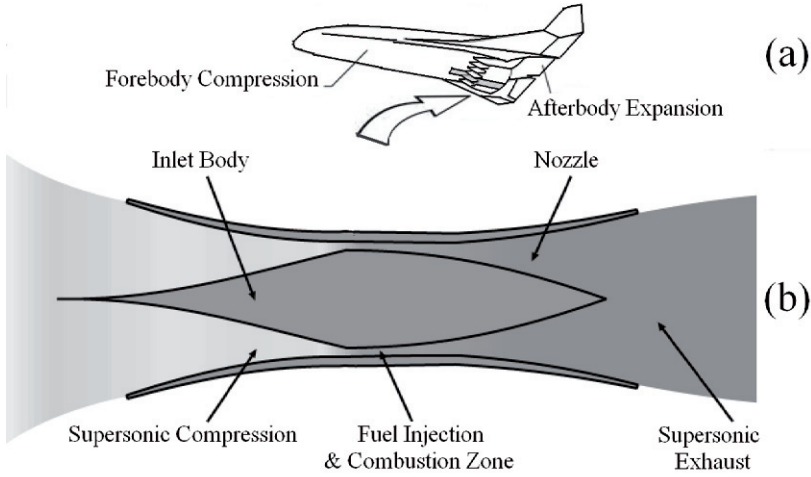


Figure 1.1: (a) Propulsion airframe Integrated Scramjet (Source : LaRC) and (b) Schematic diagram for a single model in scramjet engine (Source : Wikimedia)

1.2 Air-Fuel Mixing and Flame-Holding In Scramjet Engines

Hydrogen is considered the best choice for scramjet engine fuel, due to its high calorific value, in addition to the very fast rate of its dissociation. That ensures an efficient combustion of the supersonic air-fuel flow inside scramjet combustor. It is mostly likely to be stored in liquid state in pressurized tanks to reduce the overall storage volume.

As the residence time of the reactants inside scramjet engine is of order milliseconds, cruising at very high Mach number arises challenges in fuel-air mixing, and in flame holding and stabilization. Many techniques are suggested and studied to enhance air-fuel mixing,[58] using compression or expansion ramps, pulsed jets, or shear-layer/shock-wave interactions, etc.. . Flame-holding in the supersonic flowfield

is attained by providing the necessary activation energy for combustion initiation, in very small fraction of time. Shock-induced combustion, or plasma torches are the most feasible flame-holding candidates. However, *transverse sonic fuel injection* into supersonic air inlet flow, as shown in figure (1.2), is one of the most efficient techniques suggested to enhance both air-fuel mixing and flame holding.

As shown in figure (1.2), the supersonic inlet flow is decelerated by the high pressure gradient due to the sonic fuel injection perpendicular to the main flow stream, forming a separation shock followed by a strong bow shock, after which the decelerated air diffuses into the injected fuel through the mixing layer. When we focus on the injection zone, we find a barrel-shaped stream-tube surrounded by jet shocks, where the injected fuel is accelerated into supersonic speed and then choked again at a circular plan, which is known as “Mach Disk”. The separation shock creates a recirculation zone located in front of the injection zone, which plays a great role in air-fuel mixing and flame holding processes. The low speeds vortices are efficiently stirring the perpendicular streams of air and fuel. Also, combustion is sustained due to the effect of the upstream separation shock in deceleration the incoming supersonic air flow, and raising temperature inside the front recirculation region. In this study, mixing and combustion processes are investigated in case of using transverse sonic fuel injection technique.

1.3 Modelling Overview of Supersonic Mixing and Combustion

Since the great progress in the computational resources in 1980’s, computational fluid dynamics (CFD) has proven to be an invaluable tool for the design and analysis of high speed propulsion devices. It is capable of estimating the main design features of scramjet engines,

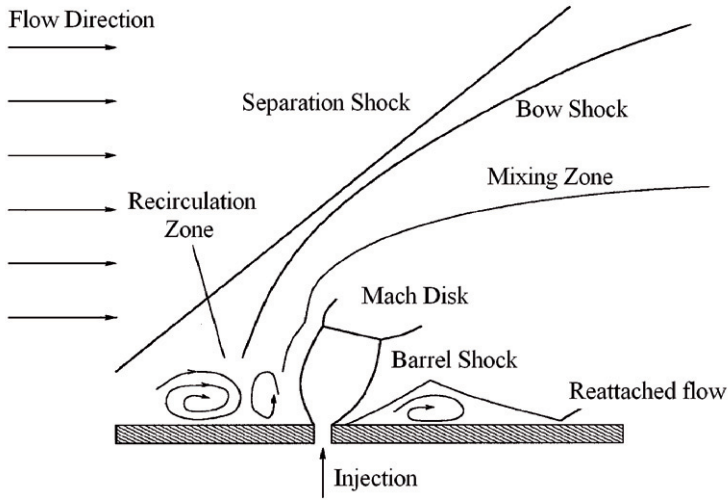


Figure 1.2: **Different aerodynamic phenomena in sonic transverse injection to supersonic flow stream, Lavante et al. [41]**

instead of implementing a great set of prototype experiments.

The unsteady Navier-Stokes equations, which are generally considered to govern turbulent flows, can be solved by Direct Numerical Simulation (DNS), Large Eddy Simulation (LES), or Reynolds-Averaged Navier-Stokes equations (RANS). RANS simulations are now routinely used in design parametric studies of scramjet engine, and in the development of the main engine features. RANS approach is based on time-averaging the turbulent fluctuations in the flow variables magnitude. Higher order modeling approaches, such as Large Eddy Simulation (LES), offer significant advantages that overcome many of the shortcomings associated with the statistical representation of time-averaged RANS closures. LES approach for turbulence closure attempts to resolve the filtered spatial-averaged large-scale components of turbulence while modeling the smaller scales. Most of the transport of mass, momentum, and energy (on the order of 90%) is done by the

large eddies, while the primary role of the small eddies is to dissipate these fluctuations. Spalart [56] found that the application of a traditional LES approach on airliner wing requires on the order of 10^{20} floating point operations. This value is roughly one million times that of the largest RANS calculations attempted today. The most accurate and the most expensive approach is the Direct Numerical Simulation (DNS) turbulence closure, where only unsteady Navier-Stokes equations are applied, to resolve all flow features with all relevant length scales be resolved from the smallest eddies to scales on the order of the physical dimensions of the problem domain. The computational effort required for DNS approach is about 10 times that required by LES closure. [59] Accordingly, RANS approach is still proven to be the efficient tool to explore the main flow features in scramjet engines.

As, the flow inside scramjet engine is mainly supersonic, the residence time of reacting species is too short to achieve chemical equilibrium. Finite-rate chemistry model is the most convenient choice for the calculations of the species source in the mixture. Over the 1980's, a number of finite rate chemistry models for the hydrogen-air system have appeared in the literature. Rogers and Schexnayder [49] proposed as many as 60 reaction paths in their model; this is certainly one of the most complete representations of hydrogen-air reaction. Unfortunately, the enormous number of reaction paths and chemical species involved in the model do not lend themselves feasible for a numerical investigation, at least with in the current capability of state-of-the-art computers. The mechanism is reduced by Hitch et al. [33] to 14 elementary reactions and 8 species. Although these models are considerable less tedious than the 60-path model, they are expected to be too costly to use for routine parametric studies. The global two-step chemistry model of Rogers and Chinitz [48] offers an alternative to numerical investigators since it is a finite rate model with only four species of reactants and products and with only two reaction paths.

The most common species production rate closures used for high-speed reacting flows are based on laminar-chemistry, eddy break-up / dissipation, [42],[57] or probability density function (PDF) [39],[51],[52] formulations. Approaches based on a laminar-chemistry assumption simply ignore turbulence-chemistry interactions by evaluating the chemical source terms based on mean flow properties. Eddy break-up models are mixing limited models where the chemical time scale is assumed to be limited by the dissipation rate of turbulent eddies. Formulations based on ideas borrowed from probability theory represent perhaps the most elegant class of models for averaging the chemical source terms.

Turbulence modeling utilized is based on Boussinesq's assumption, are divided into numerous categories according to the number of the partial differential equations added to the whole governing equations. There are the field two-equations turbulence model such as $(k - \epsilon)$ [16],[19] and $(k - \omega)$ [40] models, also there are the One-Equation Turbulence Models such as Baldwin-Barth model [3], also there is the Zero-Equation Model, or Algebraic Model which only requires an algebraic equation solution to solve the turbulent flow properties, such as Cebeci-Smith model [55], and Baldwin-Lomax model [2], which has no need to calculate the boundary-layer thickness at each station which is necessary in the former model. Because of its simplicity, Baldwin-Lomax algebraic model is widely used for turbulent chemically reacting flows. However, Baldwin-Lomax model shows overestimation of the length of attached flow in case of adverse pressure gradients, Degani and Schiff [20] add some modifications to determine more accurately when a strong vortical flow structure or a massive separation exists.

The order of magnitude of characteristic time of the chemical reactions is much less than that of flow residence time, even in case of supersonic combustion. Stiffness arises from the great gap between the time scales of the coupled governing equations. Full im-

implicit treatment for the governing equations for two-dimensional flows leads to solve simultaneous equations in pent-block diagonal matrix form, which is suggested to be carried out by the iterative method of Lower-Upper Symmetric Gauss-Siedel (LUSGS) method, suggested by Yoon and Jameson [67]. which is proved to be of highest efficiency and fastest convergence rate, as concluded by Mottura et. al [44]. Otherwise, in order to reduce the computational efforts of inverting the flow Jacobians, the convective and viscous flow fluxes are treated explicitly, where only the chemical source term is solved implicitly, this method is well-known as Chemistry-Implicit or Point-Implicit, which is first introduced by Curtiss et al. [18], to decouple between the implicit treatment of the stiff turbulent or chemical terms, from other flow terms, which are solved using explicit scheme. For Point-Implicit scheme, mono-block diagonal matrix will be solved, resulting in dramatic decrease in the computational effort, and in liberating time-stepping from chemical stiffness restriction.

There are some attempts to simplify the chemical source Jacobian formulation, as presented by Eberhardt et al. [25], [26], and Kim et al. [37],[38], where partial implicit treatment for the chemical source term is applied. As, it is proposed to write the chemical Jacobian in form of a lower or a diagonal matrices instead of the full matrix form, in order to evade the matrix inversion efforts. However, using partial formulation for the chemical Jacobian matrix leads to convergence rates slowness and makes solver robustness more restricted with time-stepping in the initial stages of the reactions.

Flux-vector and flux-difference splitting schemes was developed and numerically applied, by Grossman et. al [30], for chemically and thermally nonequilibrium one-dimensional flows. More extensions for multi-dimensional problem, were presented by Walters et al. [62], where two reacting mechanisms were studied: two-reactions H_2 -air model [48], and five-reactions N_2 - O_2 dissociation model [10]. Buss-

ing and Murman [8],[9] used a finite volume point-implicit method, with multiple grid accelerator to solve for flows over ramps and rearward facing steps. Shuen and Yoon [54] employed fully implicit finite-volume, Lower-Upper Symmetric Successive Over-Relaxation scheme (LUSSOR). Their model is coupled with chemical kinetics model of 8-species, 14-reactions model [33]. Eklund et al. [27], studied relative merits of an Adam scheme and a Runge-Kutta scheme. The partially implicit method and the global two-step chemistry model [48] was used successfully by Drummond, et al. [21] to calculate premixed Hydrogen-air reacting flow using a spectral method. Drummond and Weidner were the first who solved transverse sonic injection of hydrogen into supersonic air flow in a single strut scramjet engine, using finite difference MacCormack scheme, with complete chemical reaction model. Chitsomboon and Tiwari [11],[12] used also a finite difference method for similar problems. This particular type of reacting flow was solved again by Chitsomboon, Tiwari, Drummond and Kumar [13], using finite rate chemistry model; in the study, gaseous hydrogen fuel was injected perpendicular to the sidewalls and the fuel struts of an inlet-combustor configuration. The results reported in these studies have indicated that the semi-implicit method together with the global two-step chemistry model provides a viable tool in numerical study of Hydrogen-air reacting flow by using the full Navier-Stokes governing equations. Also, it was concluded that equilibrium chemistry assumption leads to overestimation of the net thrust of scramjet engine, as it predicts higher values of temperature, than that calculated using finite-rate chemistry model.

1.4 Study Objectives

This study is to construct a numerical code capable of resolving the flow features details of mixing and combustion processes, in scramjet engines, applying transverse sonic fuel injection technique. Also, it is aimed to analysis the role of transverse sonic injection, in mixing

enhancement, and flame stabilization. The numerical code is required to be evaluated by several different test cases, dealing with simple aerothermochemical phenomena, in order to be comprehend the nature of supersonic turbulent chemically reacting flow field.

Chapter 2

Mathematical Modeling

2.1 Introduction

For comprehensive modeling of complex flow features taking place in scramjet combustors, such as shock waves, recirculation zones and shock - boundary layer separation, full Navier-Stocks equations are adopted. Neither the thin wall approximation nor the parabolized form of Navier-Stocks equations is incapable of resolving this flow complexity.

2.2 Full Navier-Stocks Governing Equations

Full Navier Stocks equations are applied to resolve thermally equilibrium, chemically non-equilibrium flows. Favre’s weighted-based time averaging [29], which is discussed in details in appendix **B**, is implemented in order to model the turbulence effects. In Addition, flow variables non-dimensionalization is utilized to avoid *round off* errors in numerical calculations as explained in appendix **A**. The dimensionless vector form of “Reynolds averaged Navier-Stocks” Equations (RANS) for planar two-dimensional and internal axisymmetric turbu-

lent chemically reacting flows, can be expressed symbolically as:

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \alpha H = \frac{\partial E_v}{\partial x} + \frac{\partial F_v}{\partial y} + \alpha H_v + S \quad (2.1)$$

where:

$$\alpha = \begin{cases} 0, & \text{Planar two dimensional flow} \\ 1, & \text{Axisymmetric two dimensional internal flow} \end{cases} \quad (2.2)$$

Q is the vector of flow conservative variables. E and F are the convective fluxes vectors, on the other hand E_v and F_v are the diffusive fluxes vectors. The convective and diffusive additional terms for internal axisymmetric flows are H and H_v respectively. Finally, S is the source term vector. The vectors length is equal to $(3 + ns)$ corresponding to the number of equations used for chemically non-equilibrium mixture, where the number of the existing species is equal (ns) . The terms written in equation (2.1) can be expanded as follows:

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E_t \\ \rho Y_m \end{bmatrix}, E = \begin{bmatrix} \rho u \\ \rho u^2 + P \\ \rho uv \\ \rho H_t u \\ \rho Y_m u \end{bmatrix}, F = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + P \\ \rho H_t v \\ \rho Y_m v \end{bmatrix}, H = \frac{1}{y} \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 \\ \rho H_t v \\ \rho Y_m v \end{bmatrix},$$

$$E_v = \begin{bmatrix} 0 \\ \tau_{xx_p} \\ \tau_{xy} \\ \tau_{xx_p} u + \tau_{xy} v - q_x \\ -d_{mx} \end{bmatrix}, F_v = \begin{bmatrix} 0 \\ \tau_{xy} \\ \tau_{yy_p} \\ \tau_{xy} u + \tau_{yy_p} v - q_y \\ -d_{my} \end{bmatrix}, S = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \dot{\omega}_m \end{bmatrix},$$

$$H_v = \frac{1}{y} \begin{bmatrix} 0 \\ \tau_{xy} + y \frac{\partial \tau_a}{\partial x} \\ \tau_{yy_p} + \tau_a - \tau_{\theta\theta} + y \frac{\partial \tau_a}{\partial y} \\ \tau_{xy}u + \tau_{yy_p}v + \tau_a v - q_y + y \left(\frac{\partial}{\partial x} (\tau_a u) + \frac{\partial}{\partial y} (\tau_a v) \right) \\ -d_{my} \end{bmatrix}. \quad (2.3)$$

ρ and P represent the mixture density and pressure respectively. u and v are the velocity components in x and y directions. The mixture total internal energy and total enthalpy are symbolized in E_t and H_t respectively. The thermodynamic relations between flow variables for multi-species mixture will be discussed in details in section **2.3**.

Elements of viscous shear stress tensor represented in: τ_{xx} , τ_{yy} , τ_{xy} , and $\tau_{\theta\theta}$, are shown in the above equations, such that τ_{xx_p} and τ_{yy_p} are the planar two dimensional terms of τ_{xx} and τ_{yy} respectively, and τ_a is the axisymmetric extra term of the both of τ_{xx} and τ_{yy} . Viscous shear stress tensor terms are described in more details in section **2.4**. Also, Modeling of heat fluxes in x and y directions (i.e. q_x and q_y), and mass fluxes in x and y directions (i.e. d_{mx} and d_{my}) is discussed in section **2.5**

Y_m is the mass fraction of the m^{th} species. As shown above, we apply for chemically non-equilibrium mixture of ns species one global continuity equation, plus $(ns - 1)$ individual species equations. The mass fraction of the ns_{th} species Y_{ns} is calculated using the following equation:

$$Y_{n_s} = 1 - \sum_{m=1}^{n_s-1} Y_m. \quad (2.4)$$

2.3 Thermodynamic Model

The whole mixture is treated as an ideal gas governed by the following equation of state:

$$P = \frac{T_{ref}}{V_{ref}^2} \rho R_{mix} T. \quad (2.5)$$

The mixture properties are dependent on properties of the individual species in addition to their mass fractions which represent the degree of dominance of each species in the mixture. The mass fraction is defined as the ratio of the species mass to the mixture mass. Similarly, the mole fraction is the ratio between the species number of moles and the total moles of the mixture:

$$Y_m = \frac{M_m}{M_{mix}}, \quad X_m = \frac{N_m}{N_{mix}}. \quad (2.6)$$

The mixture pressure, density, and other thermodynamic properties like the mixture gas constant and specific heat coefficient at constant pressure on the mass basis are expressed by the following equations:

$$\begin{aligned} \rho &= \sum_{m=1}^{n_s} Y_m \rho_m, & P &= \sum_{m=1}^{n_s} X_m P_m, \\ R_{mix} &= \sum_{m=1}^{n_s} Y_m R_m = \mathcal{R} \sum_{m=1}^{n_s} \frac{Y_m}{\mathcal{M}_m}, & c_{p_{mix}} &= \sum_{m=1}^{n_s} Y_m c_{p_m}. \end{aligned} \quad (2.7)$$

The mixture enthalpy and internal energy are calculated from the superposition of the contributions of the individual species, where each species enthalpy or internal energy is dependent on its heat of formation, and the behavior of its specific heat coefficients with temperature, as follows:

$$\begin{aligned} h &= \sum_{m=1}^{n_s} Y_m h_m, & e &= \sum_{m=1}^{n_s} Y_m e_m, & h_m &= \frac{1}{V_{ref}^2} \left[h_{f_m}^o + \int_{T_o}^{T^*} c_{p_m} dT^* \right], \\ e_m &= \frac{1}{V_{ref}^2} \left[h_{f_m}^o + \int_{T_o}^{T^*} c_{v_m} dT^* \right] = \frac{1}{V_{ref}^2} \left[h_{f_m}^o + \int_{T_o}^{T^*} (c_{p_m} - \frac{\mathcal{R}}{\mathcal{M}_m}) dT^* \right], \end{aligned} \quad (2.8)$$

where T^* is the temperature value before non-dimensionalization:

$$T^* = T.T_{ref}. \quad (2.9)$$

We assume that specific heat coefficient for each species (c_{p_m}) is a polynomial function in the Temperature (T). According to McBride et al. [43], the polynomial coefficients for different species (i.e. O_2 , H_2O , H_2 , OH , N_2) are presented in appendix **D**, for The mixture total enthalpy (H_t) and the total internal energy are summation of the kinetic energy to the mixture enthalpy and internal energy respectively:

$$\begin{aligned} H_t &= h + \frac{1}{V_{ref}^2} \frac{(u^2 + v^2)}{2} = \frac{1}{V_{ref}^2} \left[h_{f_{mix}}^o + \int_{T_o}^{T^*} c_{p_{mix}} d\tau + \frac{(u^2 + v^2)}{2} \right], \\ E_t &= e + \frac{1}{V_{ref}^2} \frac{(u^2 + v^2)}{2} \\ &= \frac{1}{V_{ref}^2} \left[h_{f_{mix}}^o + \int_{T_o}^{T^*} (c_{p_{mix}} - R_{mix}) dT^* + \frac{(u^2 + v^2)}{2} \right], \end{aligned} \quad (2.10)$$

where the mixture enthalpy of formation is defined in the index notation as:

$$h_{f_{mix}}^o = \sum_{m=1}^{n.s} Y_m h_{f_m}^o. \quad (2.11)$$

From the previous we can conclude the relation between the total enthalpy and total internal energy as following:

$$\begin{aligned} H_t - E_t &= \frac{R_{mix}}{V_{ref}^2} (T - T_o) = \frac{P}{\rho} - \frac{R_{mix}}{V_{ref}^2} T_o, \\ h_s - e_s &= \frac{P}{\rho} - \frac{R_{mix}}{V_{ref}^2} T_o, \end{aligned} \quad (2.12)$$

where (h_s) and (e_s) are the mixture sensible enthalpy and the mixture sensible internal energy respectively, they are defined as:

$$h_s = h - h_{f_{mix}}^o = \int_{T_o}^{T^*} c_{p_{mix}} dT^*, \quad e_s = e - h_{f_{mix}}^o = \int_{T_o}^{T^*} (c_{p_{mix}} - R_{mix}) dT^*. \quad (2.13)$$

The reference temperature degree (T_o) is set to be the absolute zero, to ensure positive sensible enthalpy and sensible internal energy as recommended by Anderson [1], to enhance the stability of the numerical solution. So, the relation between the mixture pressure and density to the mixture sensible internal energy becomes:

$$\frac{P}{\rho} = (h_s - e_s) + \frac{R_{mix}}{V_{ref}^2} T_o = e_s \left(\frac{h_s}{e_s} - 1 \right) + \frac{R_{mix}}{V_{ref}^2} T_o = e_s (\gamma - 1) + \frac{R_{mix}}{V_{ref}^2} T_o \quad (2.14)$$

The ratio of the mixture sensible enthalpy to the mixture internal energy is considered as the “*equivalent*” specific ratio of the multi-species mixture to simplify the complexity of the thermodynamic relations as discussed by Shuen and Yoon [54]. So the specific heat ratio is no longer defined by the ratio of the specific heat coefficient at constant pressure to that at constant volume, (i.e. $\gamma \neq c_p/c_v$), but it is defined as follows:

$$\gamma = \frac{h_s}{e_s} = \frac{\int_{T_o}^{T^*} c_{p_{mix}} dT^*}{\int_{T_o}^{T^*} (c_{p_{mix}} - R_{mix}) dT^*} \quad (2.15)$$

2.4 Viscous Stress Tensor Modeling

The viscous shear stress tensor is dependent on the velocity spatial gradients, and on dynamic viscosity coefficient of the mixture. For planar and axisymmetric 2D flows, its diagonal elements are represented in τ_{xx} , τ_{yy} , and $\tau_{\theta\theta}$, where τ_{xy} is the off-diagonal element in

the (x, y) domain. The diagonal elements (τ_{xx} , and τ_{yy}) are given as follows:

$$\tau_{xx} = \tau_{xx_p} + \tau_a, \quad \tau_{yy} = \tau_{yy_p} + \tau_a. \quad (2.16)$$

τ_{xx_p} and τ_{yy_p} are the longitudinal viscous shear stress in planar 2D coordinates. And τ_a represent the additional term for each of τ_{xx} and τ_{yy} in case of axisymmetric 2D flows. They are expressed in dimensionless form as follows:

$$\tau_{xx_p} = \frac{1}{Re_{ref}} \mu \left[\frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right], \quad \tau_{yy_p} = \frac{1}{Re_{ref}} \mu \left[\frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} \right], \quad (2.17)$$

$$\tau_a = -\frac{2}{3} \frac{1}{Re_{ref}} \left(\frac{v}{y} \right),$$

where Re_{ref} is the reference “Reynolds number”, which is formulated in terms of the characteristic reference variables of the studied test case as in the next equation:

$$Re_{ref} = \frac{\rho_{ref} V_{ref} L_{ref}}{\mu_{ref}} \quad (2.18)$$

Also, the last diagonal element of axisymmetric 2D flows ($\tau_{\theta\theta}$) is written as:

$$\tau_{\theta\theta} = \frac{1}{Re_{ref}} \mu \left[\frac{4}{3} \frac{v}{y} - \frac{2}{3} \left(\frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) \right] \quad (2.19)$$

Finally, the off-diagonal element (τ_{xy}) is given in terms of the velocity gradients as follows:

$$\tau_{xy} = \frac{1}{Re_{ref}} \mu \left[\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \right] \quad (2.20)$$

The total dynamic viscosity (μ) is considered the summation of the laminar dynamic viscosity coefficient (μ_L), to the turbulent eddy coefficient (μ_T):

$$\mu = \mu_L + \mu_T \quad (2.21)$$

the former term, which is considered as the laminar dynamic viscosity coefficient of the mixture, is taken as the same of nitrogen, due

to the dominance of the nitrogen properties in the mixture for air-Hydrogen combustion systems. According to Chitsomboon and Tiwari [12], Sutherland’s equation for the nitrogen dynamic viscosity as a function in temperature is given as follows:

$$\mu_L = \frac{(1.458 \times 10^{-6}) T^{*\frac{3}{2}}}{T^* + 110.4} \quad (2.22)$$

On the other hand, the later term is equivalent to the effect of the velocity turbulent fluctuations, where the turbulent Reynolds’ shear stresses are modeled basing on Boussineq’s assumption [7], as shown in appendix **B**. More detailed explanation of turbulent eddy coefficient modeling is presented in section **2.7**.

2.5 Mass and Heat Fluxes Modeling

Mass concentrations and temperature gradients in space result in the transfer of diffusive mass and heat fluxes respectively, the mass fluxes d_{mx} and d_{my} of the m^{th} species in the x and y directions are written as below:

$$\begin{aligned} d_{mx} &= \frac{-1}{Re_{ref} Sc_{ref}} \left(\rho \mathcal{D}_L + \frac{\mu_T}{Sc_T} Sc_{ref} \right) \frac{\partial Y_m}{\partial x}, \\ d_{my} &= \frac{-1}{Re_{ref} Sc_{ref}} \left(\rho \mathcal{D}_L + \frac{\mu_T}{Sc_T} Sc_{ref} \right) \frac{\partial Y_m}{\partial y}. \end{aligned} \quad (2.23)$$

$\mathcal{D}_L$ is the laminar mass diffusivity coefficient of m^{th} species into the mixture. It is observable that it is set constant for all species. In addition, Sc_{ref} is the problem characteristic “Schmidt number”, which is given as:

$$Sc_{ref} = \frac{\mu_{ref}}{\rho_{ref} \mathcal{D}_{ref}}. \quad (2.24)$$

On the other hand, the heat transfer is in the x and y directions is written as follows:

$$q_x = \frac{\left[\frac{-1}{(\gamma_{ref}-1)\mathbf{M}_{ref}^2 Pr_{ref}} k_L \frac{\partial T}{\partial x} - \frac{1}{Sc_{ref}} \sum_{m=1}^{n_s} h_m \rho \mathcal{D}_L \frac{\partial Y_m}{\partial x} - \frac{\mu_T}{Pr_T} \frac{\partial h}{\partial x} \right]}{Re_{ref}}$$

$$q_y = \frac{\left[\frac{-1}{(\gamma_{ref}-1)\mathbf{M}_{ref}^2 Pr_{ref}} k_L \frac{\partial T}{\partial y} - \frac{1}{Sc_{ref}} \sum_{m=1}^{n_s} h_m \rho \mathcal{D}_L \frac{\partial Y_m}{\partial y} - \frac{\mu_T}{Pr_T} \frac{\partial h}{\partial y} \right]}{Re_{ref}} \quad (2.25)$$

k_L is considered to be the mixture laminar conductivity coefficient. $\mathbf{M}_{ref}$ and Pr_{ref} are the reference values of “Mach number” and “Prandtl number” respectively, which are expressed as:

$$Pr_{ref} = \frac{\mu_{ref} c p_{ref}}{k_{ref}} \quad \mathbf{M}_{ref} = \frac{V_{ref}}{\sqrt{\gamma_{ref} R_{ref} T_{ref}}} \quad (2.26)$$

The turbulent terms of “Schmidt number” (Sc_T) and “Prandtl number” (Pr_T) are utilized to model the mass and heat turbulent fluxes respectively as shown in appendix **B**. They are set to be constants as follows:

$$Sc_T = 0.9, \quad Pr_T = 0.9. \quad (2.27)$$

Modeling of mass and heat laminar transport coefficients (i.e. $\mathcal{D}_L$ and k_L) is based on assuming constant values of the laminar terms of “Prandtl number” and “Lewis number”. So, the laminar coefficients of mass diffusivity and heat conductivity can be easily calculated in terms of the laminar viscosity coefficient given in equation (2.22). First, the laminar “Prandtl number” is taken according to Chitsomboon and Tiwari [12] as:

$$Pr_L = 0.72 \quad (2.28)$$

And, the laminar conductivity coefficient (k_L) is determined as following:

$$k_L = \frac{c_{p_{mix}} \mu_L}{Pr_L} \quad (2.29)$$

Second, it is well-known assumption, in combustion studies, to equate between the heat and mass diffusivity coefficients, through setting the value “Lewis number” to unity:

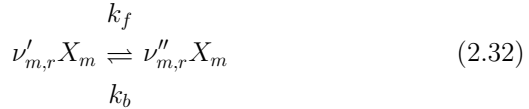
$$Le = 1 \quad (2.30)$$

So the mass diffusivity laminar coefficient is expressed in terms of the laminar conductivity coefficient as follows:

$$\mathcal{D}_L = \frac{k_L}{\rho \, Le \, c_{p_{mix}}} \quad (2.31)$$

2.6 Chemistry Modeling

Decoupling between Chemistry and Turbulence models is adopted in this study. The random fluctuations in the magnitudes of temperature and mass fractions are not considered in the calculations of the species source terms. For chemically reacting non-equilibrium air-Hydrogen system, the combustion process is modeled using a mechanism composed of a number of elementary reactions, not only one global reaction. Each elementary equation can be written as following:



(ν') and (ν'') are the stoichiometric coefficients of the reactants and products respectively of each elementary reaction of index (r) , where $r = 1, 2, \dots, n_r$, where (n_r) is the total number of elementary reactions in the mechanism. (k_f) and (k_b) are the chemical reaction rates in the forward and backward directions respectively. More elementary reactions are set, more the number of the intermediate species are considered, more species continuity equation are studied, and more complex the solution of the system of equations. The source term of each species of index $(“m”)$ is calculated using the “law of mass

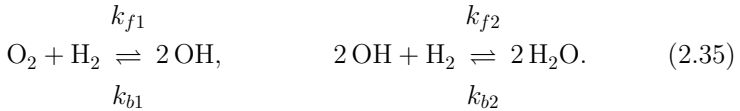
action". It is written in the dimensionless form as follows:

$$\dot{\omega}_m = \frac{L_{ref} \mathcal{M}_m \sum_{r=1}^{n_r} \left[(\nu'_{m,r} - \nu''_{m,r}) \left(k_{fr} \prod_{m=1}^{n_s} \left(\frac{\rho Y_m}{\mathcal{M}_m} \right)^{\nu'_{m,r}} - k_{br} \prod_{m=1}^{n_s} \left(\frac{\rho Y_m}{\mathcal{M}_m} \right)^{\nu''_{m,r}} \right) \right]}{\rho_{ref} V_{ref}} \quad (2.33)$$

The forward reaction rate (k_f) is highly dependent on temperature, and the thermal energy level of the mixture compared to the activation energy of each elementary reaction. It is calculated using the Arrhenius' formula whose coefficients and the temperature exponent is determined experimentally, it is written as following for each elementary reaction of index (r):

$$k_{fr} = \mathcal{A}_r T^{\mathcal{N}_r} \exp \left(\frac{-E_{actv,r}}{\mathcal{R} T} \right) \quad (2.34)$$

Air-Hydrogen combustion system is modeled by using the two reactions mechanism suggested by Rogers and Chinitz [48], this two reactions model includes four reacting species (O_2 , H_2O , H_2 , and OH), besides Nitrogen N_2 , which is assumed to be inert, because the mixture temperature in our applications is not so high to initiate the Nitrogen-Oxides formation:



The forward reaction rates for the two reactions are:

$$k_{f1} = \mathcal{A}_1 T^{-10} \exp \left(\frac{-4063.6485}{\mathcal{R} T^*} \right), \quad k_{f2} = \mathcal{A}_2 T^{-13} \exp \left(\frac{-35499.4988}{\mathcal{R} T^*} \right). \quad (2.36)$$

In equation (2.36), the calculations are set to use the universal gas constant ($\mathcal{R}$) by using [$kcal/kmole K$] units, (i.e. $\mathcal{R} = 1.98589 [kcal/kmole K]$). The pre-exponential coefficients for the elementary reaction are func-

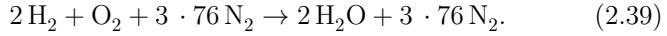
tion of the equivalence ratio (ϕ), as following:

$$\begin{aligned}\mathcal{A}_1 &= \left[8.917\phi + \frac{31.433}{\phi} - 28.95 \right] (10)^{44} [m^3/kmol \text{ sec}] , \\ \mathcal{A}_2 &= \left[2 + \frac{1.333}{\phi} - 0.833\phi \right] (10)^{58} [m^6/kmol^2 \text{ sec}] .\end{aligned}\quad (2.37)$$

The equivalence here is defined as the ratio between the ratio of actual Hydrogen to oxygen ratio, and between the stoichiometric Hydrogen to oxygen ratio:

$$\phi = \frac{F/O_{st}}{F/O}. \quad (2.38)$$

The stoichiometric Hydrogen to oxygen ratio is concluded from the one global air-Hydrogen reaction:



The stoichiometric Hydrogen to oxygen mass ratio is equal to:

$$F/O_{st} = 0.125. \quad (2.40)$$

The actual Hydrogen to oxygen ratio is defined here by the ratio of the Hydrogen content to the oxygen content in the mixture, in our study system of five species. So, the actual Hydrogen to Oxygen ratio is written as:

$$F/O = \frac{Y_{\text{H}_2} + \frac{\mathcal{M}_{\text{H}_2}}{\mathcal{M}_{\text{H}_2\text{O}}} Y_{\text{H}_2\text{O}} + \frac{\mathcal{M}_{\text{H}_2}}{\mathcal{M}_{\text{OH}}} Y_{\text{OH}}}{Y_{\text{O}_2} + 0.5 \frac{\mathcal{M}_{\text{O}_2}}{\mathcal{M}_{\text{H}_2\text{O}}} Y_{\text{H}_2\text{O}} + 0.5 \frac{\mathcal{M}_{\text{O}_2}}{\mathcal{M}_{\text{OH}}} Y_{\text{OH}}}. \quad (2.41)$$

The backward reaction rates is calculated given the rates in the forward directions, they are related by the reaction equilibrium constant (K_p) as following:

$$k_{b1} = \frac{k_{f1}}{K_{p1}} \quad k_{b2} = \frac{k_{f2}}{K_{p2}} \quad (2.42)$$

The reaction equilibrium constant, as well as, the reaction backward rate, for the two-step mechanism are given as below:

$$\begin{aligned} K_{p1} &= 26.16 \exp\left(\frac{-8992}{T^*}\right), \\ K_{p2} &= (2.682 \times 10^{-9}) (T^*) \exp\left(\frac{69415}{T^*}\right) \quad [m^3/kmol]. \end{aligned} \quad (2.43)$$

It is so important to mention that the two-step mechanism is not accurate in temperature range within 1000[K], as it wrongly predicts that chemical reaction takes below 1000[K], and does not consider the long ignition time delay as the temperature is below the ignition temperature. So, Tiwari and Chitsomboon [12]. suggest to set in the numerical solver to prevent any chemical reaction for temperature less than 1000[K].

2.7 Turbulent Dynamic Viscosity Modeling

Algebraic Baldwin-Lomax turbulence model is applied in calculating The turbulent eddy coefficient eddy (μ_T). It is considered a two-layer turbulence model; where the turbulent dynamic viscosity coefficient (μ_T) is calculated with one of two different sets of algebraic equations, depending on the position from boundary walls, or jets centerlines:

$$\mu_T = \begin{cases} \mu_{T_{in}}, & n \leq n_{cross} \\ \mu_{T_{out}}, & n > n_{cross} \end{cases} \quad (2.44)$$

where (n) the distance from the wall (or the centerline of the wake or jet), and (n_{cross}) is the minimum distance, at which the eddy viscosity coefficients for both the inner and outer regions, i.e. ($\mu_{T_{in}}$ and $\mu_{T_{out}}$). From the turbulent viscosity profile μ_T for the two-layer model is illustrated in figure (2.1), we can find that the criterion to

calculate (μ_T) as following:

$$\mu_T = \min(\mu_{T_{in}}, \mu_{T_{out}}) \quad (2.45)$$

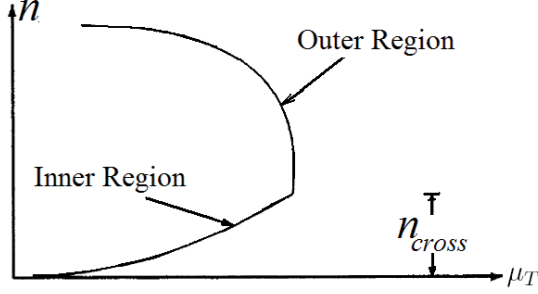


Figure 2.1: Typical Profile Turbulent Viscosity Coefficient for the Algebraic Two-Layer Turbulence (Wilcox [65])

The sets of calculations for two regions are listed as following:

- **Inner Region** The inner region eddy viscosity coefficient ($\mu_{T_{in}}$) is calculated in terms of the mixing length (l_{mix}), and the vorticity vector magnitude (ω) as following:

$$\mu_{T_{in}} = \rho l_{mix}^2 \omega \quad (2.46)$$

- **Outer Region** The eddy viscosity of the outer layer ($\mu_{T_{out}}$) is calculated as following:

$$\mu_{T_{out}} = \rho K C_p F_{wake} F_{Klep} \quad (2.47)$$

where, The vorticity vector magnitude for 2D coordinates is written as:

$$\omega = \sqrt{\left[\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right]^2} \quad (2.48)$$

As this turbulence model is based on *Prandtl's mixing length hypothesis*, we have to define the mixing length in the form proposed by Van Driest:

$$l_{mix} = \kappa n \left(1 - e^{-n^+/A^+}\right) \quad (2.49)$$

The damping factor (e^{-n^+/A^+}) is eliminated for the case of wakes and jets. (n^+) is defined as the dimensionless distance from the boundary wall, referred to the flow properties at the wall. And, it is one of the main parameters of the **law of the wall**, the other parameter is the dimensionless velocity (u^+), which is defined as the ratio between the velocity magnitude ($\tilde{V}$) to the wall friction velocity (u_τ):

$$u_\tau = \sqrt{\frac{\tau_w}{\rho_w}}, \quad n^+ = \frac{u_\tau \rho_w n}{\mu_{L_w}}, \quad u^+ = \frac{V}{u_\tau}. \quad (2.50)$$

For above equations, we have to mention that in the case of non wall-bounded regions like wakes and jets the dimensionless velocity (u^+) is also equal to zero, and to point that the friction velocity is (u_τ) is dependent on the wall shear stress (τ_w) and the mixture density at the wall ($\bar{\rho}_w$).

The other terms presented in equation (2.47) is presented as following:

$$F_{wake} = \min\left(n_{max} F_{max}, C_{wk} n_{max} \frac{u_{diff}^2}{F_{max}}\right) \quad (2.51)$$

$$F_{Kleb} = \left[1 + 5.5 \left(\frac{n C_{Kleb}}{n_{max}}\right)^6\right]^{-1} \quad (2.52)$$

where (u_{diff}) is the difference in the between the maximum and minimum velocities magnitudes in the boundary layer, i.e. ($u_{diff} = V_{max} - V_{min}$), so in the wall-bounded domains the minimum velocity equals zero and so $u_{diff} = V_{max}$. Besides, (F_{max}) is the max value of the intermediate function $F(n)$ along a certain line normal to the wall or normal to the centerline of the jet. This function is written as

following:

$$F(n) = \frac{1}{\kappa} l_{mix} \omega, \quad F_{max} = \max_n [F(n)], \quad n_{max} = n|_{F_{max}}. \quad (2.53)$$

As shown above, n_{max} is the normal distance (n) at which the function (F) reaches its maximum value. This turbulence approach consists of six closure constant listed below according to Baldwin and Lomax [2]:

$$\begin{aligned} A^+ &= 26, & C_{cp} &= 1.6, & C_{Kleb} &= 0.3, \\ C_{wk} &= 0.25, & \kappa &= 0.4, & K &= 0.0168. \end{aligned} \quad (2.54)$$

In spite of the excellent performance of the Baldwin and Lomax method in solving attached flows, it predicts incorrectly the separation point location for strong pressure gradients. Degani and Schiff [20], added some modifications to Baldwin and Lomax model to eliminate the reasons leading to the model deficiency when used in separated flows. They found that there are dramatic differences in the behavior of the intermediate function $F(n)$ in the attached and separated flows, which have considerable effects on the calculations. In part (a) of figure (2.2), it is found that there is *one local maximum point* in the function $F(n)$, where the global maximum of the function (F_{max}) can be estimated. However, in separated flows, illustrated in part (b), there will be *multiple local maxima*. By implementing equation (2.53) to get (F_{max}), the global maximum will be selected, which is not considered the right choice. That is because the local maxima far away from the wall or jets, represent recirculating zone of high vorticity magnitude. The right choice is to select the nearest local maximum from the wall or jet centerline in order to substitute in the turbulence model calculations with the physical correct values of F_{max} and n_{max} .

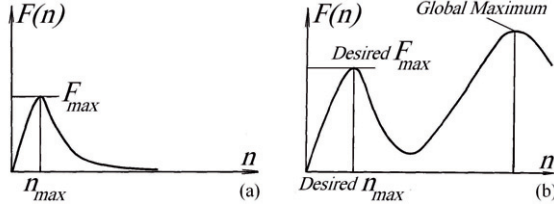


Figure 2.2: **The intermediated function $F(n)$ behavior for: (a) attached flows and (b) separated flows**

The normal distance from the wall is calculated as mentioned in reference [36]; It is defined as the normal distance from the concerned point to the wall at the point of the same vertical mesh line. For more explanation: if we have a point of spatial indices (i, j) , i.e. found at the intersection of the i^{th} vertical mesh line and the j^{th} horizontal mesh line, the normal distance to the wall is from the previously mentioned point to the point at the wall with the same (i) index. Note the mesh line of (j) indices is parallel to the wall.

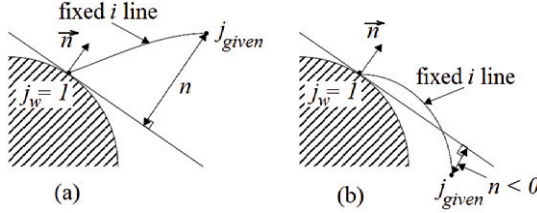


Figure 2.3: **Schematic for the calculations of the normal distance from the wall, [36]**

The normal distance is equal to the component of the vector $(\vec{r}_{wp})$ originated from the wall at the point of spatial indices (i, j_w) to the specified point of indices (i, j) , in the direction of the unit vector normal to the wall $(\hat{n}_w)$. The vector is $(\vec{r}_{wp})$ is the difference between the two position

vector: the position vector of the specified point ($\vec{r}_p$) and that of the point at the wall ($\vec{r}_w$):

$$n = \vec{r}_{wp} \cdot \hat{n}_w + (\vec{r}_p - \vec{r}_w) \cdot \hat{n}_w \quad (2.55)$$

As shown in figure (2.3), the normal distance calculations are acceptable for mesh lines having smooth curvatures, as in part (a). But for very strong curvatures, there will be incorrect estimation of the normal distance, as shown in part (b). It is recommended for the second case to utilize field equations turbulence models instead.

Chapter 3

Numerical Method

3.1 Introduction

Computational procedures to solve turbulent chemically reacting flow are represented in discretizing the domain of the test case required to be solved, into a number of cells, where the finite-volume method is applied in each cell (which is considered as a control volume) and utilize the governing equation presented in (2.1) in a discretized integral form. As a result, the equation can be written in terms of the flow variables and fluxes at the cell's centroid and faces, where the faces convective fluxes will be modeled utilizing approximate Riemann solvers proposed by Roe [47]. Furthermore, second order spatial accuracy is attained by primitive variable extrapolation using MUSCL approach "Monotone Upstream-Centered Schemes for Conservative Laws", which is first suggested by Van-Leer [60], and it is named after his numerical code applying it. On the other hand, the diffusive (or viscous) fluxes are centrally discretized satisfying the second order accuracy in space.

As we are interested in steady-state flows, the final steady-state solution can be achieved by pseudo time integrating the governing equations. The time marching is of second order temporal accurate, by implementing two-step Runge-Kutta method. And, to overcome the stiffness caused by the chemical source term, and to avoid heavy computa-

tions of inversion of huge matrices required in fully implicit schemes, it is set to treat the flow terms explicitly and chemically source term implicitly. This scheme is called the point-implicit or chemistry-implicit scheme.

Algebraic grid generator is used for domain discretization, where the mesh points are clustered in the regions near walls and around jets using different clustering functions. All computations are carried out in a Cartesian generalized domain, to which the equations are transformed from the physical domain. More detailed insight for the computational solving features will be illustrated in this chapter.

3.2 Physical to Computational Domain Transformation

To simply the discretized equations for structured meshes, it is recommended that all domain cells have the same dimensions. That is can be fulfilled by transforming the governing equations from the physical domain to a generalized domain having an equal spatial step between grid points.

3.2.1 Governing Equations in The Computational Domain

By applying the transformation relations between the physical domain (x, y) and computational domain (ξ, η) . The flux vector form of the governing equations, which is written in the physical domain as in equation (2.1), can be written in the computational domain as follows:

$$\frac{\partial \overline{Q}}{\partial t} + \frac{\partial \overline{E}}{\partial \xi} + \frac{\partial \overline{F}}{\partial \eta} + \alpha \overline{H} = \frac{\partial \overline{E}_v}{\partial \xi} + \frac{\partial \overline{F}_v}{\partial \eta} + \alpha \overline{H}_v + \overline{S}, \quad (3.1)$$

where:

$$\begin{aligned}
\overline{Q} &= \frac{1}{J}Q, \\
\overline{E} &= \frac{1}{J}(\xi_x E + \xi_y F), & \overline{F} &= \frac{1}{J}(\eta_x E + \eta_y F), \\
\overline{E}_v &= \frac{1}{J}(\xi_x E_v + \xi_y F_v), & \overline{F}_v &= \frac{1}{J}(\eta_x E_v + \eta_y F_v), \\
\overline{H} &= \frac{1}{J}H, & \overline{H}_v &= \frac{1}{J}H_v, & \overline{S} &= \frac{1}{J}S, \quad (3.2)
\end{aligned}$$

where the transformation relations between the physical domain and the computational are:

$$\begin{aligned}
J &= \frac{\partial(\xi, \eta)}{\partial(x, y)} = \frac{1}{x_\xi y_\eta - x_\eta y_\xi}, \\
\xi_x &= \frac{\partial \xi}{\partial x} = J y_\eta = J \frac{\partial y}{\partial \eta}, & \xi_y &= \frac{\partial \xi}{\partial y} = -J x_\eta = -J \frac{\partial x}{\partial \eta}, \\
\eta_x &= \frac{\partial \eta}{\partial x} = -J y_\xi = -J \frac{\partial y}{\partial \xi}, & \eta_y &= \frac{\partial \eta}{\partial y} = J x_\xi = J \frac{\partial x}{\partial \xi}. \quad (3.3)
\end{aligned}$$

For more computations simplification, the spatial step in the computational domain in either ξ or η directions (i.e. $\Delta\xi$, and $\Delta\eta$) have the same length, which is equal to unity, as illustrated in figure (3.1). Furthermore, that makes each point spatial indices in ξ and η directions, which are notated as i and j respectively determine precisely its location in the computational space.

3.2.2 Declaration of Vectors Normal to Cell Faces

Defining the vector normal to the cell faces and the structured grid lines in the physical space is necessary in our computations, to determine the normal distance from the wall as in equation (2.55), also to calculate the velocities normal to the boundary cell faces and compare them with eigenvalues at boundaries as discussed in details in section 3.5.

At first, the vector normal to a horizontal line of fixed (j) index (or fixed value of eta) must parallel to the vector ($\vec{n}$) which is defined as:

$$\vec{n}_{j-fixed} = \eta_x \vec{i} + \eta_y \vec{j}. \quad (3.4)$$

And, the unit vector in its direction is written as:

$$\hat{n}_{j-fixed} = \frac{\eta_x \vec{i} + \eta_y \vec{j}}{|\nabla\eta|}, \quad (3.5)$$

where: $|\nabla\eta| = \sqrt{\eta_x^2 + \eta_y^2}$.

In like manner for the unit vector normal to vertical line of fixed i -index (or fixed ξ) is expressed as:

$$\hat{n}_{i-fixed} = \frac{\xi_x \vec{i} + \xi_y \vec{j}}{|\nabla\xi|}, \quad (3.6)$$

where: $|\nabla\xi| = \sqrt{\xi_x^2 + \xi_y^2}$.

Similarly, when talking about the contravariant velocities, which are normal to the cell faces, and so they are perpendicular to the grid lines, they are written as follows:

$$\mathcal{U} = \vec{\nabla}\xi \cdot \vec{V} = \xi_x u + \xi_y v, \quad \mathcal{V} = \vec{\nabla}\eta \cdot \vec{V} = \eta_x u + \eta_y v, \quad (3.7)$$

where ($\mathcal{U}$) and ($\mathcal{V}$) are the contravariant velocities normal to the cell faces in the directions of ξ and η respectively. Consequently, the physical velocity components ($\mathcal{U}'$, $\mathcal{V}'$), which are normal to the mesh lines of fixed values of ξ and η respectively, and directed into the inside domain, can be expressed as:

$$\mathcal{U}' = \hat{n}_{i-fixed} \cdot \vec{V} = \frac{\xi_x u + \xi_y v}{|\nabla\xi|}, \quad \mathcal{V}' = \hat{n}_{j-fixed} \cdot \vec{V} = \frac{\eta_x u + \eta_y v}{|\nabla\eta|}. \quad (3.8)$$

3.2.3 Eigenvalues of the convective flux Jacobian in The Computational Domain

As we can write the general form of the eigenvalues in the vector notation as:

$$\begin{aligned}\lambda_1, \lambda_2, \dots, \lambda_{ns}, \lambda_{ns+1} &= \vec{V} \cdot \hat{n}, \\ \lambda_{ns+2} &= \vec{V} \cdot \hat{n} + c, \\ \lambda_{ns+3} &= \vec{V} \cdot \hat{n} - c,\end{aligned}\tag{3.9}$$

where $(\hat{n})$ is the unit vector normal to the boundary and directed inward the domain. By substitution equation (3.8) in the above equation, we can write the eigenvalues of the Jacobian matrix of the convective fluxes in ξ -direction and η -direction as follows:

- **Eigenvalues of the convective flux Jacobian in ξ -direction**

$$\begin{aligned}\lambda_{\xi_1}, \lambda_{\xi_2}, \dots, \lambda_{\xi_{ns}}, \lambda_{\xi_{ns+1}} &= \mathcal{U}' \\ \lambda_{\xi_{ns+2}} &= \mathcal{U}' + c \\ \lambda_{\xi_{ns+3}} &= \mathcal{U}' - c\end{aligned}\tag{3.10}$$

- **Eigenvalues of the convective flux Jacobian in η -direction**

$$\begin{aligned}\lambda_{\eta_1}, \lambda_{\eta_2}, \dots, \lambda_{\eta_{ns}}, \lambda_{\eta_{ns}} &= \mathcal{V}' \\ \lambda_{\eta_{ns+2}} &= \mathcal{V}' + c \\ \lambda_{\eta_{ns+3}} &= \mathcal{V}' - c\end{aligned}\tag{3.11}$$

As we know that that eigenvalues for any system have no unique values, and so they can be scaled by some factor. We can write the eigenvalues for both the convective fluxes Jacobians in ξ and η directions, after multiplying them by $|\nabla\xi|$ and $|\nabla\eta|$, respectively:

- **Eigenvalues of the convective flux Jacobian in ξ -direction**

$$\begin{aligned}\lambda_{\xi_1}, \lambda_{\xi_2}, \dots, \lambda_{\xi_{ns}}, \lambda_{\xi_{ns+1}} &= \mathcal{U}, \\ \lambda_{\xi_{ns+2}} &= \mathcal{U} + c |\nabla\xi|, \\ \lambda_{\xi_{ns+3}} &= \mathcal{U} - c |\nabla\xi|.\end{aligned}\tag{3.12}$$

• **Eigenvalues of the convective flux Jacobian in η -direction**

$$\begin{aligned}\lambda_{\eta_1}, \lambda_{\eta_2}, \dots, \lambda_{\eta_{ns}}, \lambda_{\eta_{ns}} &= \mathcal{V}, \\ \lambda_{\eta_{ns+2}} &= \mathcal{V} + c |\nabla \eta|, \\ \lambda_{\eta_{ns+3}} &= \mathcal{V} - c |\nabla \eta|.\end{aligned}\tag{3.13}$$

3.3 Spatial Discretization

Here, different elements of equations discretization in space will be considered in more details, represented in Finite-volume Method formulation of the governing equation at each cell in the computational domain, and modeling the convective and diffusive fluxes at each cell face.

3.3.1 Structured Finite-Volume Scheme

The Integral Vector Form of Governing Equations

Starting from equation (3.1) the integral vector form for cell of volume ($\mathbb{V}$) is described as:

$$\begin{aligned}\iiint_{\mathbb{V}} \left[\frac{\partial \bar{Q}}{\partial t} + \frac{\partial (\bar{E} - \bar{E}_v)}{\partial \xi} + \frac{\partial (\bar{F} - \bar{F}_v)}{\partial \eta} \right] d\mathbb{V} &= \\ &= \iiint_{\mathbb{V}} \bar{S} d\mathbb{V} - \alpha \iiint_{\mathbb{V}} (\bar{H} - \bar{H}_v) d\mathbb{V},\end{aligned}\tag{3.14}$$

where the cell's depth in the 2D computational space is unity, so the cell's volume according to figure (3.1) is equal to:

$$d\mathbb{V} = d\xi \cdot d\eta \cdot 1.\tag{3.15}$$

By applying Green's theory for volume integration for vector divergence ($\vec{\nabla} \cdot \vec{\mathbf{F}}$), where:

$$\begin{aligned}\vec{\mathbf{F}} &= (\overline{E} - \overline{E}_v) \vec{\mathbf{i}} + (\overline{F} - \overline{F}_v) \vec{\mathbf{j}}, \\ \vec{\nabla} \cdot \vec{\mathbf{F}} &= \frac{\partial (\overline{E} - \overline{E}_v)}{\partial \xi} + \frac{\partial (\overline{F} - \overline{F}_v)}{\partial \eta}.\end{aligned}\quad (3.16)$$

Green's theory states in case of 2D domain:

$$\iiint_{\mathbb{V}} \vec{\nabla} \cdot \vec{\mathbf{F}} d\mathbb{V} = \iint_{\mathbb{S}} \vec{\mathbf{F}} \cdot \hat{n}_{\mathbb{S}} d\mathbb{S} = \iint_{\mathbb{S}} [(\overline{E} - \overline{E}_v) d\eta + (\overline{F} - \overline{F}_v) d\xi]. \quad (3.17)$$

where ($\hat{n}_{\mathbb{S}}$) is the unit vector directed outgoing the control volume normal to its surface of total area ($\mathbb{S}$). Substituting in equation (3.14) yields:

$$\begin{aligned}\iiint_{\mathbb{V}} \frac{\partial \overline{Q}}{\partial t} d\xi d\eta + \iint_{\mathbb{S}} [(\overline{E} - \overline{E}_v) d\eta + (\overline{F} - \overline{F}_v) d\xi] &= \\ &= \iiint_{\mathbb{V}} \overline{S} d\xi d\eta - \alpha \iiint_{\mathbb{V}} (\overline{H} - \overline{H}_v) d\xi d\eta.\end{aligned}\quad (3.18)$$

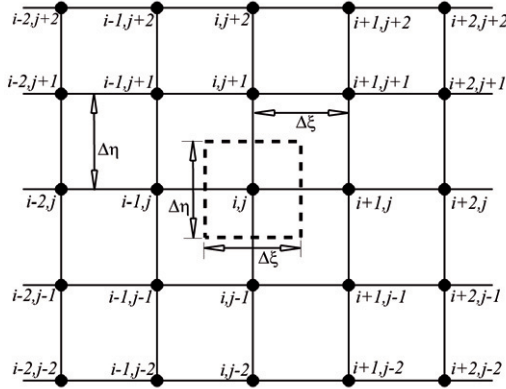


Figure 3.1: **Finite-Volume scheme terminology for the structured mesh in the computational space**

Discretized Control Volume Terminology

Finite-volume scheme can be classified into two classes: The first class, which is called *cell-centered* schemes, carry out the computations in terms of the flow variables at the centroids of the discrete control volumes. On the other hand, *cell-vertex* schemes apply the governing equations using the flow variables at the cell vertices. Also, there is another categorizing of these schemes for, the first category set the control volumes centroids at the mesh nodes. In contrast, the other group of schemes make the control volumes coincide on the mesh cells, where the control volume vertices are located at the mesh nodes.

In our numerical model, as illustrated in figure (3.1), the utilized finite-volume scheme evaluates the flow equations and store the domain variables in the *centroids* of individual control volumes, which are positioned at the mesh *nodes* of the discretized computational domain. Consequently, each *face's midpoint* is lying in the halfway between two mesh nodes, and *vertices* of the control volume is found in the middle of the surrounding *grid cells*. According to this definition, this scheme can be considered as *cell-center-nodal* finite-volume scheme.

The whole computational domain is discretized into individual control volume, whose flow properties are evaluated at their nodes. Reducing the discrete cells size, improve spatial resolution, but also increase greatly the number of calculations, and vice versa. In our model, we set that the computational domain is discretization in ξ -direction into $imax$ nodes, and in η -direction into $jmax$ nodes, such that there are $(imax - 2) \times (jmax - 2)$ interior nodes representing the control volumes centroids, at which the discretized governing equations are applied, and on the other side there are $2(imax - 2) + 2(jmax - 2) + 4$ nodes on the boundaries, where the flow variables are calculated given the equations given in section 3.5.

Discretized Vector Form of Governing Equations

By applying equation (3.18) for the control volume shown in figure (3.1), the discrete integral vector form of the flow governing equation for an individual cell is formulated as:

$$\begin{aligned} \frac{\Delta \bar{Q}_{i,j}}{\Delta t} \Delta \xi \Delta \eta &+ \left(\bar{E}_{i+\frac{1}{2},j} - \bar{E}_{v i+\frac{1}{2},j} \right) \Delta \eta - \left(\bar{E}_{i-\frac{1}{2},j} - \bar{E}_{v i-\frac{1}{2},j} \right) \Delta \eta + \\ &+ \left(\bar{F}_{i,j+\frac{1}{2}} - \bar{F}_{v i,j+\frac{1}{2}} \right) \Delta \xi - \left(\bar{F}_{i,j-\frac{1}{2}} - \bar{F}_{v i,j-\frac{1}{2}} \right) \Delta \xi + \\ &+ \alpha \left(\bar{H}_{i,j} - \bar{H}_{v i,j} \right) \Delta \xi \Delta \eta = \bar{S}_{i,j} \Delta \xi \Delta \eta. \end{aligned} \quad (3.19)$$

As discussed in section 3.4, $(\Delta \bar{Q}_{i,j})$ is the difference in the conservative variables vector between two time levels:

$$\Delta \bar{Q}_{i,j} = \bar{Q}_{i,j}^{n+1} - \bar{Q}_{i,j}^n. \quad (3.20)$$

So, equation (3.19) can be rewritten as:

$$\begin{aligned} &\frac{1}{\Delta t} \left(\bar{Q}_{i,j}^{n+1} - \bar{Q}_{i,j}^n \right) + \\ &\frac{1}{\Delta \xi} \left(\bar{E}_{i+\frac{1}{2},j} - \bar{E}_{i-\frac{1}{2},j} \right) + \frac{1}{\Delta \eta} \left(\bar{F}_{i,j+\frac{1}{2}} - \bar{F}_{i,j-\frac{1}{2}} \right) + \alpha \bar{H}_{i,j} + \\ &-\frac{1}{\Delta \xi} \left(\bar{E}_{v i+\frac{1}{2},j} - \bar{E}_{v i-\frac{1}{2},j} \right) - \frac{1}{\Delta \eta} \left(\bar{F}_{v i,j+\frac{1}{2}} - \bar{F}_{v i,j-\frac{1}{2}} \right) - \alpha \bar{H}_{v i,j} = \bar{S}_{i,j}. \end{aligned} \quad (3.21)$$

3.3.2 Convective Fluxes Discretization

Roe's Flux-Difference Splitting Upwind Scheme

Like other flux-difference splitting schemes, Roe's scheme presents an approximate solution for Riemann's problem (i.e. shock tube problem) at each cell face, in order to resolve the flow variable discontinuities. Ideal gases frozen flows can be solved by Roe's scheme [47]. This approach was extended by Grossman et. al [30] for chemically and thermally nonequilibrium one-dimensional flows, and then more exten-

sions were presented by Walters et al. [62] for multi-dimensional problem, from which we conclude the formulation of Roe's flux-difference scheme employed for chemically-nonequilibrium, thermally-equilibrium two-dimensional flows.

For the cell face convective fluxes presented in equation (3.21), where $(\bar{E}_{i+\frac{1}{2},j}, \bar{E}_{i-\frac{1}{2},j})$ are the fluxes in ξ -direction, and $(\bar{F}_{i,j+\frac{1}{2}}, \bar{F}_{i,j-\frac{1}{2}})$ are in η -direction, the general formulation of the cell interface convective flux in ξ -direction $(\bar{E}_F)$, involves the averaged value of the fluxes at the right and left sides of the face (E^R, E^L) , and the flux jump across the cell interface:

$$\bar{E}_F = \frac{1}{2} (E^R + E^L) - \frac{1}{2} |\widehat{\mathbf{A}}| (\bar{Q}^R - \bar{Q}^L) = \frac{1}{2} (E^R + E^L) - \frac{1}{2} |\widehat{\mathbf{A}}| \delta \bar{Q}. \quad (3.22)$$

The second term in equation (3.22) represents the summation of the wave speeds, where the Roe-averaged flux flow Jacobian in ξ -direction $(|\widehat{\mathbf{A}}|)$ can be decomposed into the diagonal matrix of absolute eigenvalues $(|\widehat{\Lambda}_\xi|)$, and the right and left eigenvectors $(\widehat{\mathcal{E}}_R, \widehat{\mathcal{E}}_L)$, where the flow variables are averaged between and right and left sides of the cell interface by Roe scheme technique as discussed in equations (3.34)-(3.38). So, the Roe-averaged flux Jacobian in ξ -direction is equal to:

$$|\widehat{\mathbf{A}}| \delta \bar{Q} = \widehat{\mathcal{E}}_R |\widehat{\Lambda}_\xi| \widehat{\mathcal{E}}_L \delta \bar{Q}. \quad (3.23)$$

As the characteristic variables $(\mathcal{W})$ is equal to the product of the left eigenvectors matrix and the conservative variable vector, so the jump in the characteristic variables at the cell face or the wave strengths $(\delta \widehat{\mathcal{W}})$ is equal to:

$$\delta \widehat{\mathcal{W}} = \widehat{\mathcal{E}}_L \delta \bar{Q}. \quad (3.24)$$

By substituting equation (3.24) in (3.22), we have:

$$\bar{E}_F = \frac{1}{2} (E^R + E^L) - \frac{1}{2} \widehat{\mathcal{E}}_R |\widehat{\Lambda}_\xi| \delta \widehat{\mathcal{W}} = \frac{1}{2} (E^R + E^L) - \frac{1}{2} [E]. \quad (3.25)$$

The second term of wave speeds superposition ($\llbracket E \rrbracket$) in equation (3.25) can be decomposed into three terms as follows:

$$\llbracket E \rrbracket = \llbracket E \rrbracket_A + \llbracket E \rrbracket_B + \llbracket E \rrbracket_C. \quad (3.26)$$

Before writing down the elements of wave speeds summation, it should be mentioned that the averaging of the variable (f) between the left and right sides of the cell interface is symbolized as:

$$\langle f \rangle = \frac{1}{2} (f^{\mathbf{R}} + f^{\mathbf{L}}). \quad (3.27)$$

It is important to consider what is expressed in equation (3.27), is not the accurate definition of the flow variables properties at the cell interface, as the cell face property ($f_{\mathbf{F}}$) is calculated from the arithmetic averaging between the *nearest forward and backward two mesh nodes* located on the same grid line passing through the cell face midpoint:

$$f_{\mathbf{F}} = \frac{1}{2} (f_{\text{front node}} + f_{\text{back node}}). \quad (3.28)$$

Regarding figure (3.1), the flow properties at the four cell faces are written down as:

$$\begin{aligned} f_{i+\frac{1}{2},j} &= \frac{1}{2} (f_{i+1,j} + f_{i,j}), & f_{i-\frac{1}{2},j} &= \frac{1}{2} (f_{i,j} + f_{i-1,j}), \\ f_{i,j+\frac{1}{2}} &= \frac{1}{2} (f_{i,j+1} + f_{i,j}), & f_{i,j-\frac{1}{2}} &= \frac{1}{2} (f_{i,j} + f_{i,j-1}). \end{aligned} \quad (3.29)$$

Equations (3.27) and (3.28) are identical only for first order spatial accurate schemes. But, the left and right hand sides of the cell face have different definition for higher order solutions as shown later.

On the other hand, the jump in the value of (f), across the cell interface, from the left to the right sides, will be notated as:

$$\llbracket f \rrbracket = (f^{\mathbf{R}} - f^{\mathbf{L}}). \quad (3.30)$$

In equation (3.26), $(\llbracket E \rrbracket_A)$ represents the summation of the wave speeds in ξ -direction, corresponding to the $(n_s + 1)$ eigenvalues in ξ -direction, whose value equal to $(\mathcal{U})$, where each of $(\llbracket E \rrbracket_B)$ and $(\llbracket E \rrbracket_C)$ corresponds to the two last eigenvalues $(\mathcal{U} + c |\nabla \xi|)$ and $(\mathcal{U} - c |\nabla \xi|)$ respectively, where (c) is the speed of sound, i.e. $c = \sqrt{\gamma P / \rho}$. The three vectors are expressed as follows:

$$\begin{aligned} \llbracket E \rrbracket_A &= \\ &= \frac{|\nabla \xi|_{\mathbf{F}}}{J_{\mathbf{F}}} \left| \hat{\mathcal{U}}' \right| \left\{ \left(\llbracket \rho \rrbracket - \frac{\llbracket P \rrbracket}{\hat{c}^2} \right) \begin{bmatrix} 1 \\ \hat{u} \\ \hat{v} \\ \hat{H}_t - \frac{\hat{c}^2}{(\hat{\gamma}_{mix} - 1)} \\ \hat{Y}_m \end{bmatrix} + \hat{\rho} \begin{bmatrix} 0 \\ \llbracket u \rrbracket + \llbracket \mathcal{U}' \rrbracket \xi'_{x\mathbf{F}} \\ \llbracket v \rrbracket + \llbracket \mathcal{U}' \rrbracket \xi'_{y\mathbf{F}} \\ \Theta_{\xi} \\ \llbracket Y_m \rrbracket \end{bmatrix} \right\}, \\ \llbracket E \rrbracket_{B,C} &= \frac{|\nabla \xi|_{\mathbf{F}}}{J_{\mathbf{F}}} \left| \left(\hat{\mathcal{U}}' \pm \hat{c} \right) \right| \left(\frac{1}{\hat{c}^2} \right) (\llbracket P \rrbracket \pm \hat{\rho} \hat{c} \llbracket \mathcal{U}' \rrbracket) \begin{bmatrix} 1 \\ \hat{u} \pm \hat{c} \xi'_{x\mathbf{F}} \\ \hat{v} \pm \hat{c} \xi'_{y\mathbf{F}} \\ \hat{H}_t \pm \hat{\mathcal{U}}' \hat{c} \\ \hat{Y}_m \end{bmatrix}, \end{aligned} \quad (3.31)$$

where:

$$\begin{aligned} \hat{\mathcal{U}}' &= \frac{1}{|\nabla \xi|_{\mathbf{F}}} (\xi_{x\mathbf{F}} \hat{u} + \xi_{y\mathbf{F}} \hat{v}), \\ \llbracket \mathcal{U}' \rrbracket &= \mathcal{U}'^{\mathbf{R}} - \mathcal{U}'^{\mathbf{L}}, \\ \mathcal{U}'^{\mathbf{R}} &= \frac{\mathcal{U}^{\mathbf{R}}}{|\nabla \xi|_{\mathbf{F}}}, & \mathcal{U}'^{\mathbf{L}} &= \frac{\mathcal{U}^{\mathbf{L}}}{|\nabla \xi|_{\mathbf{F}}}, \\ \xi'_{x\mathbf{F}} &= \frac{\xi_{x\mathbf{F}}}{|\nabla \xi|_{\mathbf{F}}}, & \xi'_{y\mathbf{F}} &= \frac{\xi_{y\mathbf{F}}}{|\nabla \xi|_{\mathbf{F}}}. \end{aligned} \quad (3.32)$$

Also, (Θ_{ξ}) is the expression for:

$$\Theta_{\xi} = \hat{u} \llbracket u \rrbracket + \hat{v} \llbracket v \rrbracket - \hat{\mathcal{U}}' \llbracket \mathcal{U}' \rrbracket - \sum_{m=1}^{n_s} \llbracket Y_m \rrbracket \hat{\psi}_m. \quad (3.33)$$

In equations (3.31) and (3.33), the Roe-averaged flow variables ($\hat{\rho}$, $\hat{u}$, $\hat{v}$, $\hat{H}_t$, $\hat{Y}_m$, $\hat{\psi}_m$, $\hat{\gamma}_{mix}$, $\hat{c}$) are written as:

$$\begin{aligned}\hat{\rho} &= \sqrt{\rho^{\mathbf{L}} \rho^{\mathbf{R}}}, & \hat{u} &= \frac{\langle u \sqrt{\rho} \rangle}{\langle \sqrt{\rho} \rangle}, & \hat{v} &= \frac{\langle v \sqrt{\rho} \rangle}{\langle \sqrt{\rho} \rangle}, \\ \hat{H}_t &= \frac{\langle H_t \sqrt{\rho} \rangle}{\langle \sqrt{\rho} \rangle}, & \hat{Y}_m &= \frac{\langle Y_m \sqrt{\rho} \rangle}{\langle \sqrt{\rho} \rangle},\end{aligned}\quad (3.34)$$

$$\hat{\psi}_m = \frac{\hat{T} R_m}{\gamma_{mix} - 1} \frac{T_{ref}}{V_{ref}^2} + \frac{\hat{\mathbf{q}}^2}{2} - \hat{e}_m, \quad (3.35)$$

$$\hat{\gamma}_{mix} = 1 + \frac{\hat{R}_{mix}}{c_v^*}, \quad (3.36)$$

$$\hat{c}^2 = (\hat{\gamma}_{mix} - 1) \left[\hat{H}_t - \frac{\hat{\mathbf{q}}^2}{2} + \sum_{m=1}^{n_s} \hat{Y}_m \hat{e}_m + c_v^* \hat{T} \frac{T_{ref}}{V_{ref}^2} \right], \quad (3.37)$$

where:

$$\begin{aligned}\hat{T} &= \frac{\langle T \sqrt{\rho} \rangle}{\langle \sqrt{\rho} \rangle}, & \hat{e}_m &= \frac{\langle e_m \sqrt{\rho} \rangle}{\langle \sqrt{\rho} \rangle}, & \hat{R}_{mix} &= \frac{\langle R_{mix} \sqrt{\rho} \rangle}{\langle \sqrt{\rho} \rangle}, \\ \hat{\mathbf{q}} &= \sqrt{\hat{u}^2 + \hat{v}^2}, \\ c_v^* &= \sum_{m=1}^{n_s} \hat{Y}_m c_{v_m}^* & c_{v_m}^* &= \frac{1}{\llbracket T \rrbracket} \int_{T^{\mathbf{L}}}^{T^{\mathbf{R}}} c_{v_m} dT.\end{aligned}\quad (3.38)$$

It should be reminded that all utilized variables are dimensionless and time-averaged as mentioned in chapter 2, but there are still dimensional variables such as the specific heat coefficients, heat of formation and gas constant. So, as seen in equations (3.35) and (3.37), some extra terms of reference variables are added to achieve non-dimensionalization for all terms of the model equations.

Likewise, it be concluded that the expression of the summation of the wave speeds in η -direction represented in three terms. The first is ($\llbracket F \rrbracket_A$), which corresponds to the eigenvalue ($\mathcal{V}$) in η -direction which is repeated for $(n_s + 1)$ times. And other two are ($\llbracket F \rrbracket_B$, $\llbracket F \rrbracket_C$), corre-

sponding to the remaining eigenvalues $(\mathcal{V} + c |\nabla\eta|)$ and $(\mathcal{V} - c |\nabla\eta|)$, respectively:

$$\begin{aligned}
\llbracket F \rrbracket_A &= \\
&= \frac{|\nabla\eta|_{\mathbf{F}}}{J_{\mathbf{F}}} \left| \hat{\mathcal{V}}' \right| \left\{ \left(\llbracket \rho \rrbracket - \frac{\llbracket P \rrbracket}{\hat{c}^2} \right) \begin{bmatrix} 1 \\ \hat{u} \\ \hat{v} \\ \hat{H}_t - \frac{\hat{c}^2}{(\hat{\gamma}_{mix}-1)} \\ \hat{Y}_m \end{bmatrix} + \hat{\rho} \begin{bmatrix} 0 \\ \llbracket u \rrbracket + \llbracket \mathcal{V}' \rrbracket \eta'_{x\mathbf{F}} \\ \llbracket v \rrbracket + \llbracket \mathcal{V}' \rrbracket \eta'_{y\mathbf{F}} \\ \Theta_\eta \\ \llbracket Y_m \rrbracket \end{bmatrix} \right\}, \\
\llbracket F \rrbracket_{B,C} &= \frac{|\nabla\eta|_{\mathbf{F}}}{J_{\mathbf{F}}} \left| (\hat{\mathcal{V}}' \pm \hat{c}) \right| \left(\frac{1}{\hat{c}^2} \right) (\llbracket P \rrbracket \pm \hat{\rho} \hat{c} \llbracket \mathcal{V}' \rrbracket) \begin{bmatrix} 1 \\ \hat{u} \pm \hat{c} \eta'_{x\mathbf{F}} \\ \hat{v} \pm \hat{c} \eta'_{y\mathbf{F}} \\ \hat{H}_t \pm \hat{\mathcal{V}}' \hat{c} \\ \hat{Y}_m \end{bmatrix}, \tag{3.39}
\end{aligned}$$

where:

$$\begin{aligned}
\hat{\mathcal{V}}' &= \frac{1}{|\nabla\eta|_{\mathbf{F}}} (\eta_{x\mathbf{F}} \hat{u} + \eta_{y\mathbf{F}} \hat{v}), \\
\llbracket \mathcal{V}' \rrbracket &= \mathcal{V}'^{\mathbf{R}} - \mathcal{V}'^{\mathbf{L}}, \\
\mathcal{V}'^{\mathbf{R}} &= \frac{\mathcal{V}^{\mathbf{R}}}{|\nabla\eta|_{\mathbf{F}}}, & \mathcal{V}'^{\mathbf{L}} &= \frac{\mathcal{V}^{\mathbf{L}}}{|\nabla\eta|_{\mathbf{F}}}, \\
\eta'_{x\mathbf{F}} &= \frac{\eta_{x\mathbf{F}}}{|\nabla\eta|_{\mathbf{F}}}, & \eta'_{y\mathbf{F}} &= \frac{\eta_{y\mathbf{F}}}{|\nabla\eta|_{\mathbf{F}}}, \tag{3.40}
\end{aligned}$$

$$\Theta_\eta = \hat{u} \llbracket u \rrbracket + \hat{v} \llbracket v \rrbracket - \hat{\mathcal{V}}' \llbracket \mathcal{V}' \rrbracket - \sum_{m=1}^{n_s} \llbracket Y_m \rrbracket \hat{\psi}_m. \tag{3.41}$$

Second Order Upwind Schemes Using MUSCL Approach

Determination of the spatial accuracy of the flux-difference splitting scheme is determined by the method of calculation of the right and left sides of the cell interface in terms of the nearest mesh nodes surrounding the cell face midpoint. The first order accuracy is achieved by zero order extrapolation from nearest node in each side, to deter-

mine the right and left sides of the cell interface, it can be described for the four cell faces shown in figure (3.1) for a general flow variable (f) as:

$$\begin{aligned} f_{i+\frac{1}{2},j}^{\mathbf{R}} &= f_{i+1,j}, & f_{i+\frac{1}{2},j}^{\mathbf{L}} &= f_{i,j}, & f_{i-\frac{1}{2},j}^{\mathbf{R}} &= f_{i,j}, & f_{i-\frac{1}{2},j}^{\mathbf{L}} &= f_{i-1,j}, \\ f_{i,j+\frac{1}{2}}^{\mathbf{R}} &= f_{i,j+1}, & f_{i,j+\frac{1}{2}}^{\mathbf{L}} &= f_{i,j}, & f_{i,j-\frac{1}{2}}^{\mathbf{R}} &= f_{i,j}, & f_{i,j-\frac{1}{2}}^{\mathbf{L}} &= f_{i,j-1}. \end{aligned} \quad (3.42)$$

To attain the second order accuracy in space for the upwind scheme, the flow properties of the left and right sides of the cell interface are calculated using linear extrapolation for the primitive variables from the nearest two mesh nodes from each side. This approach is also called MUSCL approach:

$$\begin{aligned} f_{i+\frac{1}{2},j}^{\mathbf{R}} &= f_{i+1,j} - \frac{1}{2}(f_{i+2,j} - f_{i+1,j}), & f_{i+\frac{1}{2},j}^{\mathbf{L}} &= f_{i,j} + \frac{1}{2}(f_{i,j} - f_{i-1,j}), \\ f_{i-\frac{1}{2},j}^{\mathbf{R}} &= f_{i,j} - \frac{1}{2}(f_{i+1,j} - f_{i,j}), & f_{i-\frac{1}{2},j}^{\mathbf{L}} &= f_{i-1,j} + \frac{1}{2}(f_{i-1,j} - f_{i-2,j}), \\ f_{i,j+\frac{1}{2}}^{\mathbf{R}} &= f_{i,j+1} - \frac{1}{2}(f_{i,j+2} - f_{i,j+1}), & f_{i,j+\frac{1}{2}}^{\mathbf{L}} &= f_{i,j} + \frac{1}{2}(f_{i,j} - f_{i,j-1}), \\ f_{i,j-\frac{1}{2}}^{\mathbf{R}} &= f_{i,j} - \frac{1}{2}(f_{i+1,j} - f_{i,j}), & f_{i,j-\frac{1}{2}}^{\mathbf{L}} &= f_{i,j-1} + \frac{1}{2}(f_{i-1,j} - f_{i-2,j}). \end{aligned} \quad (3.43)$$

Hirsch [32] points the attention that the used variables in extrapolation must not be conservative, but they may be conservative, primitive or characteristic variables. Here the *primitive variable extrapolation* is applied to ensure the second order spatial accuracy. While, the conservation of the solution is obtained in the formulation of the fluxes used in the governing equations.

Some nonphysical numerical oscillations are formed around the flow discontinuities, when using second order space accurate schemes, because of the third order spatial derivatives found in the truncation error of second order accurate schemes. To save the monotonicity of

the numerical solution to match with the physical one and to eliminate the nonphysical oscillations, Total Variation Diminishing (TVD) conditions, discussed in details by Hirsch [32], must be satisfied. They are fulfilled by using *non-linear limiters* restricting the amplitude of the gradients of the additional terms in the truncation error of the utilized scheme.

There are two types of limiters: The flux limiter, and flow variable slope limiter. We will concern in our study with the second one, which is considered simply a function of the flow variable slope at the right or left side of the cell face. So we must define first, the flow variable slope for the left and right sides of the faces of the control volume in figure (3.1) as follows:

$$\begin{aligned}
r_{i+\frac{1}{2},j}^{\mathbf{R}} &= \frac{f_{i+1,j} - f_{i,j}}{f_{i+2,j} - f_{i+1,j}}, & r_{i+\frac{1}{2},j}^{\mathbf{L}} &= \frac{f_{i+1,j} - f_{i,j}}{f_{i,j} - f_{i-1,j}}, \\
r_{i-\frac{1}{2},j}^{\mathbf{R}} &= \frac{f_{i,j} - f_{i-1,j}}{f_{i+1,j} - f_{i,j}}, & r_{i-\frac{1}{2},j}^{\mathbf{L}} &= \frac{f_{i,j} - f_{i-1,j}}{f_{i-1,j} - f_{i-2,j}}, \\
r_{i,j+\frac{1}{2}}^{\mathbf{R}} &= \frac{f_{i,j+1} - f_{i,j}}{f_{i,j+2} - f_{i,j+1}}, & r_{i,j+\frac{1}{2}}^{\mathbf{L}} &= \frac{f_{i,j+1} - f_{i,j}}{f_{i,j} - f_{i,j-1}}, \\
r_{i,j-\frac{1}{2}}^{\mathbf{R}} &= \frac{f_{i,j} - f_{i,j-1}}{f_{i,j+1} - f_{i,j}}, & r_{i,j-\frac{1}{2}}^{\mathbf{L}} &= \frac{f_{i,j} - f_{i,j-1}}{f_{i,j-1} - f_{i,j-2}}.
\end{aligned} \tag{3.44}$$

Minmode limiter is the employed slope limiter. It is defined by a logical expression in terms of the slope of the flow variable, i.e. $\psi \equiv \psi(r)$, so it belongs to the discontinuous slope limiters of flux limiters which are *not* expressed by a smooth continuous function. The minmode limiter is written as:

$$\psi(r) = \max[0, \min(1, r)]. \tag{3.45}$$

Minmode is widely used to satisfy TVD conditions [32]. That may be refer to its easy implementation, And it is also because other discontinuous slope limiters, such as superbee limiter, dramatically affect the

behavior of the solution convergence, by raising the minimum value, attained by the solution residual (or error) at convergence, in pseudo-time integration of steady state problems. Unfortunately, minmode is known of its modest capability of resolving sharp discontinuities, among other slope limiters. That may require to use bigger mesh size in problems of steep discontinuities.

Consequently, from equations (3.42)-(3.45), the general form of the primitive variable calculation for either first order accurate upwind scheme and second order upwind TVD scheme, is written as follows:

$$\begin{aligned}
f_{i+\frac{1}{2},j}^{\mathbf{R}} &= f_{i+1,j} - \frac{\varepsilon}{2} \psi(r_{i+\frac{1}{2},j}^{\mathbf{R}}) [f_{i+2,j} - f_{i+1,j}], \\
f_{i+\frac{1}{2},j}^{\mathbf{L}} &= f_{i,j} + \frac{\varepsilon}{2} \psi(r_{i+\frac{1}{2},j}^{\mathbf{L}}) [f_{i,j} - f_{i-1,j}], \\
f_{i-\frac{1}{2},j}^{\mathbf{R}} &= f_{i,j} - \frac{\varepsilon}{2} \psi(r_{i-\frac{1}{2},j}^{\mathbf{R}}) [f_{i+1,j} - f_{i,j}], \\
f_{i-\frac{1}{2},j}^{\mathbf{L}} &= f_{i-1,j} + \frac{\varepsilon}{2} \psi(r_{i-\frac{1}{2},j}^{\mathbf{L}}) [f_{i-1,j} - f_{i-2,j}], \\
f_{i,j+\frac{1}{2}}^{\mathbf{R}} &= f_{i,j+1} - \frac{\varepsilon}{2} \psi(r_{i,j+\frac{1}{2}}^{\mathbf{R}}) [f_{i,j+2} - f_{i,j+1}], \\
f_{i,j+\frac{1}{2}}^{\mathbf{L}} &= f_{i,j} + \frac{\varepsilon}{2} \psi(r_{i,j+\frac{1}{2}}^{\mathbf{L}}) [f_{i,j} - f_{i,j-1}], \\
f_{i,j-\frac{1}{2}}^{\mathbf{R}} &= f_{i,j} - \frac{\varepsilon}{2} \psi(r_{i,j-\frac{1}{2}}^{\mathbf{R}}) [f_{i+1,j} - f_{i,j}], \\
f_{i,j-\frac{1}{2}}^{\mathbf{L}} &= f_{i,j-1} + \frac{\varepsilon}{2} \psi(r_{i,j-\frac{1}{2}}^{\mathbf{L}}) [f_{i-1,j} - f_{i-2,j}],
\end{aligned} \tag{3.46}$$

where:

$$\varepsilon = \begin{cases} 0, & \text{First order spatial accuracy.} \\ 1, & \text{Second order spatial accuracy.} \end{cases} \tag{3.47}$$

3.3.3 Diffusive Fluxes Discretization

Second Order Central Discretization

Starting from equation (3.2), The cell faces diffusive fluxes ($\overline{E}_{v_{i\pm\frac{1}{2},j}}$, $\overline{F}_{v_{i,j\pm\frac{1}{2}}}$) in equation (3.18) can be written down as follows:

$$\begin{aligned}\overline{E}_{v_{i\pm\frac{1}{2},j}} &= \frac{1}{J_{i\pm\frac{1}{2},j}} \left(\xi_{x_{i\pm\frac{1}{2},j}} E_{v_{i\pm\frac{1}{2},j}} + \xi_{y_{i\pm\frac{1}{2},j}} F_{v_{i\pm\frac{1}{2},j}} \right), \\ \overline{F}_{v_{i,j\pm\frac{1}{2}}} &= \frac{1}{J_{i,j\pm\frac{1}{2}}} \left(\eta_{x_{i,j\pm\frac{1}{2}}} E_{v_{i,j\pm\frac{1}{2}}} + \eta_{y_{i,j\pm\frac{1}{2}}} F_{v_{i,j\pm\frac{1}{2}}} \right),\end{aligned}\tag{3.48}$$

where the transformation derivatives at the faces ($J_{i\pm\frac{1}{2},j}$, $J_{i,j\pm\frac{1}{2}}$, $\xi_{x_{i\pm\frac{1}{2},j}}$, $\xi_{y_{i\pm\frac{1}{2},j}}$, $\eta_{x_{i,j\pm\frac{1}{2}}}$, $\eta_{y_{i,j\pm\frac{1}{2}}}$) are calculated according to equation (3.29).

As the viscous fluxes at the cell face are composed of first order derivatives of different flow variables as discussed in chapter 2, so the spatial derivative of the diffusive fluxes themselves as in equation (3.21) is equivalent to second order spatial derivatives of flow variables. So the central discretization of the cell face viscous fluxes, implies central modeling of second order discretization, which are second order accurate in space.

Derivatives of Flow Variables at the Cell Faces

The diffusive fluxes are composed from spatial derivatives of velocities (u , v), temperature (T), enthalpy (h), and mass fraction (Y_m). For a general flow variable (f) representing anyone of these variables, its spatial derivatives in the physical domain can be expressed in terms of its derivatives in computational domain as follows:

$$\frac{\partial f}{\partial x} = \xi_x \frac{\partial f}{\partial \xi} + \eta_x \frac{\partial f}{\partial \eta}, \quad \frac{\partial f}{\partial y} = \xi_y \frac{\partial f}{\partial \xi} + \eta_y \frac{\partial f}{\partial \eta}. \tag{3.49}$$

Thus, the discretized form of the spatial derivatives can be written for the cell faces $(i \pm \frac{1}{2}, j)$ shown in figure (3.1) as follows:

$$\begin{aligned}
\left(\frac{\partial f}{\partial x}\right)_{i+\frac{1}{2},j} &= \frac{f_{i+1,j}-f_{i,j}}{\Delta\xi} (\xi_x)_{i+\frac{1}{2},j} + \frac{1}{2} \left[\frac{f_{i+1,j+1}-f_{i+1,j-1}}{2\Delta\eta} + \frac{f_{i,j+1}-f_{i,j-1}}{2\Delta\eta} \right] (\eta_x)_{i+\frac{1}{2},j} \\
\left(\frac{\partial f}{\partial y}\right)_{i+\frac{1}{2},j} &= \frac{f_{i+1,j}-f_{i,j}}{\Delta\xi} (\xi_y)_{i+\frac{1}{2},j} + \frac{1}{2} \left[\frac{f_{i+1,j+1}-f_{i+1,j-1}}{2\Delta\eta} + \frac{f_{i,j+1}-f_{i,j-1}}{2\Delta\eta} \right] (\eta_y)_{i+\frac{1}{2},j} \\
\left(\frac{\partial f}{\partial x}\right)_{i-\frac{1}{2},j} &= \frac{f_{i,j}-f_{i-1,j}}{\Delta\xi} (\xi_x)_{i-\frac{1}{2},j} + \frac{1}{2} \left[\frac{f_{i,j+1}-f_{i,j-1}}{2\Delta\eta} + \frac{f_{i-1,j+1}-f_{i-1,j-1}}{2\Delta\eta} \right] (\eta_x)_{i-\frac{1}{2},j} \\
\left(\frac{\partial f}{\partial y}\right)_{i-\frac{1}{2},j} &= \frac{f_{i,j}-f_{i-1,j}}{\Delta\xi} (\xi_y)_{i-\frac{1}{2},j} + \frac{1}{2} \left[\frac{f_{i,j+1}-f_{i,j-1}}{2\Delta\eta} + \frac{f_{i-1,j+1}-f_{i-1,j-1}}{2\Delta\eta} \right] (\eta_y)_{i-\frac{1}{2},j}
\end{aligned} \tag{3.50}$$

And the spatial derivatives of the faces $(i, j \pm \frac{1}{2})$ are written as:

$$\begin{aligned}
\left(\frac{\partial f}{\partial x}\right)_{i,j+\frac{1}{2}} &= \frac{1}{2} \left[\frac{f_{i+1,j+1}-f_{i-1,j+1}}{2\Delta\xi} + \frac{f_{i+1,j}-f_{i-1,j}}{2\Delta\xi} \right] (\xi_x)_{i,j+\frac{1}{2}} + \frac{f_{i,j+1}-f_{i,j}}{\Delta\eta} (\eta_x)_{i,j+\frac{1}{2}} \\
\left(\frac{\partial f}{\partial y}\right)_{i,j+\frac{1}{2}} &= \frac{1}{2} \left[\frac{f_{i+1,j+1}-f_{i-1,j+1}}{2\Delta\xi} + \frac{f_{i+1,j}-f_{i-1,j}}{2\Delta\xi} \right] (\xi_y)_{i,j+\frac{1}{2}} + \frac{f_{i,j+1}-f_{i,j}}{\Delta\eta} (\eta_y)_{i,j+\frac{1}{2}} \\
\left(\frac{\partial f}{\partial x}\right)_{i,j-\frac{1}{2}} &= \frac{1}{2} \left[\frac{f_{i+1,j}-f_{i-1,j}}{2\Delta\xi} + \frac{f_{i+1,j-1}-f_{i-1,j-1}}{2\Delta\xi} \right] (\xi_x)_{i,j-\frac{1}{2}} + \frac{f_{i,j}-f_{i,j-1}}{\Delta\eta} (\eta_x)_{i,j-\frac{1}{2}} \\
\left(\frac{\partial f}{\partial y}\right)_{i,j-\frac{1}{2}} &= \frac{1}{2} \left[\frac{f_{i+1,j}-f_{i-1,j}}{2\Delta\xi} + \frac{f_{i+1,j-1}-f_{i-1,j-1}}{2\Delta\xi} \right] (\xi_y)_{i,j-\frac{1}{2}} + \frac{f_{i,j}-f_{i,j-1}}{\Delta\eta} (\eta_y)_{i,j-\frac{1}{2}}
\end{aligned} \tag{3.51}$$

Flow Properties and Transport Coefficient Averaging at Cell Faces

In the formulation of each cell face diffusive flux, the flow properties at the cell face such as the laminar transport coefficients (i.e. $\mu_{L\mathbf{F}}$, $k_{L\mathbf{F}}$, and $\mathcal{D}_{L\mathbf{F}}$), and the turbulent eddy viscosity coefficient ($\mu_{T\mathbf{F}}$), which can be estimated using the properties averaging between the front and back nodes to each the control volume's interface as shown in equations (3.28) and (3.29). This method of averaging is also implemented to determine the other cell face's density and individual species heats of formation (i.e. $\rho_{\mathbf{F}}$, and $h_{m\mathbf{F}}$), which are written in equations (2.25) and (2.23).

3.4 Pseudo Time Integration

3.4.1 Chemistry-Implicit Flow-Explicit Time Integration

As mentioned before, the source of stiffness result from the chemical characteristic time is eliminated. And, the computational effort avoided using fully implicit scheme which require inversion of huge matrices, by using point-implicit scheme, which is first suggested by Curtiss et al. [18], to treat the chemical source term implicitly and flow fluxes explicitly. The discretized governing equation can be written as follows:

$$\begin{aligned} & \frac{(\bar{Q}_{i,j}^{n+1} - \bar{Q}_{i,j}^n)}{\Delta t} + \frac{(\bar{E}_{i+\frac{1}{2},j}^n - \bar{E}_{i-\frac{1}{2},j}^n)}{\Delta \xi} + \frac{(\bar{F}_{i,j+\frac{1}{2}}^n - \bar{F}_{i,j-\frac{1}{2}}^n)}{\Delta \eta} + \alpha \bar{H}_{i,j}^n + \\ & - \frac{(\bar{E}_{v_{i+\frac{1}{2},j}}^n - \bar{E}_{v_{i-\frac{1}{2},j}}^n)}{\Delta \xi} - \frac{(\bar{F}_{v_{i,j+\frac{1}{2}}}^n - \bar{F}_{v_{i,j-\frac{1}{2}}}^n)}{\Delta \eta} - \alpha \bar{H}_{v_{i,j}}^n = \bar{S}_{i,j}^{n+1}. \end{aligned} \quad (3.52)$$

Time linearization of second temporal accuracy is implemented to the chemical source term at the time level $(n+1)$ to be expressed in terms of the source term and the conservative variables vector at the time level (n) :

$$\begin{aligned} \bar{S}_{i,j}^{n+1} &= \bar{S}_{i,j}^n + \left(\frac{\partial \bar{S}}{\partial \bar{Q}} \right)_{i,j} \left(\frac{\partial \bar{Q}}{\partial t} \right)_{i,j} \Delta t + \mathcal{O}(\Delta t^2), \\ &= \bar{S}_{i,j}^n + \left(\frac{\partial \bar{S}}{\partial \bar{Q}} \right)_{i,j} \left(\frac{\Delta \bar{Q}_{i,j}}{\Delta t} \right) \Delta t + \mathcal{O}(\Delta t^2), \\ &= \bar{S}_{i,j}^n + \bar{\mathbf{H}}_{i,j} \left(\bar{Q}_{i,j}^{n+1} - \bar{Q}_{i,j}^n \right) + \mathcal{O}(\Delta t^2), \end{aligned} \quad (3.53)$$

where $(\bar{\mathbf{H}}_{i,j})$ is the chemical source Jacobian in the computational domain. So, by treating the source term implicitly, the time step taken in integration is no longer restricted by the chemical characteristic time anymore. Also, applying point-implicit scheme leads to solve mono-block diagonal matrix for a system of equations.

3.4.2 Chemical Source Jacobian Formulation

According to equation (3.2), the chemical Jacobians in both the physical and computational domains ($\mathbf{H}$, $\bar{\mathbf{H}}$) are equal according to:

$$\bar{\mathbf{H}}_{i,j} = \left(\frac{\partial \bar{S}}{\partial \bar{Q}} \right)_{i,j} = \left(\frac{\partial (S/J)}{\partial (Q/J)} \right)_{i,j} = \left(\frac{\partial S}{\partial Q} \right)_{i,j} = \mathbf{H}_{i,j}. \quad (3.54)$$

And from equation (2.33), it is noticeable that the chemical source term is not an explicit function in the conservative variables except the individual species densities (ρY_m), so the chemical Jacobian is written as:

$$\bar{\mathbf{H}}_{i,j} = \mathbf{H}_{i,j} = \begin{bmatrix} [0]_{4 \times 4} & [0]_{4 \times (n_s - 1)} \\ [0]_{(n_s - 1) \times 4} & \left[\frac{\partial \dot{\omega}_m}{\partial (\rho Y_p)} \right]_{(n_s - 1) \times (n_s - 1)} \end{bmatrix}_{i,j}. \quad (3.55)$$

$(\partial \dot{\omega}_m / \partial (\rho Y_p))$ is $(n_s - 1) \times (n_s - 1)$ matrix, and represents the degree of dependence of species formation rates to the species densities in the mixture. And, the formulation for a general chemical mechanism can be concluded as:

$$\begin{aligned} \frac{\partial \dot{\omega}_m}{\partial (\rho Y_p)} &= \\ &= \frac{L_{ref}}{V_{ref}} \mathcal{M}_m \sum_{r=1}^{n_r} \left\{ (\nu''_{m,r} - \nu'_{m,r}) \left[k_{fr} \nu'_{p,r} \frac{(\rho_{ref} \rho Y_p)^{\nu'_{p,r}-1}}{(\mathcal{M}_p)^{\nu'_{p,r}}} \prod_{\substack{q=1 \\ q \neq p}}^{n_s} \left(\frac{\rho_{ref} \rho Y_q}{\mathcal{M}_q} \right)^{\nu'_{q,r}} + \right. \right. \\ &\quad \left. \left. - k_{br} \nu''_{p,r} \frac{(\rho_{ref} \rho Y_p)^{\nu''_{p,r}-1}}{(\mathcal{M}_p)^{\nu''_{p,r}}} \prod_{\substack{q=1 \\ q \neq p}}^{n_s} \left(\frac{\rho_{ref} \rho Y_q}{\mathcal{M}_q} \right)^{\nu''_{q,r}} \right] \right\}, \end{aligned} \quad (3.56)$$

where (m, p, q) are indices for the chemical species and ranging within $(1, 2, \dots, n_s)$, and (r) is the index for chemical reaction as $(r = 1, 2, \dots, n_r)$, and species density (ρY_p) is multiplied by the reference density, because the former is dimensionless as mentioned in section 3.1. Equation (3.56) show great efficiency when using the numerical solver for

a general chemical mechanism, it can be more simplified to a shorter expression in order to derive the chemical Jacobian analytically, the simplified form is expressed as:

$$\frac{\partial \dot{\omega}_m}{\partial (\rho Y_p)} = \left(\frac{L_{ref}}{V_{ref}} \right) \frac{\mathcal{M}_m}{\rho_{ref} \rho Y_p} \sum_{r=1}^{n_r} \left\{ (\nu''_{m,r} - \nu'_{m,r}) \left[k_{fr} \nu'_{p,r} \prod_{q=1}^{n_s} \left(\frac{\rho_{ref} \rho Y_q}{\mathcal{M}_q} \right)^{\nu'_{q,r}} + \right. \right. \\ \left. \left. - k_{br} \nu''_{p,r} \prod_{q=1}^{n_s} \left(\frac{\rho_{ref} \rho Y_q}{\mathcal{M}_q} \right)^{\nu''_{q,r}} \right] \right\}. \quad (3.57)$$

3.4.3 Separate Time-Space Discretizations of Second Order Temporal & Spatial Accuracy

Unlike the combined space-time discretization like Lax-Wendroff and MacCormack schemes, separate time and space discretizations are utilized in this study. Applying Euler first order accurate time integration to our numerical scheme of second order spatial accurate is unconditionally unstable, although the instability may be considered weak as mentioned by Hirsch [32]. So, starting from equation (3.52), which can be rewritten in the following form:

$$\begin{aligned} \left[\mathbf{I} - \Delta t \bar{\mathbf{H}}_{i,j}^n \right] \frac{(Q_{i,j}^{n+1} - Q_{i,j}^n)}{J_{i,j} \Delta t} = & \\ = \frac{-\left(\bar{E}_{i+\frac{1}{2},j}^n - \bar{E}_{i-\frac{1}{2},j}^n\right)}{\Delta \xi} + \frac{-\left(\bar{F}_{i,j+\frac{1}{2}}^n - \bar{F}_{i,j-\frac{1}{2}}^n\right)}{\Delta \eta} + \alpha \bar{H}_{i,j}^n & \\ + \frac{\left(\bar{E}_{v,i+\frac{1}{2},j}^n - \bar{E}_{v,i-\frac{1}{2},j}^n\right)}{\Delta \xi} + \frac{\left(\bar{F}_{v,i,j+\frac{1}{2}}^n - \bar{F}_{v,i,j-\frac{1}{2}}^n\right)}{\Delta \eta} + \alpha \bar{H}_{vi,j}^n & \\ + \bar{S}_{i,j}^n & \\ = \mathbf{R}_I^n + \mathbf{R}_V^n + \mathbf{R}_C^n & \end{aligned} \quad (3.58)$$

where (I) is the identity matrix, which can be expressed in index notation in terms of Kronecker's delta function as ($\mathbf{I} \equiv \delta_{ij}$). And, ($\mathbf{R}_I^n$, $\mathbf{R}_V^n$, $\mathbf{R}_C^n$) are the right hand side terms of the inviscid fluxes, viscous fluxes and chemical source respectively at the time level (n).

Two-step Runge-Kutta method of second temporal accurate splits equation (3.58) into two intermediate time integration steps instead of applying one direct step, where the conservative variables at an intermediate time level $(n + \frac{1}{2})$ is determined first given the flow variables at the time level (n) , followed by calculating the conservative variables at the time level $(n + 1)$. Second order spatial and temporal accurate for this kind of independent time-space discretizations for turbulent non-reacting flows are discussed by Hirsch [32]. Besides, there are some developments achieved by Bussing and Murman [8] and others concerning with turbulent chemically reacting flows. Consequently, the two step Runge-Kutta scheme for our model can formulated as follows:

First Step :

$$Q_{i,j}^{n+\frac{1}{2}} = Q_{i,j}^n + \left[I - \frac{\Delta t}{2} \overline{\mathbf{H}}_{i,j}^n \right]^{-1} J_{i,j} \frac{\Delta t}{2} (R_I^n + R_V^n + R_C^n).$$

Second Step :

$$Q_{i,j}^{n+1} = Q_{i,j}^n + \left[I - \Delta t \overline{\mathbf{H}}_{i,j}^{n+\frac{1}{2}} \right]^{-1} J_{i,j} \Delta t \left(R_I^{n+\frac{1}{2}} + R_V^{n+\frac{1}{2}} + R_C^{n+\frac{1}{2}} \right). \quad (3.59)$$

In equation 3.59, the right hand side of the convective (invsoid) fluxes in the first step is calculated in terms of the flow variables at the time level (n) by using first order spatial accurate scheme, where the value of (ε) is set to be zero in equation (3.46). On the other hand, It is determined in the second step by employing second order spatial accurate scheme, where $\varepsilon = 1$ in (3.46). It can be written for both steps as:

$$\begin{aligned} R_I^n &= -\frac{(\overline{E}_{i+\frac{1}{2},j}^n - \overline{E}_{i-\frac{1}{2},j}^n)^{\varepsilon=0}}{\Delta \xi} + \frac{(\overline{F}_{i,j+\frac{1}{2}}^n - \overline{F}_{i,j-\frac{1}{2}}^n)^{\varepsilon=0}}{\Delta \eta} - \alpha \overline{H}_{i,j}^n. \\ R_I^{n+\frac{1}{2}} &= \frac{(\overline{E}_{i+\frac{1}{2},j}^{n+\frac{1}{2}} - \overline{E}_{i-\frac{1}{2},j}^{n+\frac{1}{2}})^{\varepsilon=1}}{\Delta \xi} + \frac{(\overline{F}_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} - \overline{F}_{i,j-\frac{1}{2}}^{n+\frac{1}{2}})^{\varepsilon=1}}{\Delta \eta} - \alpha \overline{H}_{i,j}^{n+\frac{1}{2}}. \end{aligned} \quad (3.60)$$

The viscous fluxes right hand side for both integration steps are second spatial accurate due to central discretization, and are expressed as

follows:

$$\begin{aligned} R_V^n &= \frac{(\overline{E}_{v_{i+\frac{1}{2},j}}^n - \overline{E}_{v_{i-\frac{1}{2},j}}^n)}{\Delta\xi} + \frac{(\overline{F}_{v_{i,j+\frac{1}{2}}}^n - \overline{F}_{v_{i,j-\frac{1}{2}}}^n)}{\Delta\eta} + \alpha \overline{H}_{v_{i,j}}^n, \\ R_V^{n+\frac{1}{2}} &= \frac{(\overline{E}_{v_{i+\frac{1}{2},j}}^{n+\frac{1}{2}} - \overline{E}_{v_{i-\frac{1}{2},j}}^{n+\frac{1}{2}})}{\Delta\xi} + \frac{(\overline{F}_{v_{i,j+\frac{1}{2}}}^{n+\frac{1}{2}} - \overline{F}_{v_{i,j-\frac{1}{2}}}^{n+\frac{1}{2}})}{\Delta\eta} + \alpha \overline{H}_{v_{i,j}}^{n+\frac{1}{2}}. \end{aligned} \quad (3.61)$$

Given that time-linearization of the source term $(\overline{S}_{i,j}^{n+1})$ is of second order accurate in time, so considering it in the final time step only still preserves the second order temporal accuracy. So, in order to reduce the computational effort of inversion the chemical Jacobian matrix, the two-step time integration can be written as follows:

First Step :

$$Q_{i,j}^{n+\frac{1}{2}} = Q_{i,j}^n + J_{i,j} \frac{\Delta t}{2} (R_I^n + R_V^n).$$

Second Step :

$$Q_{i,j}^{n+1} = Q_{i,j}^n + \left[I - \Delta t \overline{H}_{i,j}^n \right]^{-1} J_{i,j} \Delta t \left(R_I^{n+\frac{1}{2}} + R_V^{n+\frac{1}{2}} + R_C^n \right). \quad (3.62)$$

where:

$$R_C^{n+\frac{1}{2}} = \overline{S}_{i,j}^{n+\frac{1}{2}}, \quad R_C^n = \overline{S}_{i,j}^n. \quad (3.63)$$

3.4.4 Time Marching Step Determination

Although the chemical source term is solved implicitly, the value of the CFL number (σ) have to not exceed unity, due to the explicit treatment of the other flow terms:

$$\sigma \leq 1 \quad (3.64)$$

As mentioned by previous researchers dealing with turbulent reacting flows, as Drummond et al. [21] and Chitsomboon et al. [13], CFL (Courant-Friedrichs-Lewy) condition relates the integration time step at a given point, to the maximum eigenvalues of the convective flow Jacobian, this relation can be written in the computational domain

as:

$$\Delta t = \sigma \left\{ \left(\frac{|\mathcal{U}| + c |\nabla \xi|}{\Delta \xi} \right) + \left(\frac{|\mathcal{V}| + c |\nabla \eta|}{\Delta \eta} \right) \right\}^{-1} = \Delta t_{local} \quad (3.65)$$

As shown equation (3.65), the governing equations can be integrated using local time stepping, where the time step in each point is calculated given its flows properties. This technique is used to accelerate the iterative computations to the final solution, and it is acceptable for this model which is concerned with steady state flows.

But, when solution stability is greatly concerned, especially at the first iterations and when the solution is approaching to the steady state, the whole domain is discretized in time using the minimum value of the calculated time step in equation (3.65) for the whole domain as in the following equation:

$$\Delta t = \sigma \left\{ \max \left(\frac{|\mathcal{U}| + c |\nabla \xi|}{\Delta \xi} \right) + \max \left(\frac{|\mathcal{V}| + c |\nabla \eta|}{\Delta \eta} \right) \right\}^{-1} = \Delta t_{min} \quad (3.66)$$

3.5 Boundary Condition Treatment

Beside calculating the flow variables at the inside mesh nodes by time-integrating the governing equations, extra set of computations have to be carried out to determine their values at the boundary nodes, which obey to two kind of boundary conditions, represented in physical and numerical conditions.

The classification of the boundary conditions is dependent on the signs of the flow eigenvalues at boundaries. The physical boundary conditions, which corresponds to the positive eigenvalues, are represented in the imposed values for the flow variables. On the other hand, numerical boundary conditions are represented in the effect of the inner domain on the flow variables at boundary nodes, due to the negative

flow eigenvalues.

The number of eigenvalues of the convective flux Jacobian in our model equals $(n_s + 3)$. And by referring to sub-section **3.2.3** it be concluded that, in the boundary mesh lines of fixed (ξ) value, there are $(n_s + 1)$ repeated eigenvalue equal to $(\mathcal{U})$, and the remaining two eigenvalues are $(\mathcal{U} \pm c |\nabla \xi|)$. Similarly, in the boundary lines of constant value of (η) , there are $(n_s + 1)$ eigenvalues of value $(\mathcal{V})$ and last ones are $(\mathcal{V} \pm c |\nabla \eta|)$.

For the first type of the boundary conditions, It is found that the number of the physical imposed boundary conditions is higher in case of viscous flows than in inviscid flows. That referred to the fact that the momentum and energy equations becomes second order partial differential equations for viscous flows, and become elliptic in space and parabolic in time, where the continuity equations are still parabolic in space and hyperbolic in time. As a result, our hybrid system of the governing equations requires more boundary conditions when the velocity and energy diffusivity are considered.

On the other side, the numerical boundary condition can be estimated by employing first order extrapolation of flow variables. And, as mentioned by Hirsch [32], the overall spatial accuracy of the numerical solver is maintained, even though the variable extrapolation used to calculate the numerical boundary conditions, is lower with one order of spatial accuracy, than the utilized interior spatial discretization. Moreover, *The numerical boundary conditions are treated explicitly*, where the numerical boundary conditions are calculated using the interior flow variables extrapolation at the previous time level. The explicit treatment of the numerical boundary condition is unconditionally stable.

Two sets of calculations using *primitive* and *conservative* variables

will be presented. The both set of computations are not equivalent. However, in both cases the properties conservation is preserved as the applied governing equations are written in the conservative form.

3.5.1 Inlet And Exit Boundary Condition

According to equations (3.7) and (3.8), we can realize the flow is either incoming or outgoing the domain, depending on the sign of the velocity component normal to the boundary line directed towards the domain.

The positive values of $(\mathcal{U}', \mathcal{U})$ at the boundary line of constant value of ξ , declares that flow is coming through this boundary line into the domain. In contrast, their negative values show that the boundary line is a flow exit. In the same manner, the positive and negative values of $(\mathcal{V}', \mathcal{V})$ at the boundary line of fixed η value, corresponds to inlet and exit boundary conditions respectively.

Subsonic Inlet Flow

Here we present the subsonic inlet boundary conditions calculations for the vertical boundary line where ξ equals to zero, i.e. ($\xi = 0$, $i = 1$). , and it is easy to derive them at any another boundary line. In our case, the incoming flow is subsonic, when the velocity component normal to the boundary is less than the sonic speed, i.e. $(\mathcal{U}' < c)$, and so the signs of convective eigenvalues in ξ -direction will be declared as follows:

$$\begin{aligned}\lambda_{\xi_1}, \lambda_{\xi_2}, \dots, \lambda_{\xi_{ns}}, \lambda_{\xi_{ns+1}} &= \mathcal{U} > 0, \\ \lambda_{\xi_{ns+2}} &= \mathcal{U} + c |\nabla \xi| > 0, \\ \lambda_{\xi_{ns+3}} &= \mathcal{U} - c |\nabla \xi| < 0.\end{aligned}\tag{3.67}$$

So, for inviscid flows, we have $(ns + 2)$ imposed physical boundary conditions and one numerical condition. But, in case of viscous flows all the subsonic inlet conditions must be given. The set of calcula-

tion to determine the boundary condition using primitive variables are written as follows:

$$\begin{aligned}
P_{1,j}^{n+1} &= P_{in}, \\
\rho_{1,j}^{n+1} &= \rho_{in}, \\
u_{1,j}^{n+1} &= u_{in}, \\
v_{1,j}^{n+1} &= \begin{cases} v_{in} & , \text{Viscous flows} \\ 2v_{2,j}^n - v_{3,j}^n & , \text{Inviscid flows} \end{cases} \\
Y_{m,1,j}^{n+1} &= Y_{m_{in}}.
\end{aligned} \tag{3.68}$$

Also, the boundary conditions computations can be rewritten in terms of the conservative variables as follows:

$$\begin{aligned}
(\rho)_{1,j}^{n+1} &= \rho_{in}, \\
(\rho u)_{1,j}^{n+1} &= \rho_{in} u_{in}, \\
(\rho v)_{1,j}^{n+1} &= \begin{cases} \rho_{in} v_{in} & , \text{Viscous flows.} \\ 2(\rho v)_{2,j}^n - (\rho v)_{3,j}^n & , \text{Inviscid flows.} \end{cases} \\
(\rho Y_m)_{1,j}^{n+1} &= \rho_{in} Y_{m_{in}}, \quad m = 1, 2, \dots, n_s - 1, \\
(\rho E_t)_{1,j}^{n+1} &= \rho_{in} (h_{f_{mix}}^o)_{1,j}^{n+1} + \frac{P_{in} - \rho_{in} (R_{mix})_{1,j}^{n+1} T_o}{(\gamma_{mix})_{1,j}^{n+1} - 1}.
\end{aligned} \tag{3.69}$$

It is worthy to point the attention that terms used in calculating $(\rho E_t)_{1,j}^{n+1}$, such as the mixture thermal properties, e.g. $(R_{mix})_{1,j}^{n+1}$ and $(h_{f_{mix}}^o)_{1,j}^{n+1}$, are calculated given the species mass fractions (Y_m) , which is, in turn, determined from the species densities and total mixture density. Additionally, the boundary specific heat ratio $(\gamma_{mix})_{1,j}^{n+1}$ is evaluated from the mixture temperature, which is computed given the inlet density and pressure. This procedure will be also carried out in the similar cases for the other boundary conditions.

Supersonic Inlet Flow

Now, if we consider the inlet velocity component normal to the boundary line of ($\xi = 0$), is greater than the sonic speed, i.e. ($\mathcal{U}' > c$). So, all the convective flux Jacobian eigenvalues in ξ -direction are positive:

$$\begin{aligned}\lambda_{\xi_1}, \lambda_{\xi_2}, \dots, \lambda_{\xi_{ns}}, \lambda_{\xi_{ns+1}} &= \mathcal{U} > 0, \\ \lambda_{\xi_{ns+2}} &= \mathcal{U} + c |\nabla \xi| > 0, \\ \lambda_{\xi_{ns+3}} &= \mathcal{U} - c |\nabla \xi| > 0.\end{aligned}\tag{3.70}$$

So, for inviscid and viscous flows, the whole flow properties at the supersonic inlet must be imposed. The boundary condition for supersonic inlet is written in terms of the primitive form as:

$$\begin{aligned}P_{1,j}^{n+1} &= P_{in}, \\ \rho_{1,j}^{n+1} &= \rho_{in}, \\ u_{1,j}^{n+1} &= u_{in}, \\ v_{1,j}^{n+1} &= v_{in}, \\ Y_{m_{1,j}}^{n+1} &= Y_{m_{in}}.\end{aligned}\tag{3.71}$$

or they can be calculated in terms of the conservative variables as:

$$\begin{aligned}(\rho)_{1,j}^{n+1} &= \rho_{in}, \\ (\rho u)_{1,j}^{n+1} &= \rho_{in} u_{in}, \\ (\rho v)_{1,j}^{n+1} &= \rho_{in} v_{in}, \\ (\rho Y_m)_{1,j}^{n+1} &= \rho_{in} Y_{m_{in}}, \quad m = 1, 2, \dots, n_s - 1, \\ (\rho E_t)_{1,j}^{n+1} &= \rho_{in} (h_{f_{mix}}^o)_{1,j}^{n+1} + \frac{P_{in} - \rho_{in} (R_{mix})_{1,j}^{n+1} T_o}{(\gamma_{mix})_{1,j}^{n+1} - 1}.\end{aligned}\tag{3.72}$$

Subsonic Exit Flow

Here, it is more convenient to take the boundary line of $i = imax$ as an example for flow exit, where the exit velocity component normal to the boundary and directed towards the domain, negative. If we assume magnitude of the velocity component is less than the sonic speed, we will have only one positive eigenvalue.

$$\begin{aligned}\lambda_{\xi_1}, \lambda_{\xi_2}, \dots, \lambda_{\xi_{ns}}, \lambda_{\xi_{ns+1}} &= \mathcal{U} < 0, \\ \lambda_{\xi_{ns+2}} &= \mathcal{U} + c |\nabla \xi| > 0, \\ \lambda_{\xi_{ns+3}} &= \mathcal{U} - c |\nabla \xi| < 0.\end{aligned}\tag{3.73}$$

It is recommended in most cases to impose the value of the exit pressure at subsonic exits. The boundary properties calculation set written in terms of the primitive variables is described as:

$$\begin{aligned}P_{imax,j}^{n+1} &= P_{out}, \\ T_{imax,j}^{n+1} &= 2T_{imax-1,j}^n - T_{imax-2,j}^n, \\ u_{imax,j}^{n+1} &= 2u_{imax-1,j}^n - u_{imax-2,j}^n, \\ v_{imax,j}^{n+1} &= 2v_{imax-1,j}^n - v_{imax-2,j}^n, \\ Y_{m,imax,j}^{n+1} &= 2Y_{m,imax-1,j}^n - Y_{m,imax-2,j}^n.\end{aligned}\tag{3.74}$$

or by using the conservative variables, the boundary properties calculations will be:

$$\begin{aligned}(\rho)_{imax,j}^{n+1} &= 2(\rho)_{imax-1,j}^n - (\rho)_{imax-2,j}^n, \\ (\rho u)_{imax,j}^{n+1} &= 2(\rho u)_{imax-1,j}^n - (\rho u)_{imax-2,j}^n, \\ (\rho v)_{imax,j}^{n+1} &= 2(\rho v)_{imax-1,j}^n - (\rho v)_{imax-2,j}^n, \\ (\rho Y_m)_{imax,j}^{n+1} &= 2(\rho Y_m)_{imax-1,j}^n - (\rho Y_m)_{imax-2,j}^n, \quad m = 1, 2, \dots, n_s - 1, \\ (\rho E_t)_{imax,j}^{n+1} &= (\rho)_{imax,j}^{n+1} (h_{f,mix}^o)_{imax,j}^{n+1} + \frac{P_{out} - (\rho)_{imax,j}^{n+1} (R_{mix})_{imax,j}^{n+1} T_o}{(\gamma_{mix})_{imax,j}^{n+1} - 1}.\end{aligned}\tag{3.75}$$

Supersonic Exit Flow

For the previously mentioned example, if the magnitude of exit velocity component normal to boundary is greater than the sonic speed, all the eigenvalues in ξ -direction become negative:

$$\begin{aligned}\lambda_{\xi_1}, \lambda_{\xi_2}, \dots, \lambda_{\xi_{n_s}}, \lambda_{\xi_{n_s+1}} &= \mathcal{U} < 0, \\ \lambda_{\xi_{n_s+2}} &= \mathcal{U} + c |\nabla \xi| < 0, \\ \lambda_{\xi_{n_s+3}} &= \mathcal{U} - c |\nabla \xi| < 0.\end{aligned}\tag{3.76}$$

And, all the exit boundary conditions is determined from variable extrapolation from the interior domain, is expressed in terms of the primitive variables as:

$$\begin{aligned}P_{imax,j}^{n+1} &= 2P_{imax-1,j}^n - P_{imax-2,j}^n, \\ \rho_{imax,j}^{n+1} &= 2\rho_{imax-1,j}^n - \rho_{imax-2,j}^n, \\ u_{imax,j}^{n+1} &= 2u_{imax-1,j}^n - u_{imax-2,j}^n, \\ v_{imax,j}^{n+1} &= 2v_{imax-1,j}^n - v_{imax-2,j}^n, \\ Y_{m_{imax,j}}^{n+1} &= 2Y_{m_{imax-1,j}}^n - Y_{m_{imax-2,j}}^n.\end{aligned}\tag{3.77}$$

or in terms of the conservative flow variables as:

$$\begin{aligned}(\rho)_{imax,j}^{n+1} &= 2(\rho)_{imax-1,j}^n - (\rho)_{imax-2,j}^n, \\ (\rho u)_{imax,j}^{n+1} &= 2(\rho u)_{imax-1,j}^n - (\rho u)_{imax-2,j}^n, \\ (\rho v)_{imax,j}^{n+1} &= 2(\rho v)_{imax-1,j}^n - (\rho v)_{imax-2,j}^n, \\ (\rho Y_m)_{imax,j}^{n+1} &= 2(\rho Y_m)_{imax-1,j}^n - (\rho Y_m)_{imax-2,j}^n, \quad m = 1, 2, \dots, n_s - 1, \\ (\rho E_t)_{imax,j}^{n+1} &= 2(\rho E_t)_{imax-1,j}^n - (\rho E_t)_{imax-2,j}^n.\end{aligned}\tag{3.78}$$

3.5.2 Wall Boundary Condition

The wall boundary is characterized by the zero value of the velocity component normal to the boundary, for both cases of inviscid and viscous flows:

$$\vec{V} \cdot \hat{n} = 0. \quad (3.79)$$

That is because the slip condition at the wall surface is assumed for inviscid flows, such that the velocity vector is tangent to the wall. On the other sides, in viscous flows, the no-slip condition states that the velocity magnitude vanishes at the wall surface.

So, if take the boundary line of ($\eta = 0, j = 1$) as an example of wall boundary, the velocity component normal to the wall ($\mathcal{V}$) is equal to zero, and we will have ($n_s + 1$) zero eigenvalues, and last two will be positive and negative:

$$\begin{aligned} \lambda_{\eta_1}, \lambda_{\eta_2}, \dots, \lambda_{\eta_{n_s}}, \lambda_{\eta_{n_s+1}} &= \mathcal{V} = 0, \\ \lambda_{\eta_{n_s+2}} &= \mathcal{V} + c |\nabla \eta| > 0, \\ \lambda_{\eta_{n_s+3}} &= \mathcal{V} - c |\nabla \eta| < 0. \end{aligned} \quad (3.80)$$

The first physical imposed boundary conditions is represented in the vanishing of the velocity component normal to the wall. Also, the wall temperature status (either for adiabatic or constant temperature cases), and the gradients of species concentrations must be specified. In addition, in case of viscous flows only, the no-slip condition sets the velocity magnitude to zero. On the other side, the main property which is mainly affected by the interior domain is the pressure at the wall surface, beside the velocity magnitude at wall in case of inviscid flows only. The wall conditions calculations can be written in terms

of the primitive variables as follows:

$$P_{i,1}^{n+1} = 2P_{i,1}^n - P_{i,1}^n,$$

For inviscid flows :

$$V_{i,1}^{n+1} = 2V_{i,2}^n - V_{i,3}^n \Rightarrow u_{i,1}^{n+1} = \frac{\eta_{y_{i,1}}}{|\nabla\eta|_{i,1}} V_{i,1}^{n+1}, \quad v_{i,1}^{n+1} = \frac{-\eta_{x_{i,1}}}{|\nabla\eta|_{i,1}} V_{i,1}^{n+1},$$

For viscous flows :

$$V_{i,1}^{n+1} = 0 \Rightarrow u_{i,1}^{n+1} = 0, \quad v_{i,1}^{n+1} = 0$$

$$T_{i,1}^{n+1} = \begin{cases} T_{i,2}^n & , \text{ Adiabatic Wall.} \\ T_w & , \text{ Constant Temperature Wall.} \end{cases}$$

$$Y_{m_{i,1}}^{n+1} = Y_{m_{i,2}}^n. \tag{3.81}$$

From the equations above, the pressure at the wall surface is determined by simple linear extrapolation, instead of using the momentum equation, in order to reduce the computational effort. Also, we find that the slope of the species concentration variation is set to zero at the wall, because we are concerned only with non-reacting wall surfaces. Besides, we also note that for inviscid flows we extrapolate only the velocity magnitude ($V_{i,1}^{n+1}$), and decompose it into two components given that the velocity vector is tangent to surface. But, in case of viscous flows, we equate both velocity components to zero due to the no-slip condition.

3.5.3 Far-field Boundary Condition

In solving external flows with computational aerodynamics techniques, the far-field boundary treatment becomes more essential when the size of the computational domain is more limited. In cases of study, we consider that the far-field conditions is totally affected by the interior domain. However, the kind of this boundary treatment is highly de-

pendent on the aerodynamic problem and the range of the domain of study.

If take the far-field boundary at the line of ($j = jmax$), the flow variables at far-field boundary is calculated in terms of the primitive variables as:

$$\begin{aligned}
P_{i,jmax}^{n+1} &= 2P_{i,jmax-1}^n - P_{i,jmax-2}^n, \\
\rho_{i,jmax}^{n+1} &= 2\rho_{i,jmax-1}^n - \rho_{i,jmax-2}^n, \\
u_{i,jmax}^{n+1} &= 2u_{i,jmax-1}^n - u_{i,jmax-2}^n, \\
v_{i,jmax}^{n+1} &= 2v_{i,jmax-1}^n - v_{i,jmax-2}^n, \\
Y_{m,i,jmax}^{n+1} &= 2Y_{m,i,jmax-1}^n - Y_{m,i,jmax-2}^n.
\end{aligned} \tag{3.82}$$

On the other side, the calculations can employ the conservative variables as follows:

$$\begin{aligned}
(\rho)^{n+1}_{i,jmax} &= 2(\rho)^n_{i,jmax-1} - (\rho)^n_{i,jmax-2}, \\
(\rho u)^{n+1}_{i,jmax} &= 2(\rho u)^n_{i,jmax-1} - (\rho u)^n_{i,jmax-2}, \\
(\rho v)^{n+1}_{i,jmax} &= 2(\rho v)^n_{i,jmax-1} - (\rho v)^n_{i,jmax-2}, \\
(\rho Y_m)^{n+1}_{i,jmax} &= 2(\rho Y_m)^n_{i,jmax-1} - (\rho Y_m)^n_{i,jmax-2}, \quad m = 1, 2, \dots, n_s - 1, \\
(\rho E_t)^{n+1}_{i,jmax} &= 2(\rho E_t)^n_{i,jmax-1} - (\rho E_t)^n_{i,jmax-2},
\end{aligned} \tag{3.83}$$

3.5.4 Symmetry Boundary Condition

In case the flow properties are mirrored across a given line, we split our domain into the two identical parts and solve one of them, in order to reduce the computational cost beside increasing the solving resolution. The symmetry line is characterized by two properties: the first is represented in the zero gradients of all the flow variables across it, and the other is velocity vector tangency to the symmetry line. So the

velocity component normal to the symmetry line is zero.

For instance, if we take the horizontal boundary line which is parallel to x -axis, and has a constant value of ξ , e.g. ($\xi = 0$, $i = 1$) is considered as a symmetry boundary. The boundary flow variables are calculated in terms of the primitive variables as:

$$\begin{aligned} P_{i,jmax}^{n+1} &= P_{i,jmax-1}^n, \\ \rho_{i,jmax}^{n+1} &= \rho_{i,jmax-1}^n, \\ u_{i,jmax}^{n+1} &= u_{i,jmax-1}^n, \\ v_{i,jmax}^{n+1} &= 0, \\ Y_{m_{i,jmax}}^{n+1} &= Y_{m_{i,jmax-1}}^n. \end{aligned} \tag{3.84}$$

or in terms of the conservative variables as:

$$\begin{aligned} (\rho)_{i,1}^{n+1} &= (\rho)_{i,2}^n, \\ (\rho u)_{i,1}^{n+1} &= (\rho u)_{i,2}^n, \\ (\rho v)_{i,1}^{n+1} &= 0, \\ (\rho Y_m)_{i,1}^{n+1} &= (\rho Y_m)_{i,2}^n, \quad m = 1, 2, \dots, n_s - 1, \\ (\rho E_t)_{i,1}^{n+1} &= (\rho E_t)_{i,2}^n. \end{aligned} \tag{3.85}$$

3.6 Grid Generation & Clustering Techniques

Algebraic grid generator is utilized in our model, due to its simple implementation and because its clustering techniques are easily controlled and modified. A detailed explanation is presented for different clustering techniques, which intensify the structured mesh lines within specified regions, where it is necessary that the spatial resolution is high enough to simulate complicated flow features.

First, we must point that in the primary steps, the behavior of the boundary grid lines is specified in order to cover the required domain of study, so the grid lines of indices $(1, j)$, $(imax, j)$, $(i, 1)$, and $(i, jmax)$ are determined. Then, the arithmetic progression technique generates, in an intermediate stage, a structured mesh for the preliminary coordinate system $(\mathbf{X}, \mathbf{Y})$ in the physical domain, where arithmetic progression is applied to create equally spaced grid line in each direction, such that:

$$\mathbf{Y}_{i,j} = \mathbf{Y}_{i,j-1} + \frac{\mathbf{Y}_{i,jmax} - \mathbf{Y}_{i,1}}{jmax - 1}, \quad \mathbf{X}_{i,j} = \mathbf{X}_{i-1,j} + \frac{\mathbf{X}_{imax,j} - \mathbf{X}_{1,i}}{imax - 1}, \quad (3.86)$$

In the transformation process from the intermediate coordinate system $(\mathbf{X}, \mathbf{Y})$ to the final coordinate system (x, y) in the physical domain, the boundary lines are identical, but the mesh nodes are stretched to obtain the required clustering, using different transformation functions.

3.6.1 Clustering At the Wall-Bounded Regions

Here, we will introduce the employed transformation function to cluster the grid lines near the walls in case of viscous flows, in order to resolve more accurately complex flow phenomena such as boundary layer, flow separation, and the boundary layer-shock wave interactions.

Clustering Using Geometric Progression for One Wall-Sided Domain

In this clustering technique, no need to generate an intermediate coordinate system $(\mathbf{X}, \mathbf{Y})$. Grid line stretching in certain direction is achieved by multiplying each spatial interval with a certain factor to determine the successor interval in the same direction. The multiplication factor is known as geometric progression rate ($\mathbf{r}$). If we are

clustering the grid lines in y -direction starting from ($j = 1$) which is the index of the wall boundary, the stretching function can be written as:

$$y_{i,j} = y_{i,j-1} + \delta_1 \mathbf{r}^{j-2}. \quad (3.87)$$

The summation of all intervals in y -direction will equal distance between the extreme points, i.e ($i, 1$) and ($i, jmax$). So the total distance (L_y) is expressed as:

$$L_y = \mathbf{y}_{i,jmax} - \mathbf{y}_{i,1} = \delta_1 + \delta_1 \mathbf{r} + \delta_1 \mathbf{r}^2 + \dots + \delta_1 \mathbf{r}^{jmax-3} + \delta_1 \mathbf{r}^{jmax-2}, \quad (3.88)$$

where (δ_1) is the first and smallest spatial interval next to the wall surface. It is considered the base of the geometric series written in equation (3.88). Its value is set to be order of (10^{-4}) for laminar flows, and of order (10^{-5}) or even (10^{-6}) for turbulent flows. When equation (3.88) is written in the compact form as:

$$L_y = \delta_1 \left(\frac{\mathbf{r}^{jmax-1} - 1}{\mathbf{r} - 1} \right). \quad (3.89)$$

We can conclude the value of the progression rate ($\mathbf{r}$), given the number of intervals ($jmax - 1$), the first spatial step (δ_1), and the total distance (L_y), by applying this iterative procedure:

1. Assume value of the progression rate $\mathbf{r}$.
2. According to equation (3.89), calculate the new value of the progression rate as:

$$\mathbf{r}_{new} = \left\{ 1 + (\mathbf{r} - 1) \frac{L_y}{\delta_1} \right\}^{\frac{1}{jmax-1}}. \quad (3.90)$$

3. Calculate the error between the old and new values of the progression rate:

$$\text{error} = \frac{|\mathbf{r}_{new} - \mathbf{r}|}{\mathbf{r}}. \quad (3.91)$$

4. If the error exceeds the allowable error limit, repeat the calculation

from (1) again.

For smooth stretching, the progression rate $\mathbf{r}$ is preferred to be limited such that ($\mathbf{r} \leq 1.3$). That is can be achieved by selecting the suitable number of grid line (j_{max}).

Clustering Using First Robert's Transformation Function For One wall-sided Domain

Roberts [46] suggested a transformation function from $(\mathbf{X}, \mathbf{Y})$ coordinate system to the (x, y) axes, to cluster the grid line towards one side only as shown in figure (3.2), The transformation technique is explained as:

$$\Gamma = 1 - \frac{\mathbf{Y}_{i,j} - \mathbf{Y}_{i,1}}{\mathbf{Y}_{i,j_{max}} - \mathbf{Y}_{i,1}},$$

$$y_{i,j} = \mathbf{Y}_{i,1} + (\mathbf{Y}_{i,j_{max}} - \mathbf{Y}_{i,1}) \frac{1 + \beta_y - (\beta_y - 1) \left\{ \frac{\beta_y + 1}{\beta_y - 1} \right\}^\Gamma}{\left(1 + \left\{ \frac{\beta_y + 1}{\beta_y - 1} \right\}^\Gamma \right)}. \quad (3.92)$$

where (β_y) is ranging from 1 to ∞ , the clustering intensity increases as β_y approaches to 1

Clustering Using Second Robert's Transformation Function For Two wall-sided Domain

For two wall-sides domains, such as ducts, the grid lines can be clustered towards the two opposite sides, as illustrated in figure (3.3), by using another function from the general stretching transformations

proposed by Roberts, which is written in details as follows:

$$\Gamma = \left(\frac{\mathbf{Y}_{i,j} - \mathbf{Y}_{i,1}}{\mathbf{Y}_{i,jmax} - \mathbf{Y}_{i,1}} - \alpha_y \right) / (1 - \alpha_y),$$

$$y_{i,j} = \mathbf{Y}_{i,1} + (\mathbf{Y}_{i,jmax} - \mathbf{Y}_{i,1}) \frac{2\alpha_y - \beta_y + (\beta_y + 2\alpha_y) \left\{ \frac{\beta_y + 1}{\beta_y - 1} \right\}^\Gamma}{(2\alpha_y + 1) \left(1 + \left\{ \frac{\beta_y + 1}{\beta_y - 1} \right\}^\Gamma \right)}. \quad (3.93)$$

For this transformation if $(\alpha_y = 0)$ the mesh will be refined only near the index $(i, jmax)$, but if $(\alpha_y = \frac{1}{2})$, the mesh will equally cluster towards the opposite both wall boundaries of indices $(i, 1)$ and $(i, jmax)$.

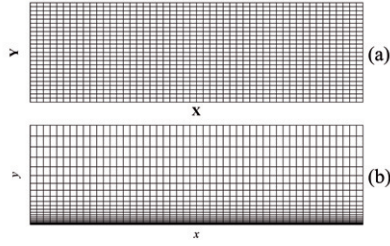


Figure 3.2: **Clustering to the one wall-bounded side.** (a) Intermediate domain (X, Y) . (b) Physical domain (x, y)

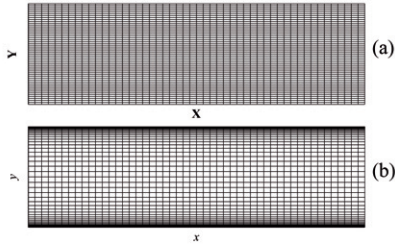


Figure 3.3: **Clustering to the two wall-bounded sides.** (a) Intermediate domain (X, Y) . (b) Physical domain (x, y)

3.6.2 Clustering Around Jet Centerlines

As shown later in next chapters, it is necessary to refine the mesh line around the axis of the transverse jet, as the interaction of high speed flows interrupt by transverse sonic injection results a complex system of shocks and separation vortices. When it is required to generate mesh near the vertical line ($\mathbf{X} = x = x_o$), as shown in figure (3.4), the vertical lines clustering is carried out using a the following transformation technique, which is based on Hyperbolic Sine function:

$$A_o = \frac{1}{2\beta_x} \ln \left(\frac{1 + (e^{\beta_x} - 1)(x_o/L_x)}{1 + (e^{-\beta_x} - 1)(x_o/L_x)} \right), \quad (3.94)$$

$$x_{i,j} = x_o \left[1 + \frac{\sinh \{ \beta_x (\mathbf{X}_{i,j}/L_x) - A_o \}}{\sinh \{ \beta_x A_o \}} \right],$$

where (A_o) is an intermediate function in the transformation process, and (β_x) is considered as clustering intensity constant, it is greater than 1, for acceptable mesh refinement, it ranges between 2 to 15. We should note that we can combine between two clustering transformation functions in different directions starting from the arithmetic generated domain ($\mathbf{X}, \mathbf{Y}$) to the final form of the physical domain (x, y).

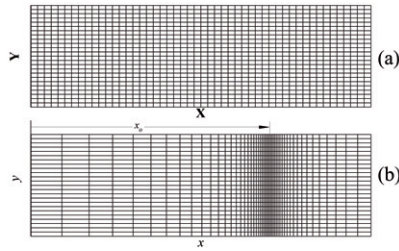


Figure 3.4: **Clustering around an interior vertical line.** (a) **Intermediate domain ($\mathbf{X}, \mathbf{Y}$).** (b) **Physical domain (x, y).**

Chapter 4

Results and Discussions

4.1 Introduction

The Hydrogen-Air mixing and combustion processes in scramjet engine includes numerous complicated flow features (i.e. shock waves - boundary layer interactions and shock induced chemical reactions,... etc.). The numerical code is developed to solve combination of these complicated phenomena. The code is validated by solving simpler test cases that are concerned with each specific flow feature. The selected problems to validate the numerical solver of chemically reacting turbulent flows, as follows:

- Laminar and turbulent air flows over a flat plate.
- Complete and over expansions of premixed hydrogen-air inviscid chemically reacting in axisymmetric nozzle.
- Premixed hydrogen-air turbulent chemically reacting two-dimensional flow in ramped duct with different inlet temperatures.
- Sonic transverse Helium injection to supersonic two-dimensional air flow.

Then, the numerical code is applied to solve the problem of hydrogen sonic transverse injection into supersonic air flow in a two-dimensional

single strut scramjet engine, for non-reacting and reacting test cases to study air-hydrogen mixing and combustion in scramjet combustors.

4.2 Laminar & Turbulent Flows Over Flat Plate

Evaluating the calculations dealing with viscous terms can be carried first by solving the simple problem of viscous air flows over a flat plate with a zero angle of attack. The plate's length is taken to be unity, which is taken to be the reference length ($L_{ref} = 1 [m]$). The reference values of density, temperature, velocity, and the laminar transport conditions are set to equal those of air at inlet, as follows:

$$\rho_{ref} = \rho_{in}, \quad T_{ref} = T_{in}, \quad V_{ref} = V_{in}, \quad \mu_{ref} = \mu_{Lin}, \quad k_{ref} = k_{Lin}. \quad (4.1)$$

Two different values of reference Reynolds number are selected for laminar and turbulent cases, as given in the following:

$$Re_{ref} = \begin{cases} 4.3 \times 10^5, & \text{for laminar flow test case.} \\ 5.4 \times 10^6, & \text{for turbulent flow test case.} \end{cases} \quad (4.2)$$

In addition, the value of inlet Mach number, is preferred to be high enough to avoid using preconditioning matrix, which is required for viscous flows of very low Mach number for both laminar and turbulent test cases. So, the assumed value of inlet Mach number, which is considered also as the reference value of Mach number, as follows:

$$\mathbf{M}_{in} = \mathbf{M}_{ref} = 0.4. \quad (4.3)$$

In this problem, air is considered as a homogenous mixture all over the domain, where the mass diffusive fluxes and chemical reactions are not considered. In other words, it is considered to be single-species flows (i.e. $n_s = 1$). Besides, the air transport coefficients are assumed

to be constants, as shown below:

$$\mu_L = 15 \times 10^{-6} [N.sec/m^2], \quad k_L = 20 \times 10^{-3} [W/m.K]. \quad (4.4)$$

4.2.1 Laminar Flow Test Case

For the case of laminar air flow over a flat plate, Reynolds number is taken less than the transition limit, i.e. ($Re_{ref} = 4.3 \times 10^5 < 5 \times 10^5$). And, as the inlet Mach number is assumed to be (0.4), the rest of the inlet flow variables are selected as follows:

$$\begin{aligned} P_{in} &= 4000 [Pa], & \rho_{in} &= 0.04 [kg/m^3], \\ u_{in} &= 150 [m/sec], & v_{in} &= 0 [m/sec]. \end{aligned} \quad (4.5)$$

The numerical solution of Navier-Stocks equations is compared to the analytical solution of Blasius laminar boundary-layer, which is written in terms of the non-dimensional normal distance from the wall (η) and its function $f(\eta)$, which can be expressed as:

$$\eta = y \sqrt{\frac{U_\infty \rho}{2 \mu x}}, \quad u = U_\infty \frac{\partial f}{\partial \eta} = U_\infty f'. \quad (4.6)$$

such that, the laminar velocity profile is obtain in solving third order ordinary non-linear partial differential equation as following:

$$f''' + f f'' = 0. \quad (4.7)$$

given these boundary condition:

$$\eta = 0 \Rightarrow f = 0, \quad f' = 0, \quad \eta = \infty \Rightarrow f' = 1. \quad (4.8)$$

The last boundary condition can be replace by ($\eta = 0 \Rightarrow f'' = 0.4696$). The results of velocity profile at different stations match with that derived by Blasius equation, as shown in figure(4.4).

In order to testify the numerical code in determining the local skin

friction drag (c_f), which is generally expressed as:

$$c_f = \frac{\tau_w}{\frac{1}{2}\rho U_\infty^2 L_{ref}}. \quad (4.9)$$

The results are compared with the derived formulation from Blasius equation, which is written as follows:

$$c_f = \frac{0.664}{\sqrt{Re_x}} = \frac{0.664}{\sqrt{\frac{\rho U_\infty x}{\mu}}}. \quad (4.10)$$

Clustering of grid lines near the wall is applied employing geometric progression technique mentioned in sub-section **3.6.1**, such that the minimum grid size is set to be 10^{-4} [m]. In order to estimate grid sensitivity of the numerical code to determine the local friction coefficient, the laminar flow is resolved using two grids of sizes 51×55 and 101×55 , as shown in figures (4.1) and (4.2) respectively. The progression rate (r) is about 1.12, to generate smooth increase in the spatial intervals in the normal direction from the wall surface.

Local time stepping is applied, where CFL coefficient is constant and set to be ($\sigma = 0.9$). The density normalized residual is plotted versus the solution iterations, as illustrated in figure (4.3). For the mesh size of 51×55 , The solution convergence of the laminar flow case is approximately achieved after 30×10^3 iterations, where sharp fluctuations of the normalized residual value around 10^{-6} are observed. That can be referred to the use of discontinuous slope limiter to satisfy TVD condition.

According to figure (4.5), the numerical calculations overestimate the local friction coefficient, especially near the leading edge. And it approaches the analytical solution by increasing the number of mesh nodes. It is concluded that it is recommended to cluster the grid lines near the leading edge for more accurate estimation of the skin friction.

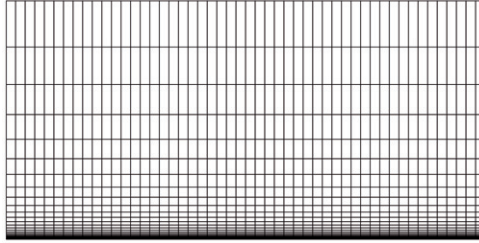


Figure 4.1: The mesh of size 51×55 utilized for solving viscous flows over a flat plate.

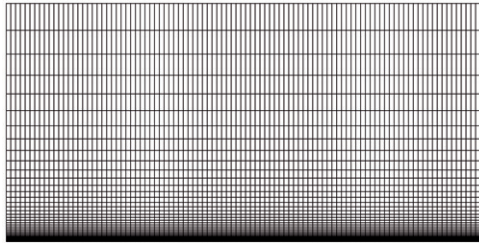


Figure 4.2: The mesh of size 101×55 utilized for solving viscous flows over a flat plate.

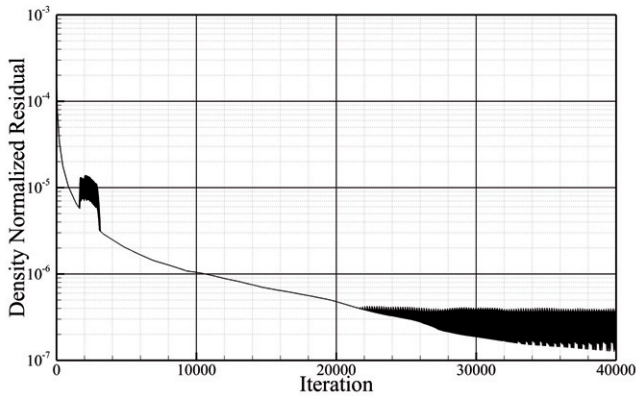


Figure 4.3: Convergence history of the laminar flow test case.

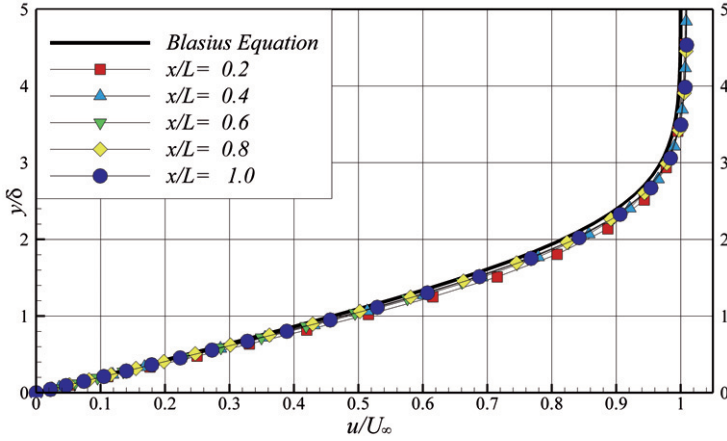


Figure 4.4: Velocity profile for laminar flow solved by Blasius equations versus numerical solution at different stations

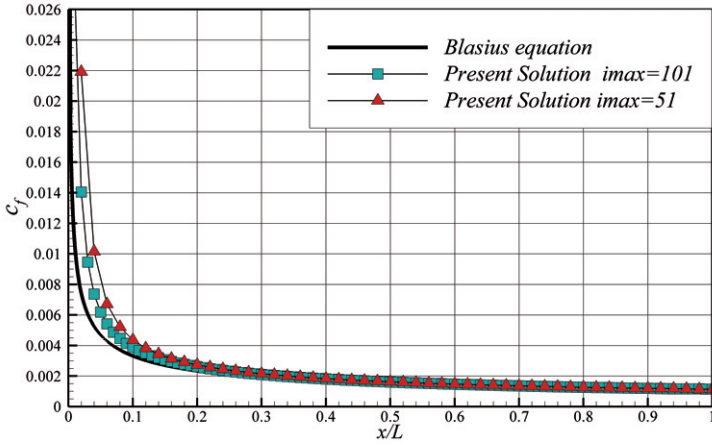


Figure 4.5: Local skin friction Coefficient for laminar flows using Blasius equation beside numerical solver for two different discretizations

4.2.2 Turbulent Flow Test Case

For viscous flows over flat plates, full transition to turbulent condition is completely assured when Reynolds number exceeds 5×10^6 . For this problem, inlet Reynolds number is set as ($Re = 5.4 \times 10^6 > 5 \times 10^6$), and fix the value of the Mach number as in the previous case, i.e. ($M_{in} = 0.4$), the inlet conditions for turbulent flow case are:

$$\begin{aligned} P_{in} &= 50000 [Pa], & \rho_{in} &= 0.5 [kg/m^3], \\ u_{in} &= 150 [m/sec], & v_{in} &= 0 [m/sec]. \end{aligned} \quad (4.11)$$

The typical turbulent velocity profile near to the wall surface can be described in the universal graph of *law of the wall*, which is drawn using the dimensionless flow variables (n^+ , u^+), which are mentioned before in section 2.7, and they are referred to the wall surface conditions, such that:

$$n^+ = \frac{u_\tau \rho_w n}{\mu_w}, \quad u^+ = \frac{V}{u_\tau}. \quad (4.12)$$

where $u_\tau = \sqrt{\tau_w / \rho_w}$. The turbulent velocity profile can be divided into a number of sub-layers, starting with the *viscous sublayer*, where the dimensionless velocity (u^+) is linearly proportional to dimensionless normal distance from the wall (n^+). And after an intermediate region known as the *buffer zone*, they are related in logarithmic relation in the *fully turbulent zone*.

$$\begin{aligned} \text{Viscous Sublayer :} & \quad u^+ = n^+, \\ \text{Fully Turbulent Zone :} & \quad u^+ = \frac{1}{0.41} \ln(n^+) + 5.15. \end{aligned} \quad (4.13)$$

In addition, the local skin friction coefficient for turbulent flow (c_f) can be determined analytical by the one fifth power law, or by White's

empirical law, which are written as follows:

$$\text{One Fifth Power Law : } c_f = \frac{0.058}{Re_x^{1/5}} = \frac{0.058}{\left(\frac{\rho U_\infty x}{\mu}\right)^{1/5}}.$$

$$\text{White's Law : } c_f = \frac{0.455}{[\ln(0.06 Re_x)]^2} = \frac{0.455}{\left[\ln\left(0.06 \frac{\rho U_\infty x}{\mu}\right)\right]^2}. \quad (4.14)$$

Geometric progression technique is used to cluster the grid lines near the wall side, such that the minimum grid size is set 10^{-6} , in order to resolve more grid points in the viscous sublayer. The turbulent flow is resolved using a mesh of size 51×55 , as shown in figure (4.1). The progression rate ($\mathbf{r}$) is raised to be 1.24, as the order of magnitude of the minimum grid size is reduced compared to that of the laminar test case. But, the gradual progression in the grid size is still preserved.

Time marching is implemented using local time stepping, with constant CFL coefficient approaching to unity (i.e., $\sigma = 0.9$). The density normalized residual is plotted versus the solution iteration, in figure (4.6) for the turbulent flow case. Convergence for the mesh of size 51×55 is achieved after 2×10^6 iterations. This slow convergence is due to applying explicit time integration for the flow convective and viscous terms.

And, it is found that numerical solutions at different stations coincide with velocity profile of the analytical solution of the law of the wall, as shown in figure (4.7). It is observed that the “*fully turbulent log-law zone*” increases downstream, as the boundary layer thickness increases along the flat plate. Additionally, there is a numerical over-estimation of the local skin friction coefficient for turbulent flow by mesh of size (51×55) compared to the solutions of the one fifth power law and White’s law as shown in figure (4.8).

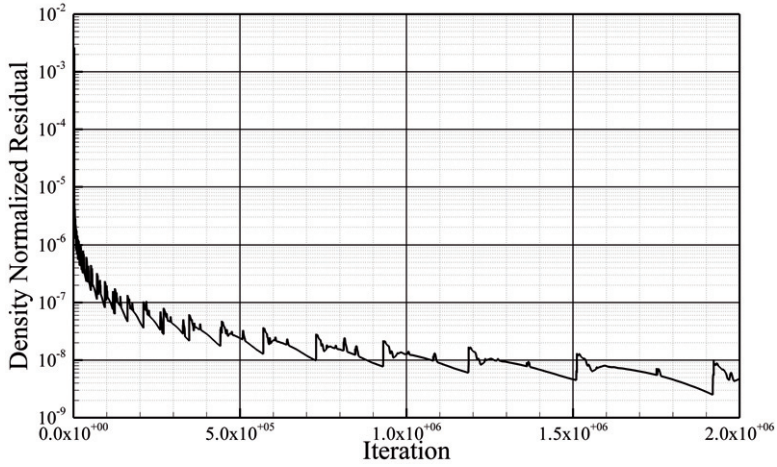


Figure 4.6: **Convergence history of the turbulent flow test case.**

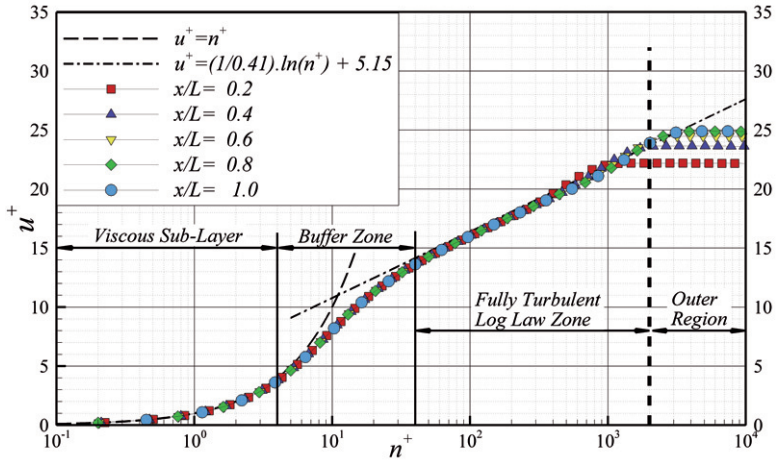


Figure 4.7: **Typical turbulent velocity profiles for the analytical solution and numerical results at different stations**

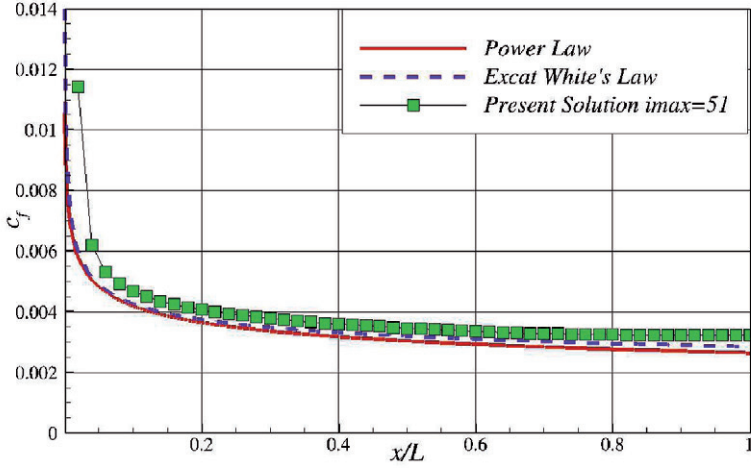


Figure 4.8: Turbulent local skin friction coefficient over a flat plate of the numerical solver and analytical solutions of Power and White's laws

4.3 Inviscid Chemically-Reacting and Supersonic Flow in 2-D Axisymmetric Nozzle

In the following test cases, the numerical code is evaluated to solve inviscid premixed hydrogen-air chemically reacting flows with and without shocks. As shown in figure (4.9), the schematic diagram illustrates the test case of premixed hydrogen-air reacting flow with an equivalence ratio of ($\phi = 0.29841$), in axisymmetric conduit of adiabatic walls. And, the inlet conditions are given as follows:

$$\begin{aligned}
 T_{in} &= 1884.3 [K], & P_{in} &= 0.8026 \times 10^5 [Pa], \\
 u_{in} &= 1245 [m/sec], & v_{in} &= 0 [m/sec].
 \end{aligned} \tag{4.15}$$

It is required to solve 2D invscid flow through the divergent part of axisymmetric nozzle, whose length is set to be the reference length, and equals to 2 meters. Besides, the reference values of transport coefficients, density, velocity, and temperature are equal to the air-hydrogen mixture properties at the inlet.

$$\begin{aligned} L_{ref} = 2 [m], \quad \rho_{ref} = \rho_{in}, \quad T_{ref} = T_{in}, \quad V_{ref} = V_{in}, \\ \mu_{ref} = \mu_{Lin}, \quad k_{ref} = k_{Lin}, \quad \mathcal{D}_{ref} = \mathcal{D}_{Lin}. \end{aligned} \quad (4.16)$$

And, the nozzle radius is a sinusoidal function of the longitudinal distance along the nozzle axis as:

$$r = 0.125L \left[1 + \sin \left(\frac{\pi x}{2L} \right) \right]. \quad (4.17)$$

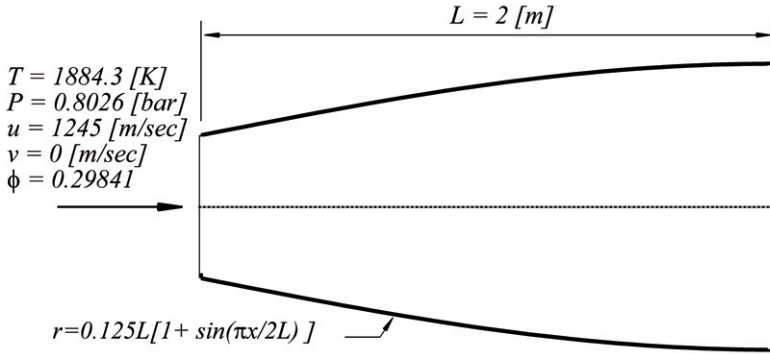


Figure 4.9: Schematic diagram for the test case of invscid flow of chemically reacting hydrogen-air mixture in axisymmetric nozzle

4.3.1 Complete Expansion Test Case

In this case, the symmetry condition is applied at the nozzle center-line, where the spatial discretization size is (41×11) . The grid size is sufficient, there is no expected shock wave in this invscid flow problem. As shown in figure (4.10), the structured mesh is generated by using arithmetic progression function which is described by equation (3.86).

Time-integration is carried out using minimum time stepping with CFL number equals to $(\sigma = 0.1)$, in order to avoid any instability result from incorrect guess of the initial conditions of the computations. The convergence history is displayed in figure (4.11). Local peaks of order of 10^{-1} arise in the intermediate iterations due to the inaccurate assumption of the initial flow condition. It is shown that the convergence is attained approximately after 5000 iterations. Also, it is noticed that there are fluctuations in the value of the normalized residual at convergence near the value 10^{-6} , due to using *minmode* slope limiter. It is expected, that the convergence value of the residual would be raised to order of magnitude 10^{-4} or 10^{-3} , if other slope limiter is applied.

Numerical solution for the species mass fraction distribution is presented in figures (4.12)-(4.15). It is shown that rapid rates of termination of the main reactants (i.e. Hydrogen and atoms molecules), and of formation of the main product (i.e water), approximately in one tenth of the nozzle length. Also, figure (4.14) illustrates steep rise in the Hydroxyl mass fraction (Y_{OH}) at the inlet. That is not a surprise, as the characteristic time of formation of this intermediate species is of order 10^{-11} seconds. After that, the species concentrations seem to be not significantly changed. That leads to realize that chemical equilibrium model is model efficient than finite-rate chemistry model in this test case, which typically represents the supersonic expansion inside rocket engines. That is due to the residence time of reacting species

is long enough to achieve chemical equilibrium state, even though the flow exceeds sonic speed.

Due to the exothermic reaction of OH-group formation, figures (4.16) and (4.17) show the rise in pressure and temperature. The pressure increase starts from the flow inlet, in a semi-circular region, wherein the maximum pressure is reached at the centerline. Likewise, the temperature is raised just after the abrupt increase in OH mass fraction.

It is noticed in figure (4.18) that the value of Mach number (M) slightly drops in the region of pressure/temperature rise, followed by supersonic expansion, to reach its maximum value at the centerline, at the nozzle exit. In figure (4.19), the distribution of the mixture specific heat ratio (γ_{mix}) shows that the relative maximum variation does not exceed 3%. Hence, applying constant value of specific heat ratio in gas dynamic relations, is not far deviated from the accurate solution, in this type of reacting flow.

The solutions at the nozzle axis and wall, in addition to the cross-sectional weighted-averaged solution along the nozzle axis, are compared with of the quasi one dimensional flow solution introduced by Drummond et al. [21], where spectral method is applied, with only 17 nodes. It is noticeable that there is semi-coincidence between the present and previous results for species mass fractions in figures (4.20)-(4.23). It is concluded that the chemical reactions rates is slightly higher at the nozzle axis than that at the nozzle wall. As, it is illustrated in figures (4.20)-(4.21), that the hydrogen and oxygen mass fractions is higher than that at the nozzle centerline, while the case it is completely the opposite for water mass fraction, as shown in figure (4.23). However, it is observed that there is no significant change in the species concentration along the nozzle radius.

In figure (4.24), the averaged solution of pressure matches with the

quasi 1D solution of Drummond et al. [21], except in the magnitude of the maximum pressure, with a relation difference of order 10%. Also, it is shown that the maximum value of pressure, attained at the nozzle centerline. On the other hand, the wall pressure drop is followed by a small rise, before the flow is completely expanded at the nozzle exit. That shows the difference in the pressure distribution behavior, between the quasi 1D solution, and the axisymmetric 2D solution, illustrated in figure (4.16).

Also, it should to note that the 1D calculations of Drummond et al. [21] overestimates temperature along nozzle, as presented in figure (4.25). That is because of the difference between the present and previous calculations in the formula of the specific heat coefficient (c_p) of different species. As mentioned in section **2.3**, the specific heat coefficients are calculated using fifth order polynomial functions, whose coefficient are given by McBride et al. [43], and presented in appendix **D**. On the other hand, Drummond et al. [21] calculated them using linear function, whose coefficients are not mentioned in their study.

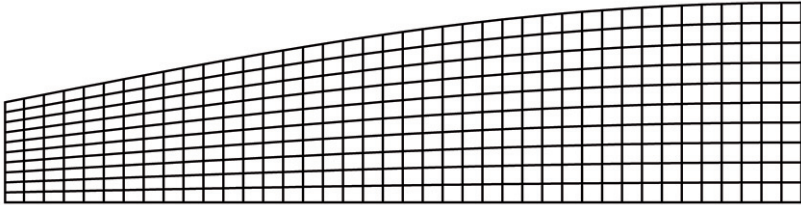


Figure 4.10: **The mesh of size 41×11 , utilized in solving complete expansion case**

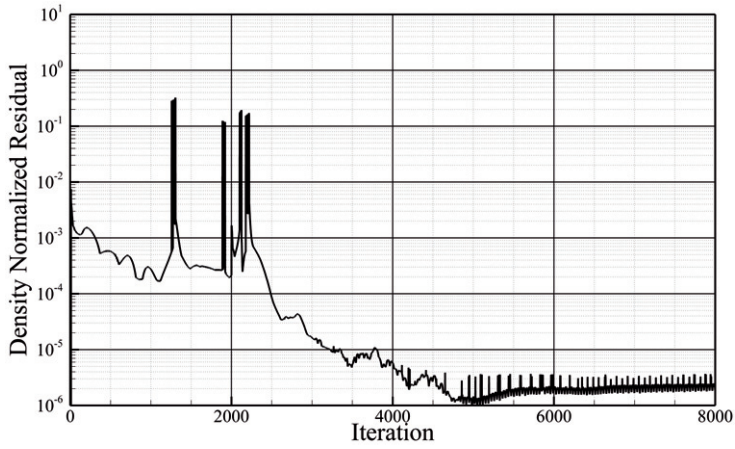


Figure 4.11: Convergence history of the chemically reacting invscid complete expansion in axisymmetric nozzle.

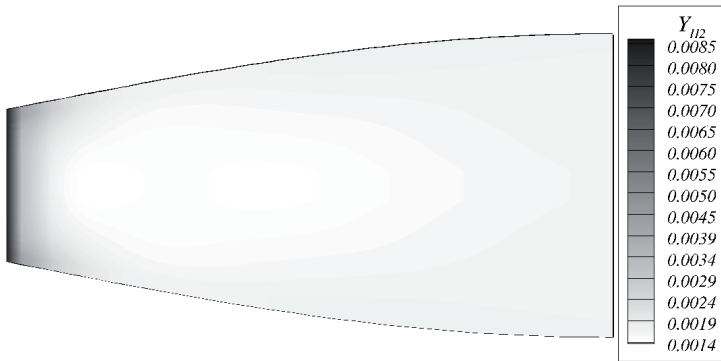


Figure 4.12: Mass fraction contours of Hydrogen (Y_{H_2}) for complete expansion through axisymmetric nozzle

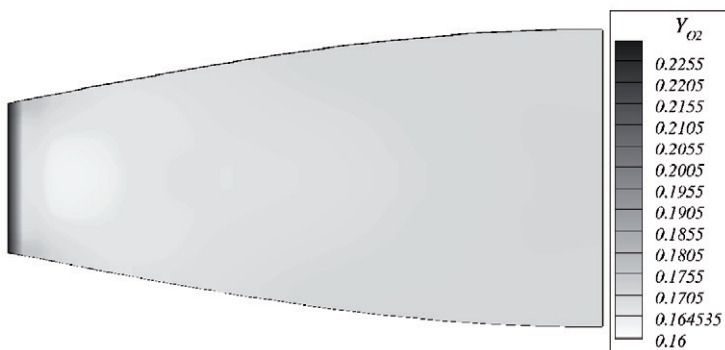


Figure 4.13: Mass fraction contours of Oxygen (Y_{O_2}) for complete expansion through axisymmetric nozzle

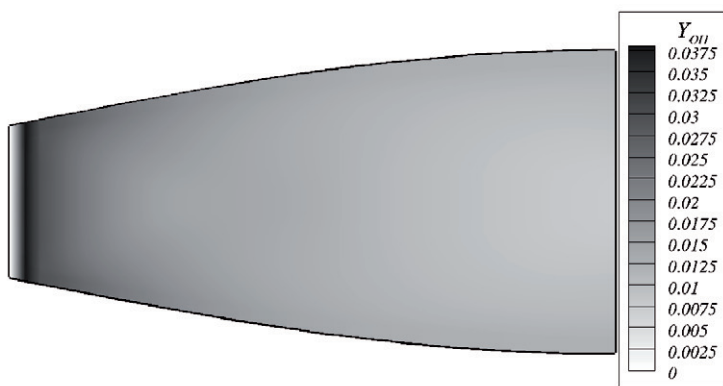


Figure 4.14: Mass fraction contours of Hydroxyl group (Y_{OH}) for complete expansion through axisymmetric nozzle



Figure 4.15: Mass fraction contours of water (Y_{H_2O}) for complete expansion through axisymmetric nozzle

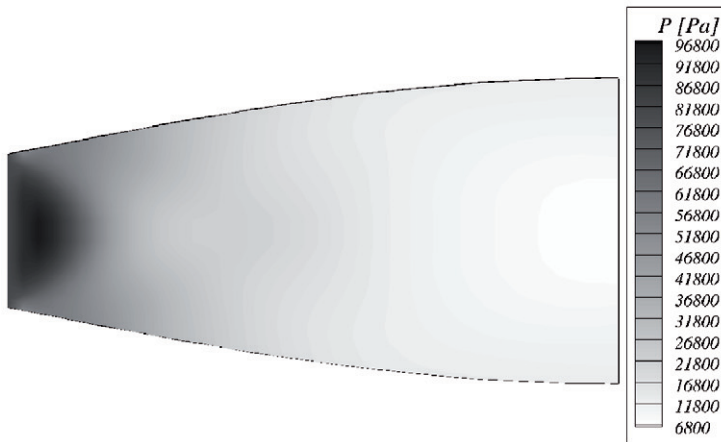


Figure 4.16: Pressure (P) contours for complete expansion through axisymmetric nozzle

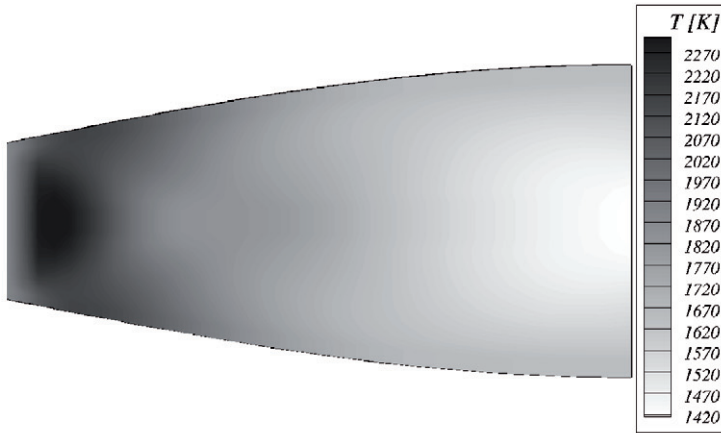


Figure 4.17: Temperature (T) contours for complete expansion through axisymmetric nozzle

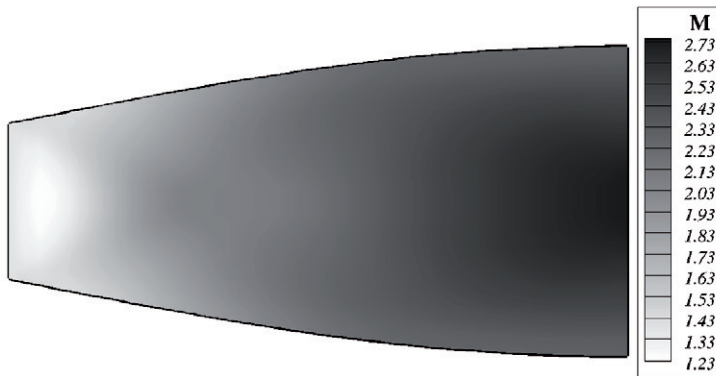


Figure 4.18: Mach Number (M) contours for complete expansion through axisymmetric nozzle

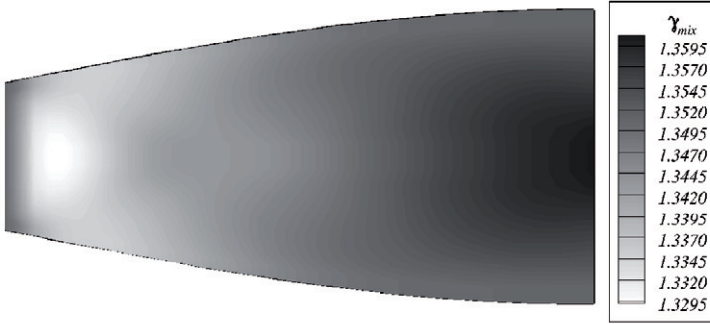


Figure 4.19: Mixture specific heat ratio (γ_{mix}) contours for complete expansion through axisymmetric nozzle

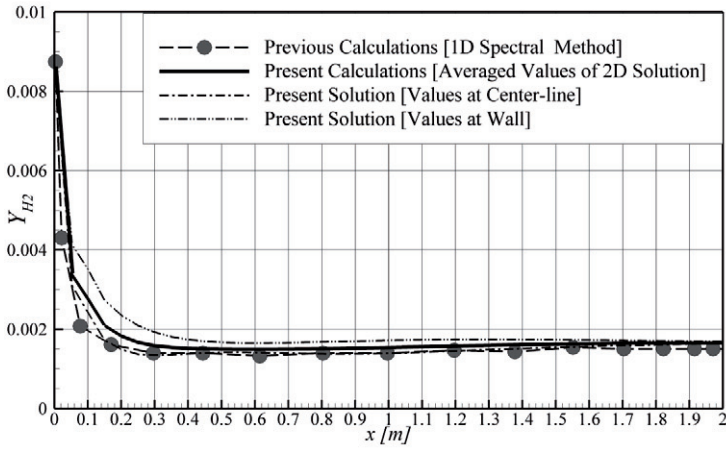


Figure 4.20: Present solution compared to previous calculations of Drummond et al. [21] for Hydrogen mass fraction (Y_{H_2})

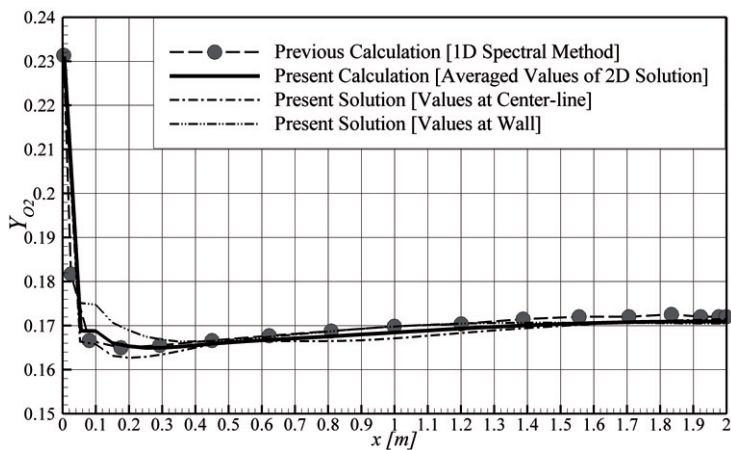


Figure 4.21: Present solution compared to previous calculations of Drummond et al. [21] for Oxygen mass fraction (Y_{O_2})

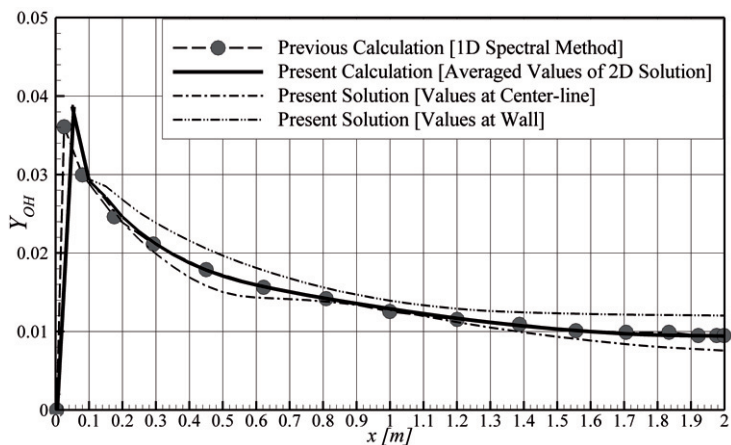


Figure 4.22: Present solution compared to previous calculations of Drummond et al. [21] for Hydroxyl mass fraction (Y_{OH})

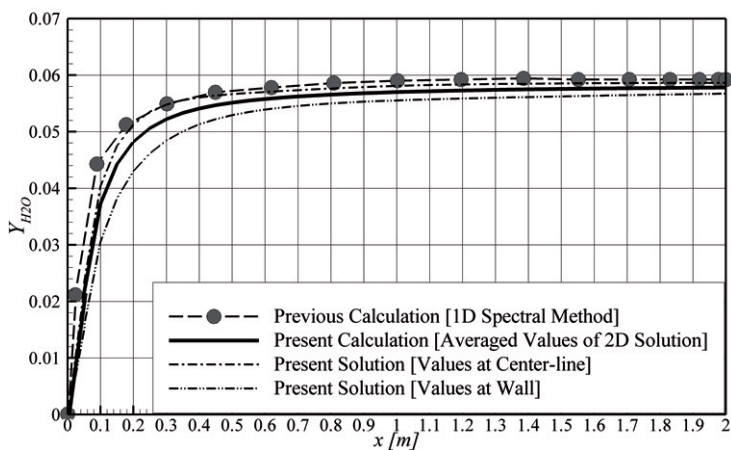


Figure 4.23: Present solution compared to previous calculations of Drummond et al. [21] for water mass fraction (Y_{H_2O})

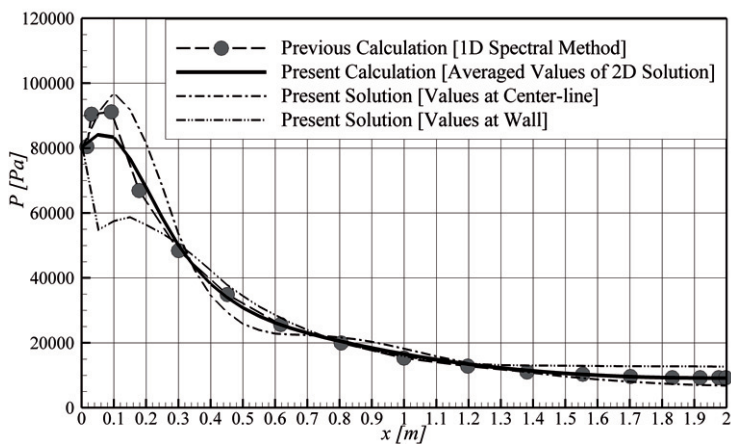


Figure 4.24: Present solution compared to previous calculations of Drummond et al. [21] for pressure (P)

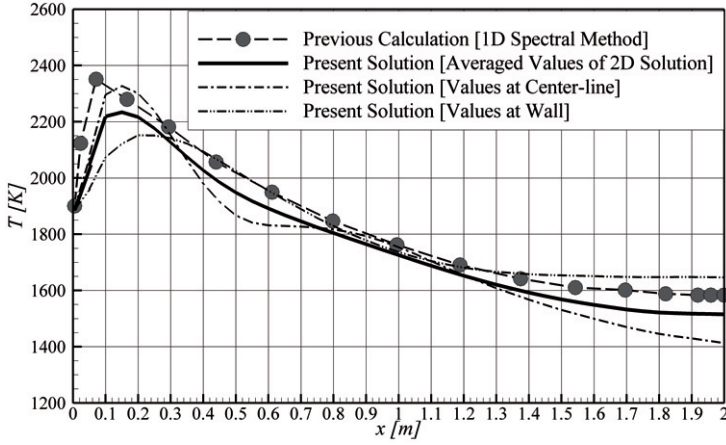


Figure 4.25: **Present solution compared to previous calculations of Drummond et al. [21] for temperature (T)**

4.3.2 Over-Expansion Test Case

Imposing atmospheric back pressure, i.e ($P_{out} = 101325 [Pa]$), a normal shock wave is formed inside the axisymmetric nozzle to match the exit pressure with back pressure. Three meshes of different sizes (101×25 , 151×25 , and 201×25) are applied, to evaluate the solution sensitivity to the grid size. They are illustrated in figures (4.26)-(4.28), where the discretization in x -direction is increased, in order to testify the code capability of resolving transverse shock waves. It is observed that the cell aspect ratio is still acceptable, even after the mesh size is enlarged in one direction only.

Minimum time stepping with CFL number equals to 0.1, in order to avoid any instability result from incorrect guess of the initial conditions of the computations. The convergence history is displayed in figure (4.29). It is observable the solution convergence is achieved after approximately 13000 iterations. However, the value of normalized residual of density does not exceed 10^{-5} , and its magnitude continues

in fluctuations above 10^{-5} .

As illustrated in figures (4.30)-(4.36), the normal shock wave in the case of 2D axisymmetric flow, takes the shape of spherical shell, where the location of flow variable discontinuity varies with the radial distance from the nozzle axis. The distribution behaviors of the mass fraction of Hydrogen (Y_{H_2}) and oxygen (Y_{O_2}) are almost the same as shown in figures (4.30)- (4.31). The shock effect in accelerating the chemical reactions is observable. And, the species mass concentrations becomes unchanged after the shock. It should be to mention that the mass fraction of water (Y_{H_2O}) seems to be unaffected with the presence of the transverse shock wave, which indicates that water reaches its chemical equilibrium, and it is no longer sensitive to the static temperature increase provided by the normal shock wave. Additionally, the Hydroxyl sudden rise takes place in the grid points, which come just after the flow inlet, as shown in figure (4.32). That leads to conclude that the solution of Hydroxyl concentration, is greatly dependent on the mesh size, especially at the regions of combustion initiation.

It is shown from the Mach number contours, in figure (4.34), that the flow begins to expand after the main combustion regime, whose length is about 10% of the nozzle length. Then, the flow expansion is interrupted with the normal shock wave, to be decelerated to subsonic speeds. It is shown that the pressure and temperature seem to be unchanging after the shock as shown in figures (4.35)-(4.36).

In figures(4.37)-(4.41), the present results are compared with the previous calculations of Grossman and Cinnella [30], for the same test case, except they solved it using quasi 1D flow model. The present solutions at the centerline and wall, beside the cross-sectional averaged solution, are all plotted versus the results for the one dimensional flow. Also, the grid sensitivity analysis is carried out, where the solutions for different discretization size in x -direction are presented. It is ob-

served that the averaged solution matches with the general trend of the 1D flow. However, the flow discontinuity at the centerline is the closet to the shock wave of the previous calculation. The flow variables discontinuity seems to be smooth, as the normal shock wave takes the shape of the spherical shell instead of planar surface in the case of 2D axisymmetric flow. As illustrated in figures (4.37)-(4.39), the shock wave contributes in accelerating the rates of termination of Oxygen and formation of Hydroxyl-group, while the water mass fraction (Y_{H_2O}) seems to be unaffected, except the wall surface.

In figures (4.40) and (4.41), it is shown that variables discontinuity at the normal shock are not so sharp, even though second order spatial accurate scheme is applied. That is because of the diffusive effect of minmode limiter at sharp flow discontinuities, as mentioned before in subsection 3.3.2. The present solutions show observable secondary peak at the nozzle centerline after the main combustion zone, where temperature and pressure reaches their maximum values, and before the normal shock. That is due to the inefficiency of the use discontinuous slope limiter in modeling continuous local maxima or minima in the flow field, as previously mentioned by Hirsch [32].

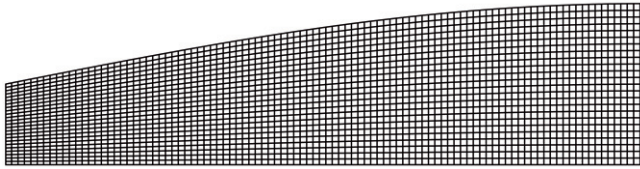


Figure 4.26: 101×25 mesh, used in solving over-expansion case

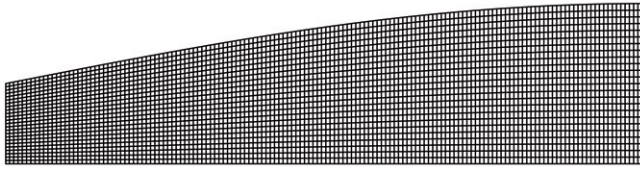


Figure 4.27: 151×25 mesh, used in solving over-expansion case

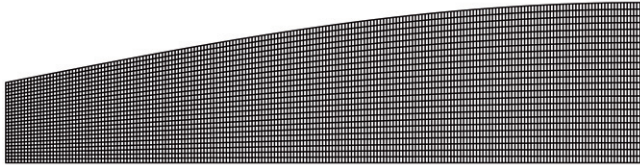


Figure 4.28: 201×25 mesh, used in solving over-expansion case

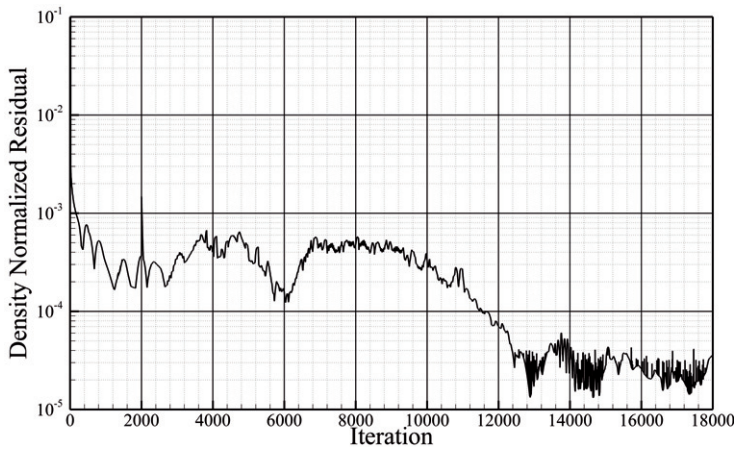


Figure 4.29: **Convergence history of the chemically reacting inviscid over-expansion in axisymmetric nozzle.**

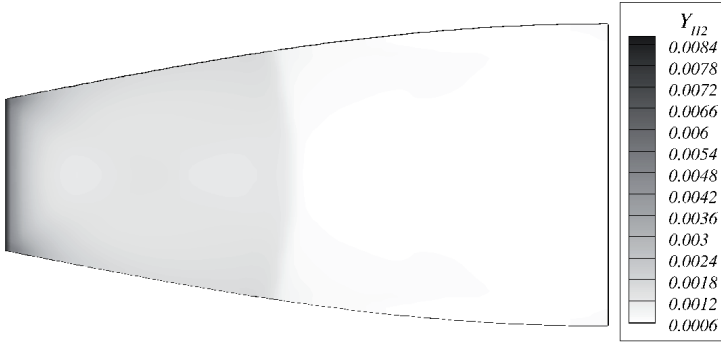


Figure 4.30: Mass fraction contours of Hydrogen (Y_{H_2}) for over-expansion through axisymmetric nozzle

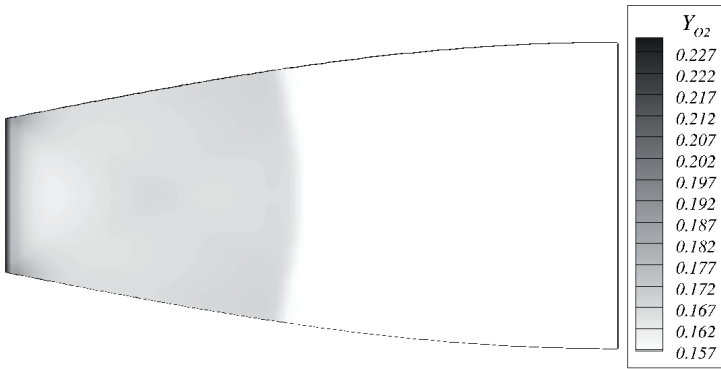


Figure 4.31: Mass fraction contours of Oxygen (Y_{O_2}) for over-expansion through axisymmetric nozzle

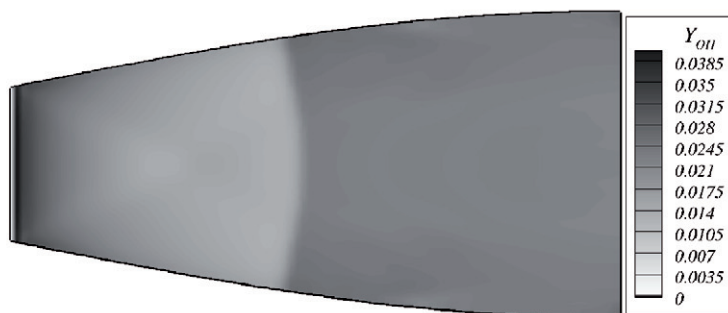


Figure 4.32: Mass fraction contours of Hydroxyl (Y_{OH}) for over-expansion through axisymmetric nozzle



Figure 4.33: Mass fraction contours of water (Y_{H_2O}) for over-expansion through axisymmetric nozzle

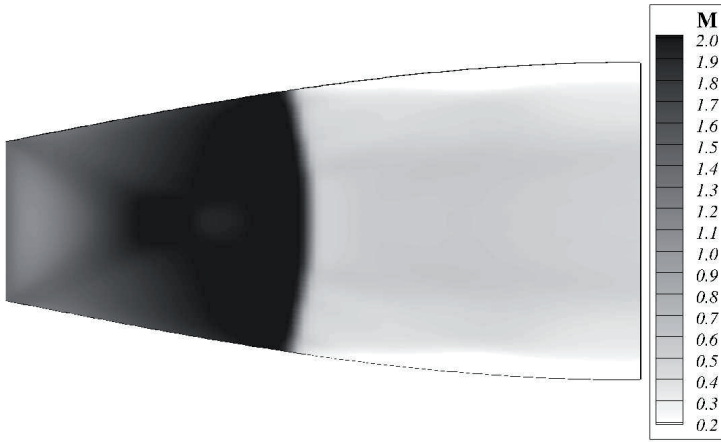


Figure 4.34: Mach number (M) contours for over-expansion through axisymmetric nozzle

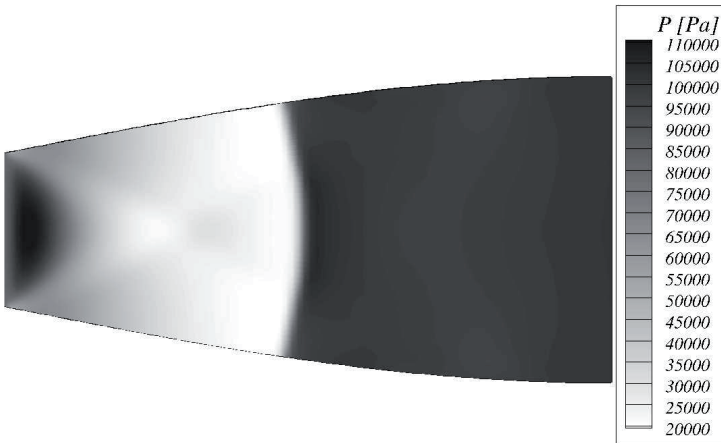


Figure 4.35: Pressure (P) contours for over-expansion through axisymmetric nozzle

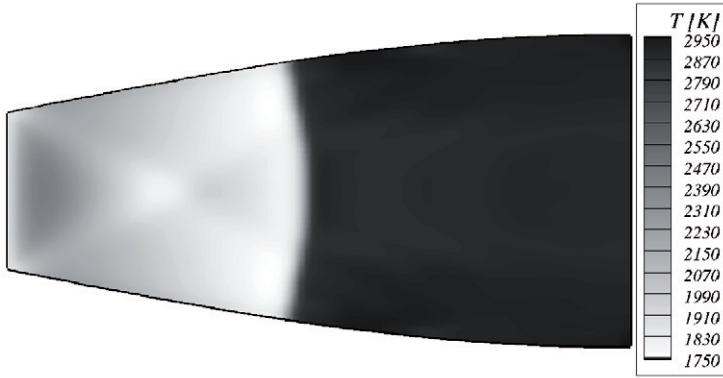


Figure 4.36: Temperature (T) contours for over-expansion through axisymmetric nozzle

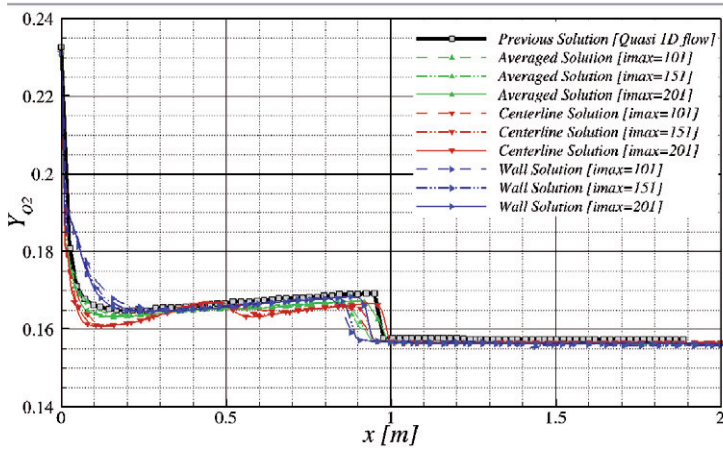


Figure 4.37: Present solution compared to previous calculations of Grossman et al. [30] for Oxygen mass fraction (Y_{O_2})

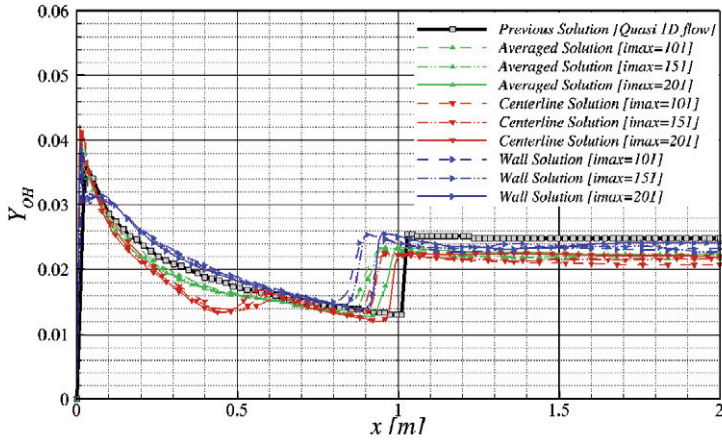


Figure 4.38: **Present solution compared to previous calculations of Grossman et al. [30] for Hydroxyl mass fraction (Y_{OH})**

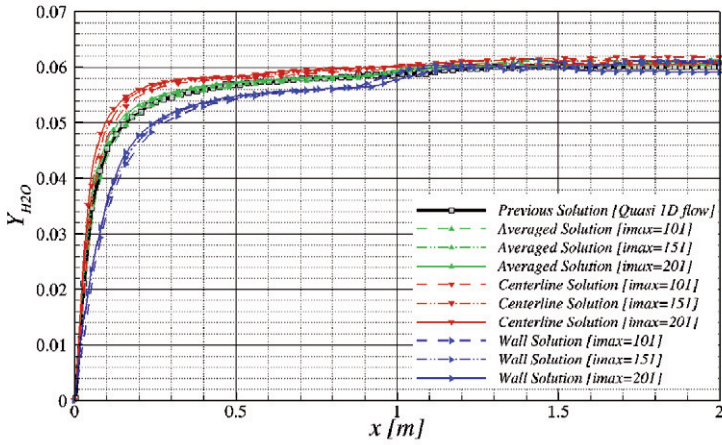


Figure 4.39: **Present solution compared to previous calculations of Grossman et al. [30] for water mass fraction (Y_{H_2O})**

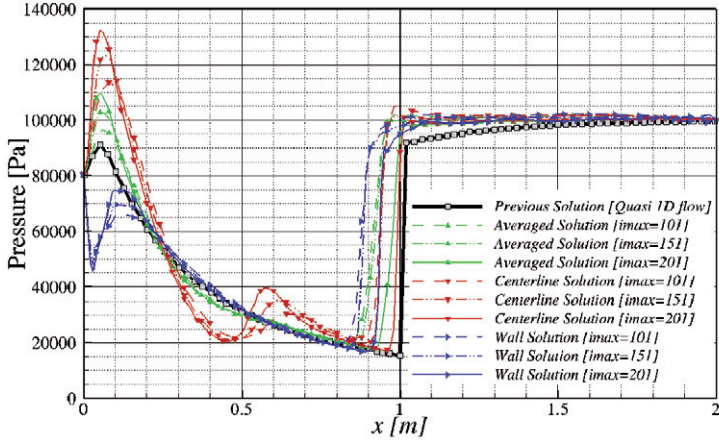


Figure 4.40: Present solution compared to previous calculations of Grossman et al. [30] for pressure (P)

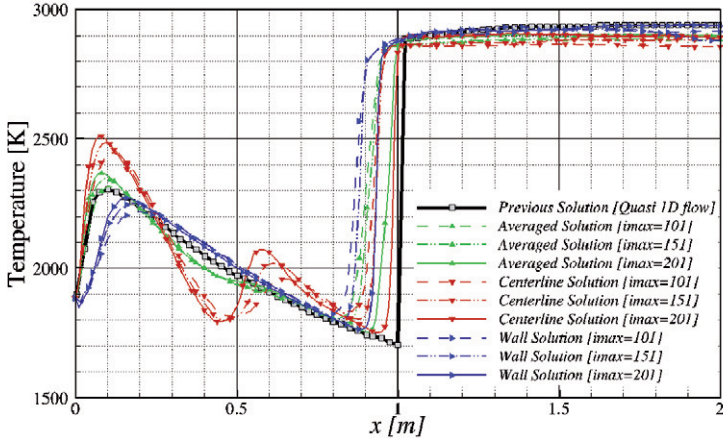


Figure 4.41: Present solution compared to previous calculations of Grossman et al. [30] for temperature (T)

4.4 Turbulent Chemically Reacting Flows in a Ramped Duct

The numerical code is also evaluated to solve turbulent premixed Hydrogen-air supersonic flow in a two-dimensional ramped duct, which shown in figure (4.42). The duct walls are assumed to be adiabatic. And, the incoming flow is premixed hydrogen-air at stoichiometric ratio. The problem is solved for two different inlet temperatures; below and above the ignition threshold which is equal to 1000 [K]. The inlet conditions are described as follows:

$$\begin{aligned}
 T_{in} = \begin{cases} 900 \text{ [K]}, & \text{Test Case 1.} \\ 1200 \text{ [K]}, & \text{Test Case 2.} \end{cases} & P_{in} = 101325 \text{ [Pa]}, \\
 \mathbf{M}_{in} = 4.0, & \phi_{in} = 1.0.
 \end{aligned} \tag{4.18}$$

The reference length is set to be the longitudinal length of the duct, while the other reference variables to equal to the inlet flow properties as shown below:

$$\begin{aligned}
 L_{ref} = 3 \text{ [cm]}, \quad \rho_{ref} = \rho_{in}, \quad T_{ref} = T_{in}, \quad V_{ref} = V_{in}, \\
 \mu_{ref} = \mu_{L_{in}}, \quad k_{ref} = k_{L_{in}}, \quad \mathcal{D}_{ref} = \mathcal{D}_{L_{in}}.
 \end{aligned} \tag{4.19}$$

For each of the two cases, three different sets of calculations using different meshes, whose sizes are 31×51 , 61×51 and 91×51 , as shown in figure (4.43)-(4.45). Arithmetic progression is used in spatial discretization in x -direction, according to equation (3.86). While discretization in y -direction is carried out using second Roberts transformation function, mentioned before in **3.6.1**, where the clustering coefficient are set to be ($\beta_y = 1.009$) and ($\alpha_y = 0.5$).

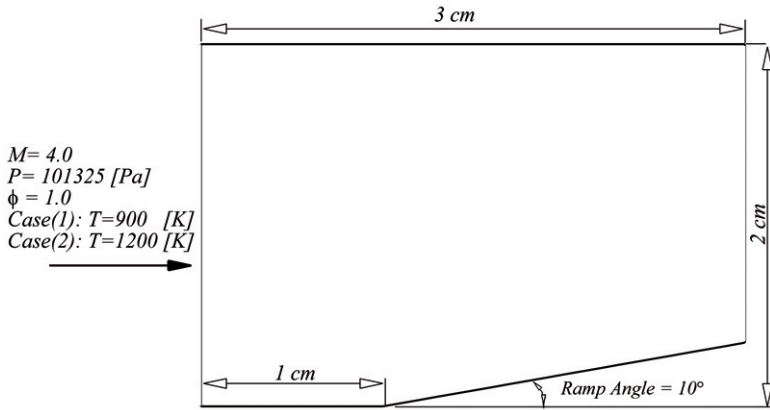


Figure 4.42: Schematic diagram of hydrogen-air flow in 2D ramped duct

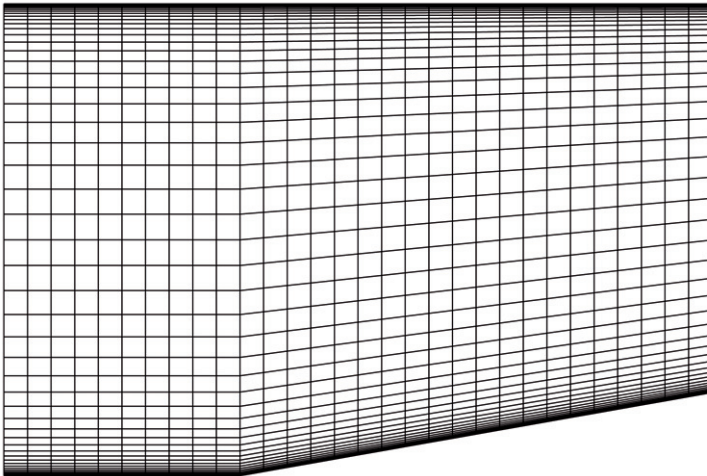


Figure 4.43: 31×51 mesh, used in solving turbulent flow in a ramped duct

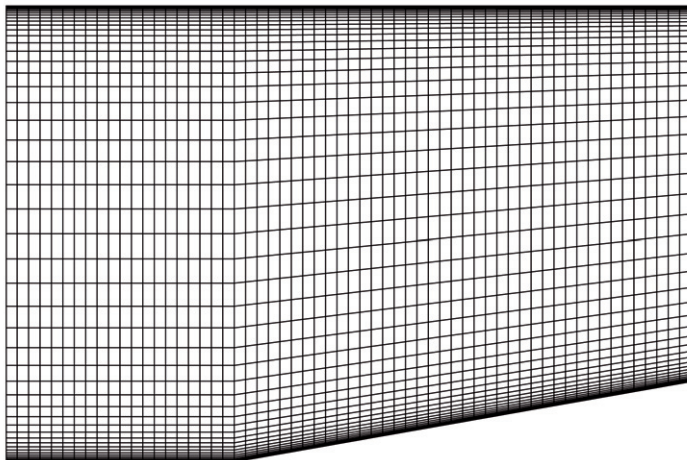


Figure 4.44: 31×51 mesh, used in solving turbulent flow in a ramped duct

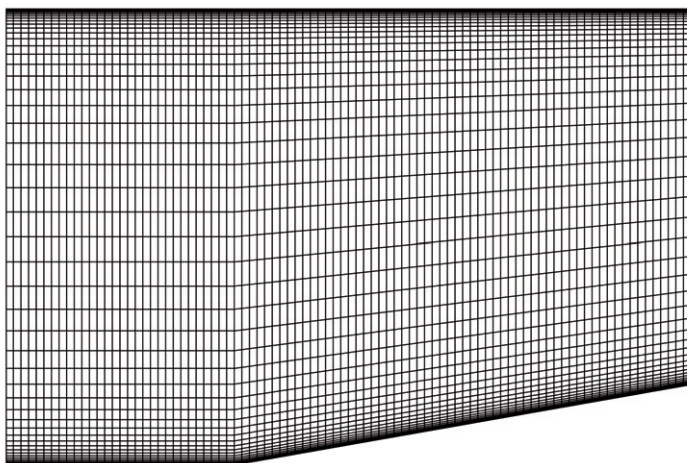


Figure 4.45: 31×51 mesh, used in solving turbulent flow in a ramped duct

4.4.1 Non-reacting Inlet Flow Test Case

In the first test case the inlet temperature is below the ignition threshold of hydrogen-air combustion system (1000 [K]). But, it rises after the oblique shock wave and in the viscous layers near wall surface, to become high enough, i.e. (greater than 1000 [K]), for combustion initiation. It is important to point that the formed oblique shock is considered as *detonation wave*, as it is responsible in the reaction excitation and sustainability.

Local time-stepping is used in the pseudo time-integration, where CFL number equals to ($\sigma = 0.1$). It is shown that convergence is attained after a relatively few number of iterations, as illustrated in figure (4.46). That is because the integration time step is locally calculated, instead of using its minimum value to be the global time-step. It is shown that the convergence in the value of the density normalized residual, is attained approximately after 1500 iterations, followed by fluctuations around 6×10^{-6} .

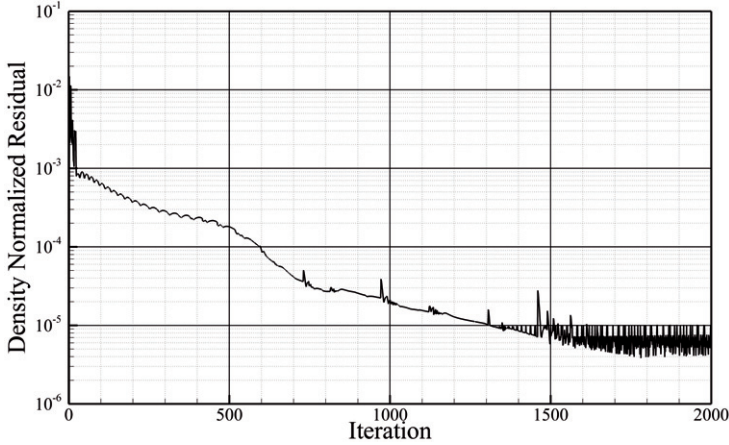


Figure 4.46: Convergence history of the case of turbulent pre-mixed flow in a ramped duct for $T_{in} = 900$ [K].

As shown in the species mass fractions contours, in figures (4.47)-(4.50), chemical reaction actually begin after the oblique shock wave and in the shear layer near the lower and upper walls. As the inlet temperature is not high enough to combustion excitation (i.e. $T_{in} = 900 [K] < 1000 [K]$). Some fluctuation are observable in the Oxygen and Hydroxyl mass fractions, along the oblique shock wave, as the shock-initiated reactions of O_2 termination and OH formation are characterized by its very high rates, in Rogers and Chinitz model. [48]. In figure (4.52), it obvious that some weak shocks formed at the leading edge of the duck in the lower and upper walls, followed by a stronger oblique shock wave, which reduce flow Mach number (M) about 50% of its value at the duct inlet. Besides, the boundary layer growth is observed, especially at the upper wall, where the boundary layer thickness reach its maximum value at the duct exit. It is shown that the maximum variation in the mixture specific heat ratio (γ_{mix}), is about 7.6% relative to its minimum value, which should be considered in evaluation of frozen flow models, which use constant value of the mixture heat ratio. The pressure and temperature distributions are illustrated in figures (4.53) and (4.54), respectively. There is rise in the static pressure, following the oblique shock. It considered as evidence of the shock-induced combustion effect in raising the static pressure, just after the oblique shock wave. However, the maximum temperature attained at the viscous layers in the lower wall behind the shock, where static temperature is raised above 3300 [K], due to the flow deceleration by the shock wave, in addition to the shear effect at the adiabatic walls.

Figures (4.55)-(4.60) present the numerical solutions at normal distance of 0.13 [cm] from the wall, which is approximately at the grid line of index ($j = 14$). The present numerical solutions of the three different meshes sizes (31×51 , 61×51 , and 91×51) are compared to the previous solutions of Chitsomboon et al. [14], and Shuen and

Yoon [54]. The first conclusion is that the present solutions are insensitive to grid resolution, which is a proof of the code efficiency in using small grid size. Also, there is observable qualitative and quantitative approaching between the present solutions and the previous solution of Chitsomboon et al. [14]. It is noted that the OH mass fraction solution, is greatly dependent on the grid resolution. As, there are sharp fluctuations in its value, initiated at the shock regions. It is observed that by increasing the grid size in longitudinal direction, the fluctuations amplitude diminish, but their number increase. This is due to the poor estimation of Rogers and Chinitz model [48], as discussed by Chitsomboon et al. [12]. As both sets the previous calculations did not apply any TVD scheme, some oscillations in pressure and temperature are observed after the shock, as shown in figure (4.59) and (4.60). In addition, the present solutions give smooth rise in pressure across shock, due to the diffusive effect of TVD scheme. Except in the shock region, there is coincidence between in the temperature soliton between the present calculations and that of ref. [14].



Figure 4.47: Mass fraction contours of Hydrogen (Y_{H_2}) in case of turbulent reacting flow in a ramped duct for $T_{in} = 900$ [K].



Figure 4.48: Mass fraction contours of Oxygen (Y_{O_2}) in case of turbulent reacting flow in a ramped duct for $T_{in} = 900$ [K].



Figure 4.49: Mass fraction contours of Hydroxyl (Y_{OH}) in case of turbulent reacting flow in a ramped duct for $T_{in} = 900$ [K].



Figure 4.50: Mass fraction contours of water (Y_{H_2O}) in case of turbulent reacting flow in a ramped duct for $T_{in} = 900$ [K].

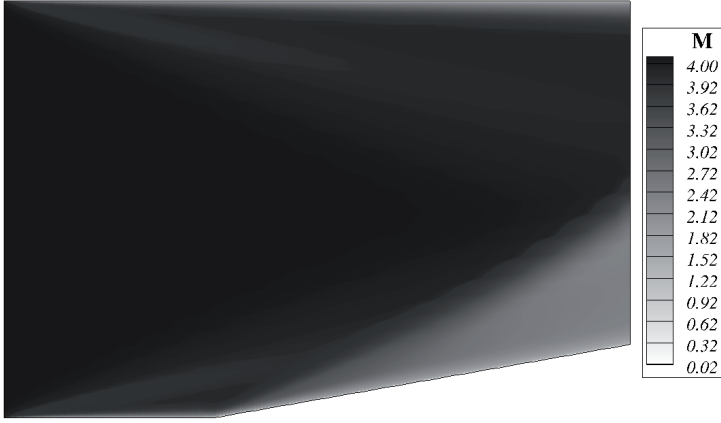


Figure 4.51: Mach Number (M) contours in case of turbulent reacting flow in a ramped duct for $T_{in} = 900$ [K].



Figure 4.52: Mixture specific heat ratio (γ_{mix}) contours in case of turbulent reacting flow in a ramped duct for $T_{in} = 900$ [K].



Figure 4.53: **Pressure (P) contours in case of turbulent reacting flow in a ramped duct for $T_{in} = 900$ [K].**



Figure 4.54: **Temperature (T) contours in case of turbulent reacting flow in a ramped duct for $T_{in} = 900$ [K].**

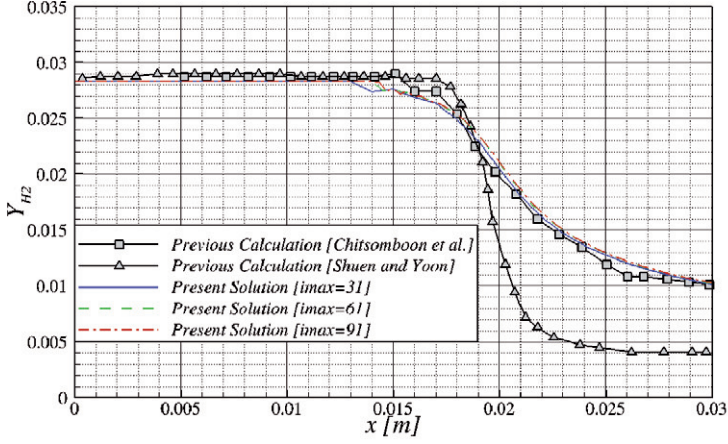


Figure 4.55: Present solution compared to previous calculations of ref. [14] and [54] for H_2 mass fraction at 0.13 cm from the lower wall

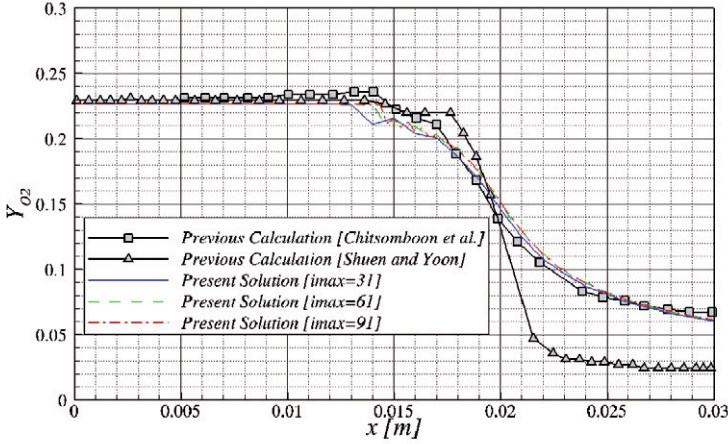


Figure 4.56: Present solution compared to previous calculations of ref. [14] and [54] for O_2 mass fraction at 0.13 cm from the lower wall

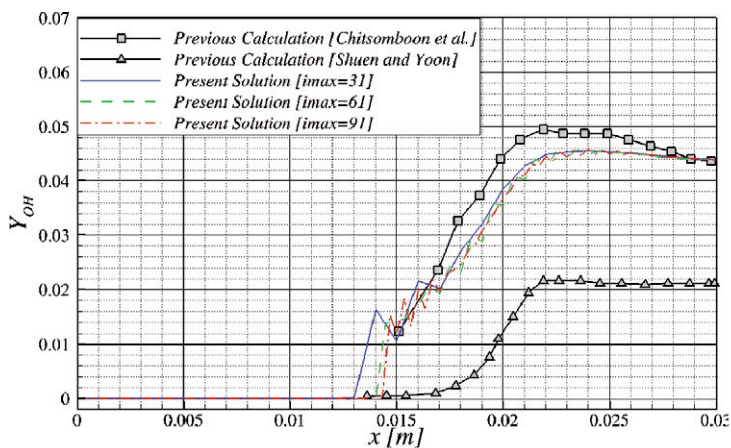


Figure 4.57: Present solution compared to previous calculations of ref. [14] and [54] for OH mass fraction at 0.13 cm from the lower wall

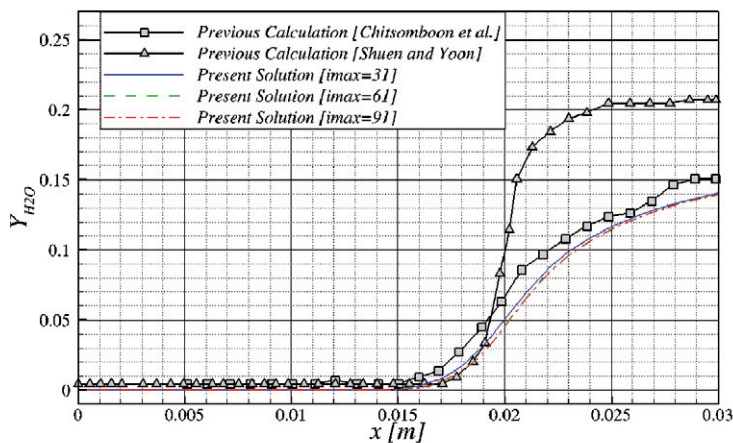


Figure 4.58: Present solution compared to previous calculations of ref. [14] and [54] for H₂O mass fraction at 0.13 cm from the lower wall

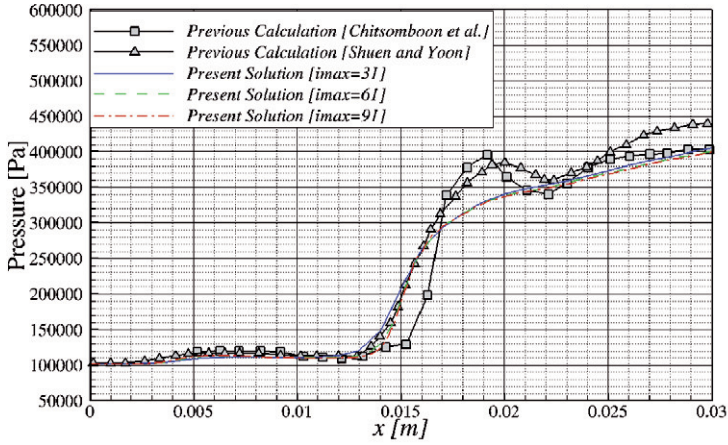


Figure 4.59: Present solution compared to previous calculations of ref. [14] and [54] for pressure at 0.13 cm from the lower wall

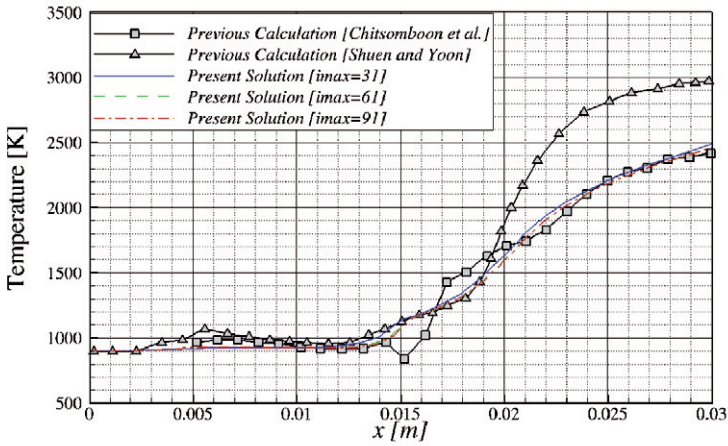


Figure 4.60: Present solution compared to previous calculations of ref. [14] and [54] for temperature at 0.13 cm from the lower wall

4.4.2 Reacting Inlet Flow Test Case

In the second case, when the inlet temperature exceeds the minimum limit of combustion initiation, (i.e. $T_{in} = 1200 [K] > 1000 [K]$), chemical reactions takes place starting from the duct inlet. However, the static temperature rise at the formed oblique shock wave, accelerates significantly the chemical reaction rates.

Pseudo time-integration is also applying here local time step, with CFL number equals to ($\sigma = 0.1$). It is shown that convergence is attained fast after 1200 iterations, as illustrated in figure (4.61). After that, the density normalized residual is fluctuating below 10^{-5} , where the troughs of this fluctuations (the minimum values of the fluctuating residual) decrease by time-integration.

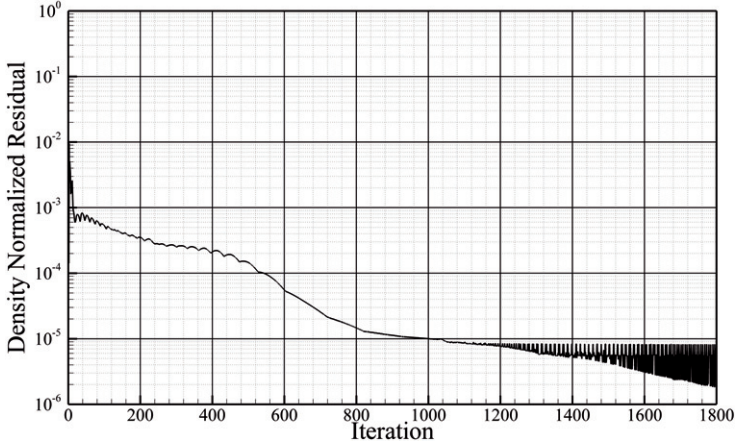


Figure 4.61: **Convergence history of the case of turbulent premixed flow in a ramped duct for $T_{in} = 1200 [K]$.**

As shown figures (4.62)-(4.65), it is found that the reduction in Oxygen and Hydrogen mass fractions, and the increase in Hydroxyl and water mass fractions, start from the duct inlet. However, it is observ-

able that the O_2 and H_2 termination, and OH and H_2O formation, are accelerated after the oblique shock wave. As it is noticed that the mass fractions of O_2 and H_2 is reduced after the shock by about 75% and 50% respectively, relative to their values at the inlet.

It is noticed in figure (4.66), that the waves at the duct leading edges becomes weaker than that in the first case. The variation in flow Mach number (M) and the specific heat ratio (γ_{mix}) before the shock becomes smoother, as shown in figures(4.66)-(4.67). That is due to the heat released from the exothermic chemical reactions, initiated at the duct inlet. It is important to mention that the maximum static pressure attained in this problem does not exceed 4.0 [bar], which is lower than that achieved by the previous test case of lower inlet temperature. Even though the total inlet total pressure is higher in the second test case, the higher static pressure is achieved in the first one. That is because in the first case, the sudden reaction initiation across the shock wave, in addition of the shock compression effect, leads to sharp rise in static pressure only after the oblique shock wave, and the thermal energy produce from the exothermic reactions is distributed in smaller region.

Figures (4.70)-(4.74) present the numerical solutions for three meshes, where the discretization in y -direction is constant (i.e. $jmax = 51$), and the mesh sizes in x -direction are $imax = 31, 61, \text{ and } 91$. The present solutions are introduced at a distance of 0.13 [cm] from the lower wall, which at the grid line of index ($j = 14$). And they are compared to the previous results of Yee and Shinn [66] and that of Shuen and Yoon [54]. It is noticeable that the numerical solver overestimates the reactions reactions. That appears in figures (4.70)-(4.72), where there is a sudden decrease in Oxygen and Hydrogen mass fraction, and very steep rise in Hydroxyl concentration, at the duct inlet. It is shown that solutions of O_2 and OH are greatly sensitive to the grid resolution at the duct inlet. However, there is matching between

the present solution and that of Yee and Shinn [66]. In figure (4.74), the solution of Shuen and Yoon [54], has nonphysical oscillations after the shock, due to its scheme did not satisfy TVD conditions. On, the other hand, the present solutions and that of ref. [66], have no oscillation, but the diffusive effect of their TVD schemes is obvious. In figure (4.75), there is no solution available for temperature from ref. YS, and there is about 20 % variation from the present solution and that of ref. [54]. That leads to the conclusion, that the pressure and temperature are overestimated by Shuen and Yoon [54], in the both discussed cases (i.e. $T_{in} = 900 [K]$ and $1200 [K]$), after the comparison the results to that of Chitsomboon et al. [14] in the first case, and that of Yee and Shinn [66] in the second one.



Figure 4.62: Mass fraction contours of Hydrogen (Y_{H_2}) in case of turbulent reacting flow in a ramped duct for $T_{in} = 1200$ [K].



Figure 4.63: Mass fraction contours of Oxygen (Y_{O_2}) in case of turbulent reacting flow in a ramped duct for $T_{in} = 1200$ [K].



Figure 4.64: Mass fraction contours of Hydroxyl (Y_{OH}) in case of turbulent reacting flow in a ramped duct for $T_{in} = 1200$ [K].



Figure 4.65: Mass fraction contours of water (Y_{H_2O}) in case of turbulent reacting flow in a ramped duct for $T_{in} = 1200$ [K].



Figure 4.66: Mach number (M) contours in case of turbulent reacting flow in a ramped duct for $T_{in} = 1200$ [K].



Figure 4.67: Mixture specific heat ratio (γ_{mix}) contours in case of turbulent reacting flow in a ramped duct for $T_{in} = 1200$ [K].



Figure 4.68: **Pressure (P) contours in case of turbulent reacting flow in a ramped duct for $T_{in} = 1200$ [K].**



Figure 4.69: **Temperature (T) contours in case of turbulent reacting flow in a ramped duct for $T_{in} = 1200$ [K].**

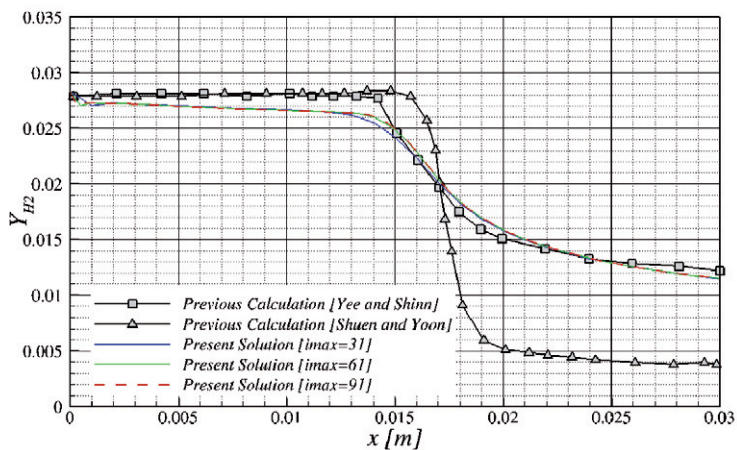


Figure 4.70: Present solution compared to previous calculations of ref. [66] and [54] for H_2 mass fraction at 0.13 cm from the lower wall

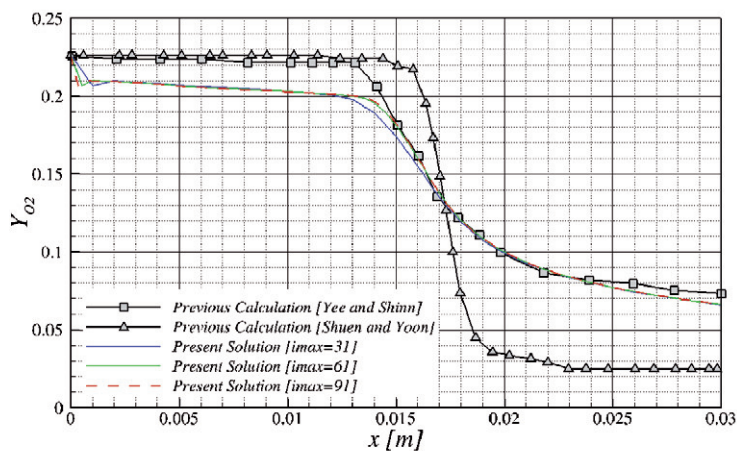


Figure 4.71: Present solution compared to previous calculations of ref. [66] and [54] for O_2 mass fraction at 0.13 cm from the lower wall

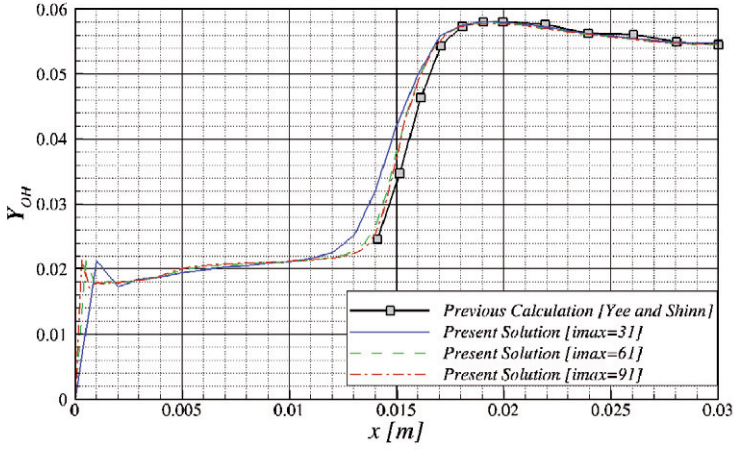


Figure 4.72: Present solution compared to previous calculations of ref. [66] for OH mass fraction at 0.13 cm from the lower wall

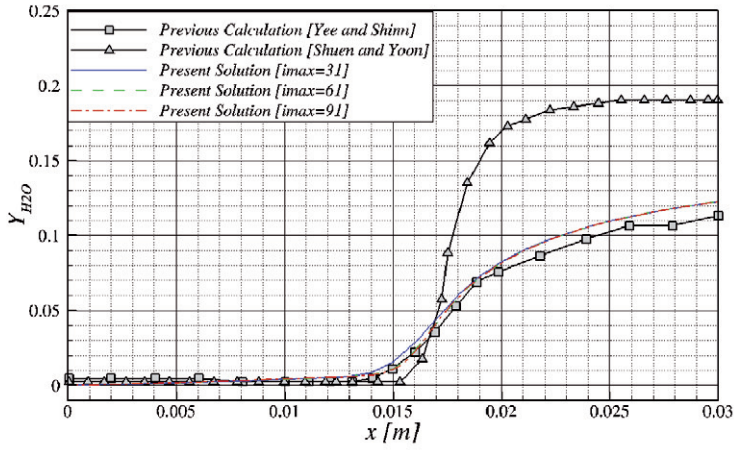


Figure 4.73: Present solution compared to previous calculations of ref. [66] and [54] for H₂O mass fraction at 0.13 cm from the lower wall

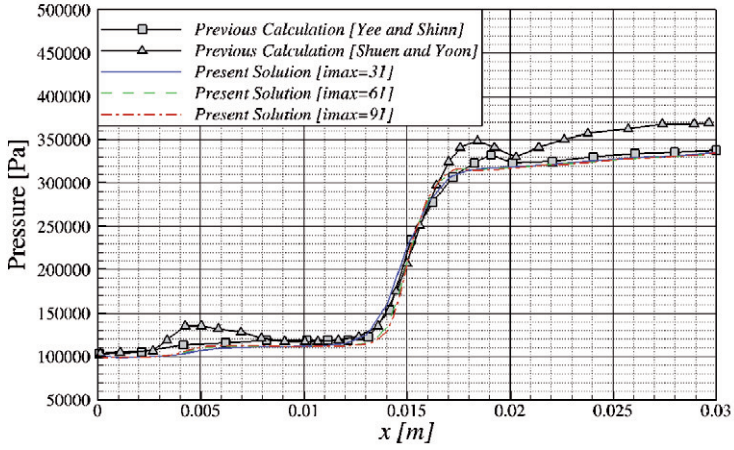


Figure 4.74: Present solution compared to previous calculations of ref. [66] and [54] for pressure at 0.13 cm from the lower wall

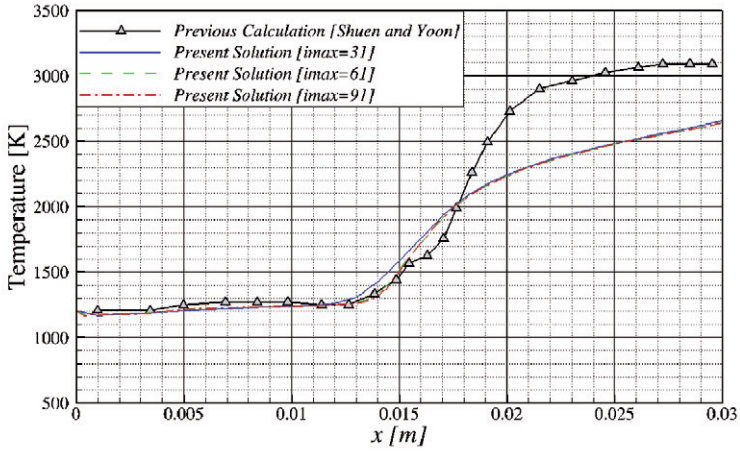


Figure 4.75: Present solution compared to previous calculations of ref. [54] for temperature at 0.13 cm from the lower wall

4.5 Sonic Transverse Helium Injection to Supersonic Air Flows

Fuel-air mixing mechanism in scramjet engines using fuel sonic transverse injection into the supersonic air flow, have a very complicated system of shocks and separation vortices. The developed code reliability is testified to solve the two-dimensional non-reacting problem case of Helium injection at sonic speed perpendicular to supersonic air flow from a slot of width 0.0559 [cm], as illustrated in figure (4.76). The conditions of inlet air and injected Helium are given as:

$$\begin{array}{lll} \mathbf{M}_{in_{air}} = 2.9 & T_{in_{air}} = 108.0 [K] & P_{in_{air}} = 0.0663 [MPa] \\ \mathbf{M}_{in_{He}} = 1.0 & T_{in_{He}} = 217 [K] & P_{in_{He}} = 1.24 [MPa] \end{array} \quad (4.20)$$

Air is assumed to be completely homogenous. That enable to apply two species model. Where the air is considered as an individual species beside Helium. The thermodynamic properties of both air and Helium are assumed to constants, as given below:

$$\begin{array}{ll} \mathcal{M}_{air} = 28.98 [\frac{kg}{kmole}] & h_{f_{air}}^o = -31457.64 [\frac{J}{kg}] \\ \mathcal{M}_{He} = 4.0026 [\frac{kg}{kmole}] & h_{f_{He}}^o = -1548557.0 [\frac{J}{kg}] \end{array} \quad (4.21)$$

$$\gamma_{air} = \gamma_{He} = 1.4$$

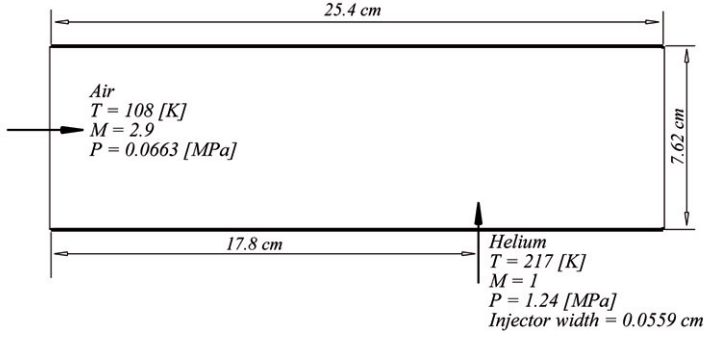


Figure 4.76: **Schematic diagram of Helium sonic transverse injection into supersonic air flow**

The longitudinal length of the duct is taken as the reference length (L_{ref}), while the air inlet properties is set to be the other reference variables, as follows:

$$\begin{aligned}
 L_{ref} &= 0.254 \text{ [m]} & \rho_{ref} &= \rho_{in_{air}} & T_{ref} &= T_{in_{air}} & V_{ref} &= V_{in_{air}} \\
 \mu_{ref} &= \mu_{L_{in_{air}}} & k_{ref} &= k_{L_{in_{air}}} & \mathcal{D}_{ref} &= \mathcal{D}_{L_{in_{air}}}
 \end{aligned} \tag{4.22}$$

The domain discretization is shown in figure (4.77), where second Roberts transformation function, discussed in **3.6.1**, is applied for grid line stretching in y -direction, where the hyperbolic sine transformation function, mentioned in **3.6.2** is employed to cluster the grid line in x -direction around the vertical line of ($x = x_o = 0.178 \text{ [m]}$), where Helium is injected from the lower wall. The clustering constants written in equations (3.94) and (3.93) have the following values:

$$\beta_x = 13 \qquad \beta_y = 1.001 \qquad \alpha_y = 0.5 \tag{4.23}$$

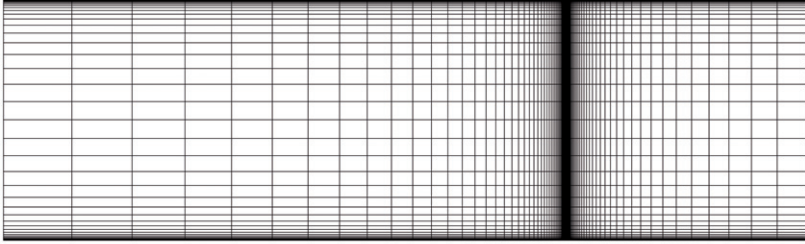


Figure 4.77: **The mesh of size 101×51 utilized to solve the transverse injection test case.**

Figure (4.78) show the history of density normalized residual, plotted versus the time-integration iterations. It is important point the attention that the flow phenomena accompanying sonic transverse injection are quite unsteady, in spite of the steadiness of the flow properties at both inlets. The normalized residuals of the solution do not converge to a final steady state. Instead, their values fluctuate around mean values, which is much higher than that of the previous discussed problems. In problems of these complicated flow feature, minimum time stepping is applied, where CFL number equals to ($\sigma = 0.1$), as recommended by Chitsomboon and Tiwari [12].

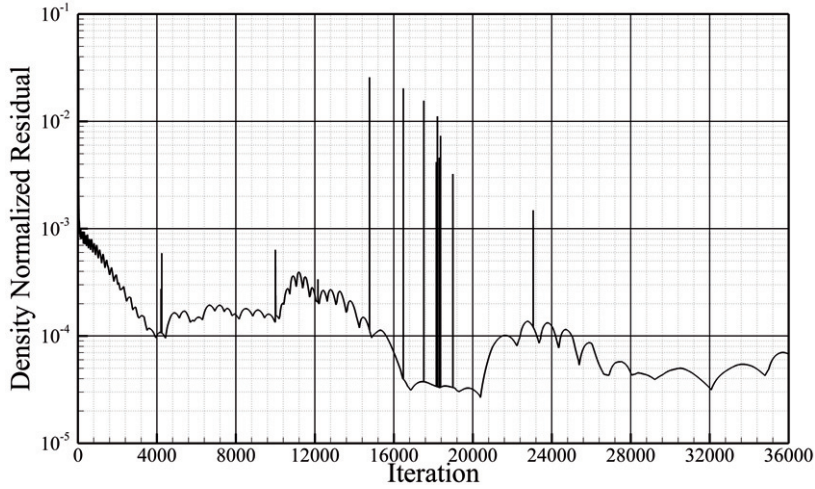


Figure 4.78: **History of density normalized residual with time-integration iterations in the case of He sonic transverse injection.**

As shown in figures (4.79) and (4.80), the flow shock system can be demonstrated from the domain contours of flow Mach number (M) and mixture density (ρ). It is shown that the separation shock is formed upstream with respect to the perpendicular injection zone. The flow speeds are obviously low, after the separation shock, and in front of the injectant Helium. Then, it is followed by a strong bow shock, which is reflected on the opposite upper wall.

An enlarge view near the Helium injection zone is given in figure (4.83) to illustrate the recirculation zones formed surrounding the perpendicularly injected Helium stream. It is shown that the separation shock prevents the transverse flow from being swept by the supersonic air stream. In addition, the front low-speed recirculation zone has a significant role in the air-injectant mixing process. Also, it is illustrated that the back-

ward vortices of higher speeds is followed by flow reattachment. One of the most characteristic phenomena of transverse sonic injection, can be recognized; as the sonic injected flow is accelerated inside a barrel-shaped stream tube, surrounded with bow shocks and then decelerated to sonic speed again at the Mach disk. The numerical solver potential is proved in modeling this complicated system of flow features, which is discussed before in section 1.2, and illustrated by a schematic diagram in figure (1.2).

The performance of transverse sonic inject in flame holding and mixing, can be also more explored in figures (4.81) and (4.82). The contours of temperature (T) presented in figure (4.81) shows the considerable effect of the front recirculation zone in flame holding, as static temperature is sustained high in the vortices region, after its rise thanks to the separation shock. Also, the mixing process represented in Helium mass fraction distribution is illustrated in figure (4.82), where the main mixing process is carried out in the front recirculation zone. In addition, He-air mixing takes place, by diffusive He-transfer through the mixing free shear layer.

It is observed that the injection pressure is about 20 times the air inlet flow pressure. The injectant pressure is much higher than air flow pressure, in order to enable the injected flow to decelerate the supersonic flow around the injection zone. Hence, raising the injection pressure, strengthen the formed shock system surrounding the injection regime, and improve the injectant penetration into the main stream.

The numerical code results is validated with the experimental results of Kraemer, G.O, and Rogers, R.C., which were reported by Drummond and Weidner [22], and introduced also by Shuen and Yoon [54], and with the previous calculations of the later reference. Comparison is carried out in the pressure solution at the lower wall around the

injection zone, at the transverse section at $x = 216$ [mm] from the duct inlet, or other words at 3.81 [cm] from the injector. There is observable matching between the present solution of pressure at the wall surface and experimental results, as shown in figure (4.84). Shuen and Yoon calculations [54], obviously overestimated the wall pressure. The present solution show a sharp pulse, indicating the pressure of the injected Helium, which is equal to 1.26×10^6 [Pa]. Despite the good prediction of the present numerical code for the wall pressure, figure (4.85) illustrates observable difference between the present solution, and the experimental results. The maximum variation relative to the local value of the present solution, is estimated about 25% near the lower wall, while it reaches to 50% near the upper wall. That is because the effect of using minmode limiter to satisfy TVD conditions, as the numerical code is inaccurately capable of resolving successive sharp changes in pressure along y -direction. However, the numerical results matches both the previous solution of ref. [54], and the experimental results in the mixing free shear layer.

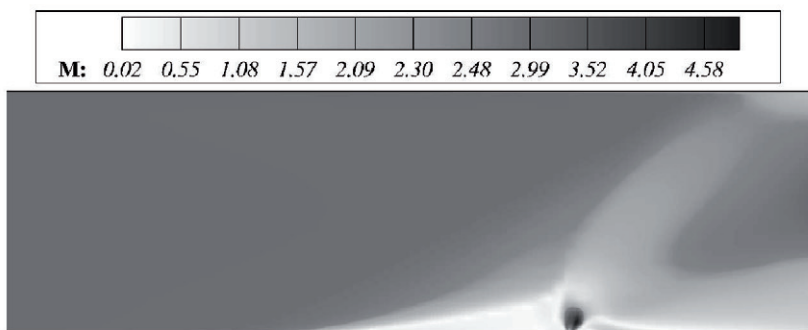


Figure 4.79: Mach Number (M) contours for the test case of Helium sonic transverse injection

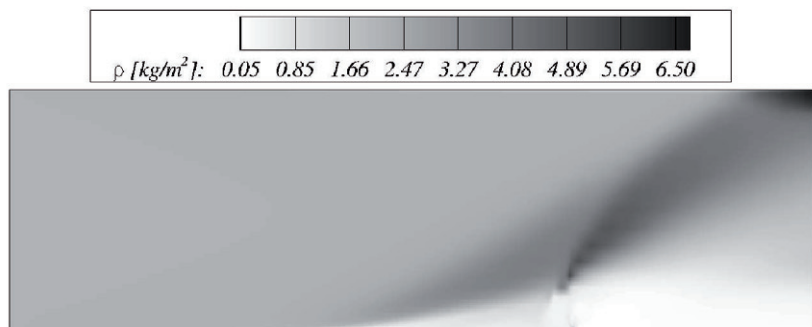


Figure 4.80: Density (ρ) contours for the test case of Helium sonic transverse injection

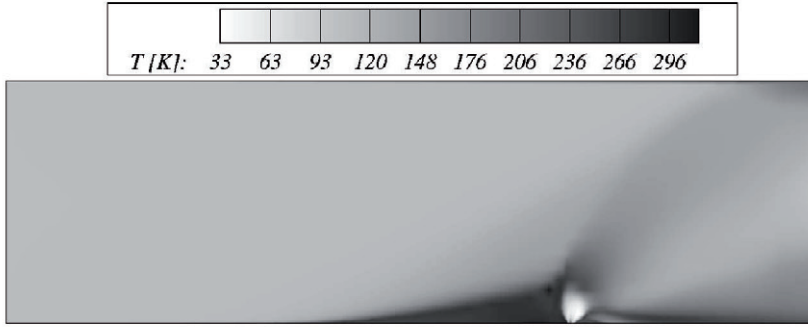


Figure 4.81: **Temperature (T) contours for the test case of Helium sonic transverse injection**

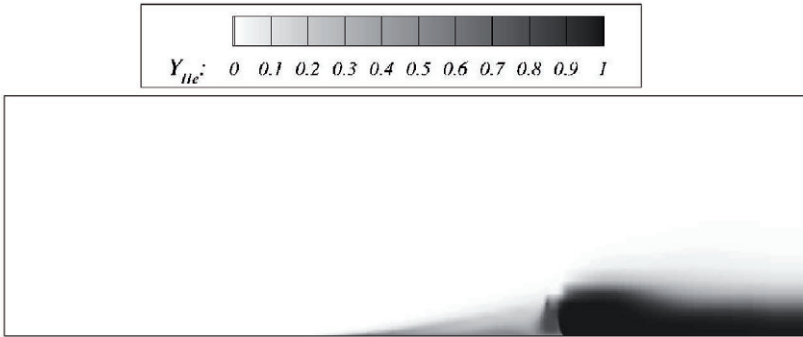


Figure 4.82: **Contours of the mass fraction of Helium (Y_{He}), which transversely injected to air supersonic flow.**

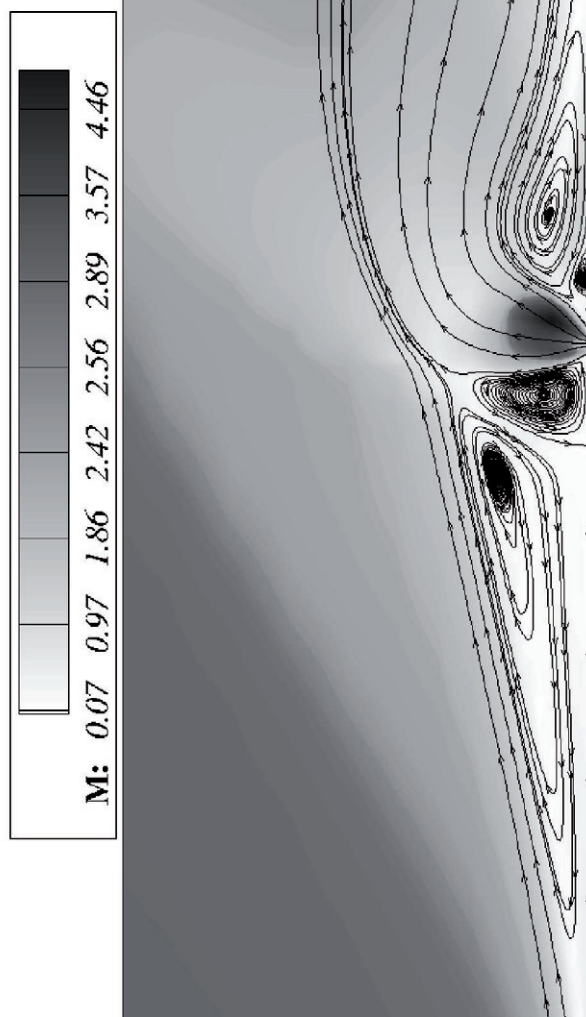


Figure 4.83: Detailed view around the injection zone, showing the contours of the Mach number (M), showing the formed recirculation zones

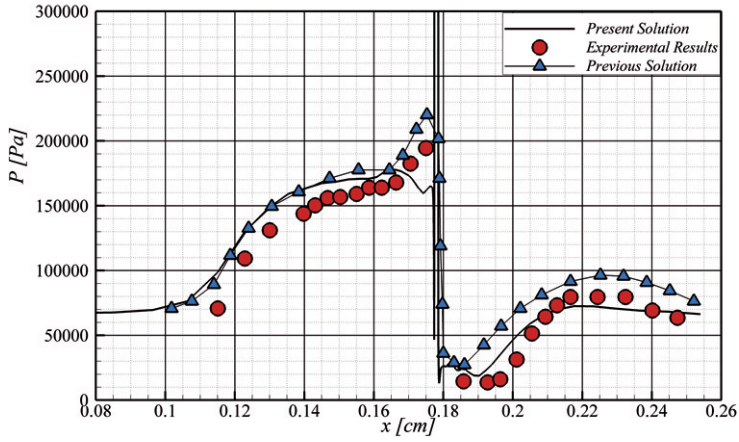


Figure 4.84: The solution of pressure at the lower wall around injector, compared to experimental results and previous calculations (ref. [54])

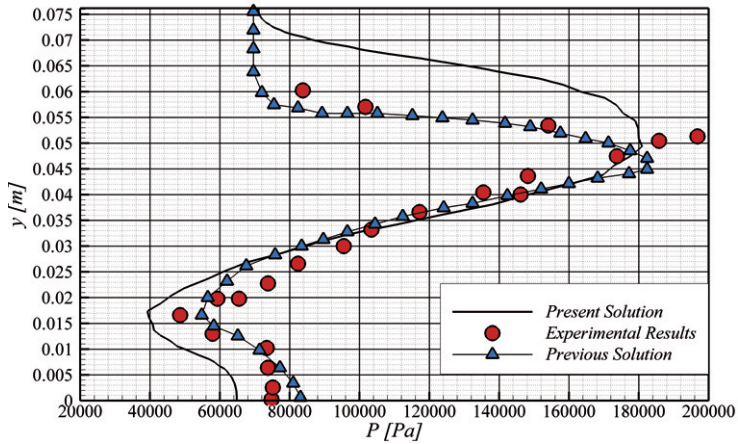


Figure 4.85: The solution of pressure at $x = 216$ [mm] from the duct inlet, compared to experimental results and previous calculations (ref. [54])

4.6 Mixing and Combustion Processes in Single-Strut Scramjet Engines

The last test case considers the non-reacting/reacting turbulent flow field in a 2D single strut scramjet engine model problem, which is introduced first by Drummond and Weidner [22]. The configuration for the problem is described in figure (4.86). The engine length is $0.78 [m]$, while its width at the inlet leading edge is $0.15 [m]$. The middle fuel injection strut is $0.258 [m]$ long and is centered about the module minimum cross-section, which is located at $0.378 [m]$ from the inlet leading edge. The half angles of the inclination of engine and injection-strut walls are 7.1 degrees. This geometry is a two-dimensional projection for an individual module of an actual scramjet engine design. Supersonic air flow enters from the intake, where gaseous Hydrogen is injected transversely at sonic speeds from four ports at the middle injection-strut and the engine wall, located at $0.06 [m]$ downstream from the minimum cross-section. The injection opening is equal to $0.1 [cm]$, which results in global equivalence ratio of unity. The inlet conditions of both air and Hydrogen are given as follows:

$$\begin{aligned} M_{in_{air}} &= 5.03, & T_{in_{air}} &= 335.0 [K], & P_{in_{air}} &= 3546.0 [Pa], \\ M_{in_{H_2}} &= 1.05, & T_{in_{H_2}} &= 246.0 [K], & P_{in_{H_2}} &= 254824.0 [Pa]. \end{aligned} \quad (4.24)$$

The longitudinal module length is taken as the reference length (L_{ref}), while the air inlet properties is set to be the other reference variables, as given below:

$$\begin{aligned} L_{ref} &= 0.78 [m], & \rho_{ref} &= \rho_{in_{air}}, & T_{ref} &= T_{in_{air}}, & V_{ref} &= V_{in_{air}}, \\ \mu_{ref} &= \mu_{L_{in_{air}}}, & k_{ref} &= k_{L_{in_{air}}}, & \mathcal{D}_{ref} &= \mathcal{D}_{L_{in_{air}}}. \end{aligned} \quad (4.25)$$

Only upper half of the scramjet model is only considered, and symmetry condition is applied at the engine centerline. Meshes of sizes 87×31 and 200×51 , are employed for domain discretization as shown in figures (4.87) and (4.88), where second Roberts transformation function,

discussed in **3.6.1**, is applied for grid line stretching in y -direction, where the hyperbolic sine transformation function, mentioned in **3.6.2** is employed to cluster the grid line in x -direction around the vertical line of ($x = x_o = 0.178$ [m]), where Helium is injected from the lower wall. The clustering constants written in equations (3.94) and (3.93) have the following values:

$$\begin{aligned} \text{For } 87 \times 31 \text{ mesh : } \quad & \beta_x = 13, & \beta_y = 1.0001, & \alpha_y = 0.5. \\ \text{For } 200 \times 51 \text{ mesh : } \quad & \beta_x = 7, & \beta_y = 1.001, & \alpha_y = 0.5. \end{aligned} \quad (4.26)$$

Clustering in x -direction is applied for the station of indices ($i = 3, 4, 5, \dots, imax$), to cover the flow domain starting from the intake leading edge to the nozzle trailing edge. The resolution of intake upstream is contained by the first two stations of the generated mesh. To ensure the smoothness of the transformation derivatives between the physical and computational domain, the axial spatial step between the first x -stations is equal to the successive step inside the scramjet module. That can be expressed in the following:

$$\left. \begin{aligned} x_{2,j} - x_{1,j} \\ x_{3,j} - x_{2,j} \end{aligned} \right\} = x_{4,j} - x_{3,j}. \quad (4.27)$$

The smaller mesh is utilized as it is of the same size of mesh used by Drummond and Weidner [22], and Chitsomboon et. al [13], to solve the same problem. The employed mesh is not identical to theirs. So, point-to-point comparison cannot be carried out, as the clustering coefficients of the transformation functions, generating their mesh are not presented.

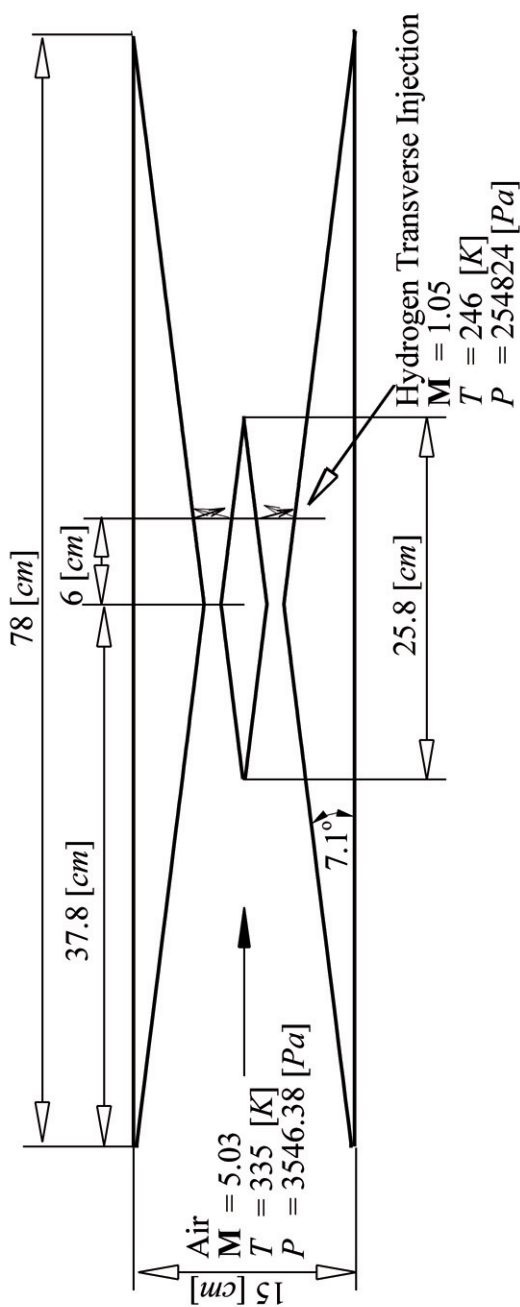


Figure 4.86: Schematic diagram for single two-dimensional strut Scramjet Engine

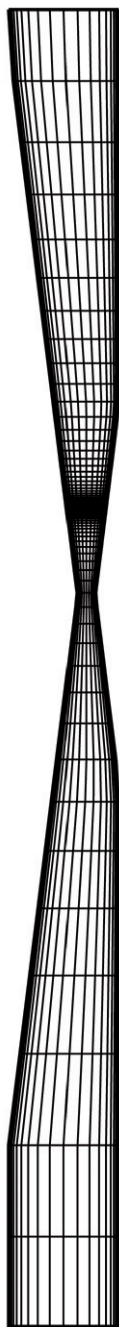


Figure 4.87: 87×31 mesh, used in solving turbulent 2D flow in single strut scramjet engine

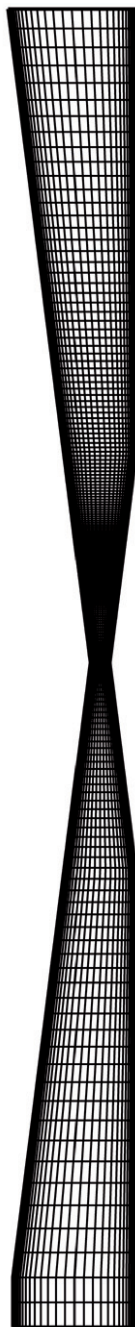


Figure 4.88: 200×51 mesh, used in solving turbulent 2D flow in single strut scramjet engine

4.6.1 Non-reacting Turbulent Flow Case

The non-reacting case is solved first, in order to demonstrate the role of shock system and recirculation zones, created around the perpendicular injectant, in fuel-air mixing and in flame holding. It is required to explore the distribution of Hydrogen mass fraction, as an indication of the mixing process efficiency, as well as to study the static temperature distribution in the non-reacting case to find the combustion-stabilized zones. It is recognized that the main design features concerning the injectant conditions, is aiming to guarantee effective mixing process. That is represented in placing the two opposite injectors near the engine cross-section minimum. Also, the mixing is enhanced by raising the injectant pressure relative to the air flow, to reinforce the fuel penetration into the main flow. It is observable the injectant pressure is about 70 times the air flow static pressure, while in the previous test case, Helium inlet pressure is only 20 times of air flow static pressure

The governing equations are integrated in time using the global and minimum value of time step, with CFL number equals to ($\sigma = 0.1$). It is not recommended to apply time stepping, as mentioned by Chitsomboon et Tiwari [12]. As this problem is considered as unsteady, the running time to solve the non-reacting test case, for mesh size 87×31 , is extended for 219 hours (i.e. 12 days approximately), while it takes about 768 hours (i.e. 32 days), for mesh size 200×51 . Then time integration is stopped after 800×10^3 iterations, for both meshes, where the unsteady flow undergoes cyclic repetitive variations, and the flow variables seem to be fluctuating around steady magnitudes.

The solution of Mach number, temperature, and Hydrogen mass fraction, for non-reacting case, for 87×31 mesh, are presented in figures (4.89)-(4.92). Due to the poor grid resolution at the intake regime, the shock waves system are not accurately represented, as shown in figure (4.89). Due to shock-wave/boundary-layer interactions, recir-

culation zone is created in the engine intake. The vortical flow speed is considered higher than that of the other downstream recirculation zones. That results in static temperature rise up to about $2300[K]$, in the turbulent shear layers. The recirculation zone, located in front of the injectant at the middle strut wall, extends upstream to pass through the minimum cross-section. H_2 -air mixing is carried out in the vortical flow front of the injection region, as illustrated in figures (4.91) and (4.92). where there is obvious resemblance in the structure of the leading recirculation zones. After the injection region, the mixture is then expanded, where Hydrogen diffusively transfers into air as mixing layers.

The non-reacting problem is resolved again, for a mesh size of 200×51 , the distribution of Mach number, static temperature, and H_2 mass fraction is presented in figures (4.93)-(4.97). There is observable improvement in the present results resolution. Mach number contours show clearly an oblique shock wave originated from the intake leading edge, then reflected at the middle strut apex to the upper wall again. Shock wave reflection creates a relatively high speed recirculation zone, whose size is *smaller* than that predicted for the smaller-sized mesh. Then the flow undergo downstream through complicated system of shock reflection and separation shock, starting from the module minimum cross-section. The flow separation at the minimum cross-section, has bigger size, compared to previous solution, indicating more Hydrogen extension upstream. However, the recirculation zone in front of the injected Hydrogen from the middle strut, becomes much more smaller, because of shock reflections. As they deflect airflow direction parallel to the injection strut walls, leading to enlarge vortical flows zone adjacent to the engine wall in front of the injector. The vortical flow structure becomes more complicated in both regions, and completely distinct from each other.

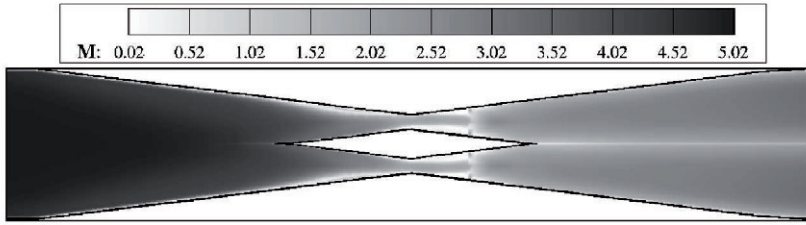


Figure 4.89: Mach number (M) contours of the non-reacting case solution, for mesh size 87×31

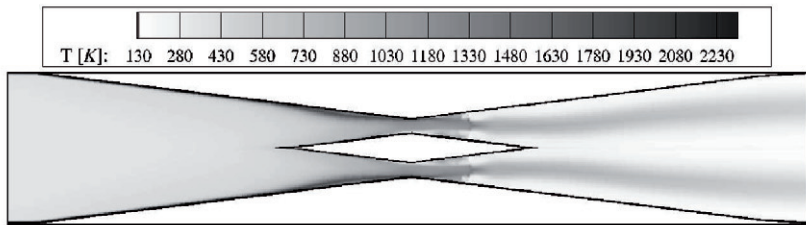


Figure 4.90: Temperature (T) contours of the non-reacting case solution, for mesh size 87×31

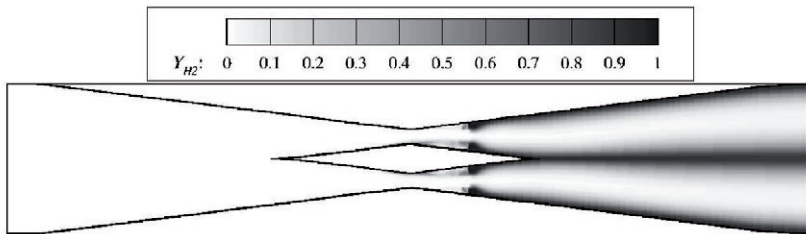


Figure 4.91: Hydrogen mass fraction (Y_{H_2}) contours of the non-reacting case solution, for mesh size 87×31

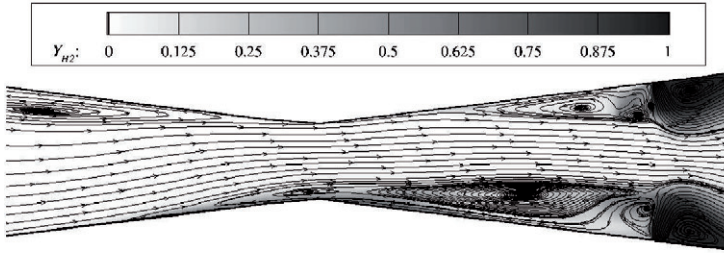


Figure 4.92: Hydrogen mass fraction (Y_{H_2}) contours within the upper injection zone, for the non-reacting case solution, for mesh size 87×31

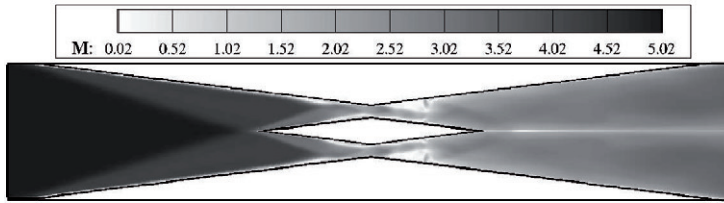


Figure 4.93: Mach number (M) contours of the non-reacting case solution, for mesh size 200×51

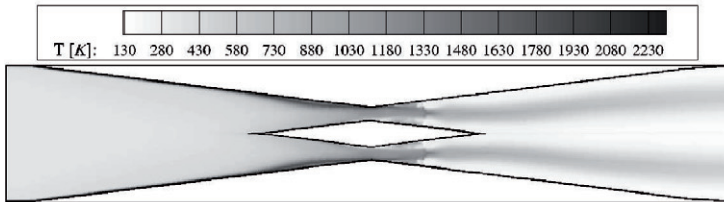


Figure 4.94: Temperature (T) contours of the non-reacting case solution, for mesh size 200×51

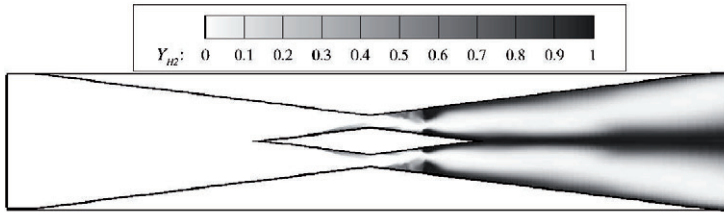


Figure 4.95: **Hydrogen mass fraction (Y_{H_2}) contours of the non-reacting case solution, for mesh size 200×51**

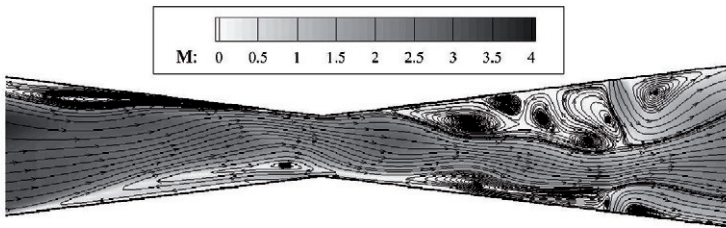


Figure 4.96: **Mach number (M) contours within the upper injection zone, for the non-reacting case solution, for mesh size 200×51**

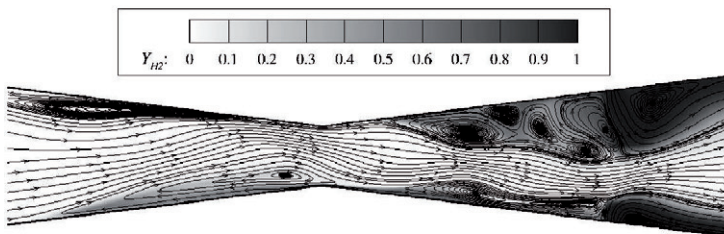


Figure 4.97: **Hydrogen mass fraction (Y_{H_2}) contours within the upper injection zone, for the non-reacting case solution, for mesh size 200×51**

4.6.2 Reacting Turbulent Flow Case

After solving the problem of non-reacting H_2 -air turbulent flow inside scramjet engine. The computational solutions of the flow variables, are set to their initial values, for the first iteration of reacting test case calculations. Unsteady Navier-Stocks equations are solved in time using minimum time step of CFL number equals to 0.1. The system of equations is composed of eight coupled non-linear partial differential equations are solved, as there is four chemically reacting species (i.e. O_2 , H_2 , OH , and H_2O), while Nitrogen is considered inert, similar to the previous non-reacting case.

The reacting case is first solved, starting the numerical solution of the non-reacting case of mesh size 87×31 , which the same size employed in Drummond and Weidner [22], and Chitsomboon et al. [13]. A *continuous growth* in the separation vortical flow in the intake region, becomes more observable by marching in time. That is because of the few cells covering the intake domain, while most of the grid nodes are intensified near the injection zone. The bad resolution leads the numerical solver to be unable to capture correct size of the intake vortices. It is estimated that the running time utilizing this mesh size, takes about 434 hours (i.e. 18 days), for only 70×10^3 iterations.

Hence, time-integration of the reacting case, utilizes the computational results of the non-reacting case of mesh size 200×51 , for the first iteration. The unsteady reacting solution seems to be repetitive, after 350×10^3 iterations, which requires about 1344 hours (i.e. 56 days).

The solution of chemically reacting turbulent H_2 -air flow inside scramjet engine is illustrated in figures (4.98)-(4.103). The recirculation zones upstream the minimum cross-section, becomes larger compared to the non-reacting case, due to the rise of the static temperature

downstream, within the injection zone. The static temperature is of order 3300 [K] in the flow-separation regimes before the injectors. Static temperature increases by going closer to the impact zone of the vortex flow with perpendicular H_2 injection, where it reaches in singular few points to 5000 [K]. In addition, the water mass fraction, is raised up to 0.72 in a singular point, downstream the front recirculations zone, at the start of the free mixing layer, leading to decreasing the static pressure and raising flow Mach number up to 6.0. That is referred to the calculations of the forward rates of the elementary reactions, of Rogers and Chinitz mechanism, have poor accuracy in the combustion initiation regimes, as concluded in section 4.4.

Hydrogen mass fraction in the reacting case is approximately vanished in the front recirculation zones, also it obviously reduce in the free mixing layer along the engine module, as shown in figure (4.101). The magnitude of water mass fraction demonstrates the extent of the combustion, along the flow field. Therefore, as shown in figure (4.100), that combustion is mainly initiated and sustained by means of the separations shocks in front of the injected H_2 stream. It is illustrated in figures (4.102) and (4.103) that the flame-holders recirculation zones have simpler eddy-structure, compared to the non-reacting test case, because the separation intensity is diminished due to the rise of the total temperature in the combustion zone. Also, it is noticeable that the flow is thermally choked the flow within the injection zone, which must be avoided in scramjet engine design and development.

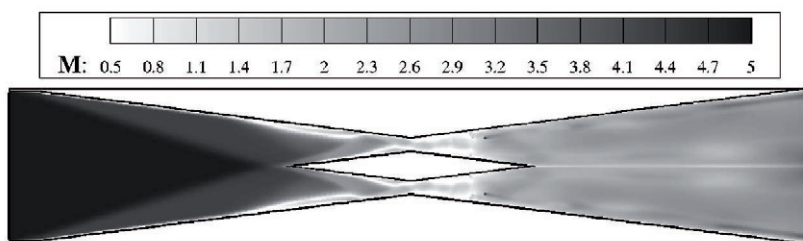


Figure 4.98: Mach number (M) contours of the reacting case solution, for mesh size 200×51

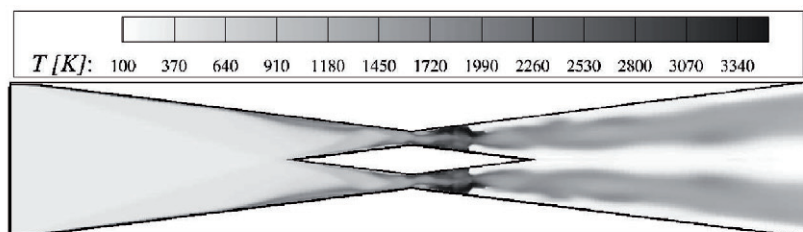


Figure 4.99: Temperature (T) contours of the reacting case solution, for mesh size 200×51

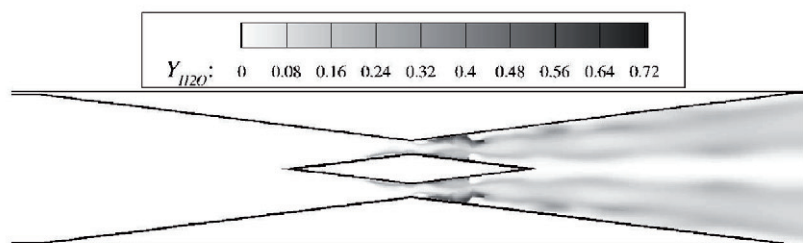


Figure 4.100: Water mass fraction ($Y_{\text{H}_2\text{O}}$) contours of the reacting case solution, for mesh size 200×51

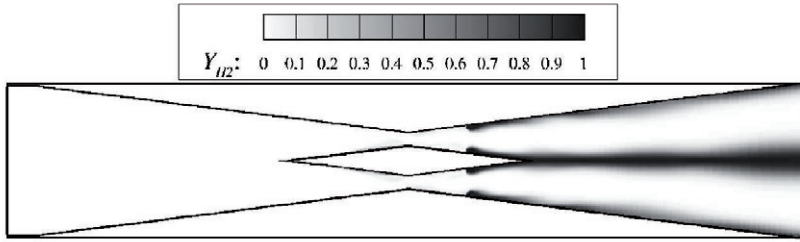


Figure 4.101: **Hydrogen mass fraction (Y_{H_2}) contours of the reacting case solution, for mesh size 200×51**

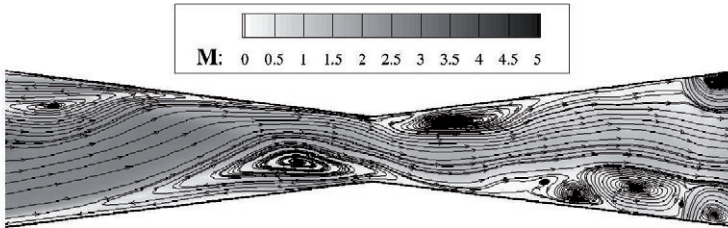


Figure 4.102: **Mach number (M) contours within the upper injection zone, for the reacting case solution, for mesh size 200×51**

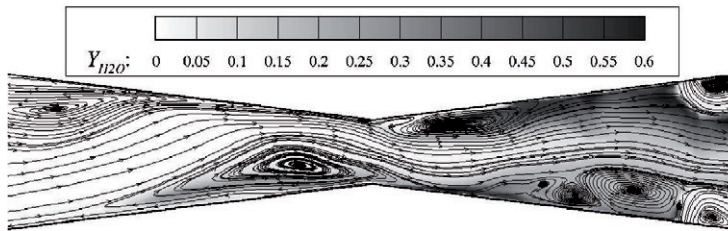


Figure 4.103: **Water mass fraction (Y_{H_2O}) contours within the upper injection zone, for the reacting case solution, for mesh size 200×51**

4.6.3 Comparison between the Results

In this section, the numerical solutions for turbulent flow in scramjet engine are more deeply analyzed and compared to each others, to previous calculations of the same problem. First of all, the comparisons are mostly carried out in terms of normalized variables, refereed to the main features of the specified test case. That facilitates to evaluate different sets of results. The utilized normalized variables are the axial and transversal normalized distance; x_{norm} , and y_{norm} respectively, in addition to the normalized pressure (P_{norm}). They are expressed as follows:

$$x_{norm} = \frac{x - x_{\text{intake leading edge}}}{x_{\text{intake leading edge}} - x_{\text{nozzle trailing edge}}},$$

$$y_{norm} = \frac{y - y_{min}}{y_{max} - y_{min}}, \quad (4.28)$$

$$P_{norm} = \frac{P - P_{\text{air inlet}}}{P_{\text{H}_2 \text{ injection}} - P_{\text{air inlet}}}.$$

First comparison is applied between the solutions of the non-reacting case for mesh sizes: 87×31 and 200×51 , at different stations upstream and downstream the injection ports, such that the distance between the injection ports and the intake leading edge is about 0.56 of the total engine length. So, two sets solutions of H_2 mass fraction, and static temperature, at different axial normalized distances, are plotted in figure (4.104) and (4.105). Stations of axial normalized distance ranging between 0.51 and 0.55 represent the flow domain upstream the injection ports, while those ranging between 0.57 and 0.61 represent the downstream flowfield.

The solutions of 87×31 -sized mesh underestimate the H_2 mass fraction upstream the injection port. On the other side, the more refined mesh, predict mass fraction Hydrogen equals to unity at normalized distance 0.1% upstream the injector. Also, the 200×51 solution shows that H_2 -air mixing is more effective at the module wall than that at

the middle strut surface, because of the recirculation zone formed adjacent to the upper wall is much bigger, as presented in figure (4.97). The two sets solutions becomes closer to each other downstream.

Then the solutions of temperature and water mass fraction are compared for the solved reacting test case for mesh size 200×51 , and the previous results represented by Chitsomboon et al [13], which is given at specific grid lines, as shown in figure (4.106) and (4.108). So, point-to-point comparison cannot be carried out, as the parameters of the applied grid generating functions are given in ref. [13]. Moreover, the temperature solution is given in the normalized form, relative to certain maximum value, which is not also mentioned. Hence qualitative and quantitative comparison is carried out in H_2O solution, while temperature solution is only qualitatively evaluated.

As illustrated in figures (4.106) and (4.107), the H_2O mass fraction solution of the 87×31 -sized mesh of Chitsomboon et al. [13], is greatly less than predicted by the present solution utilizing 200×51 -sized mesh. However, the general behaviors of water distribution in both solutions are close to each other, upstream and downstream the injection zone. And it is noted that the magnitude of H_2O does not significantly change, as an evidence of fuel-air mixing efficiency in the recirculation zones in front of the injectant. In addition, qualitative analysis between the normalized temperature of previous solution, and the static temperature of the present solution, shows resemblance in temperature field downstream the injectors. While the present solution, predict almost constant static temperature in the front recirculation zones.

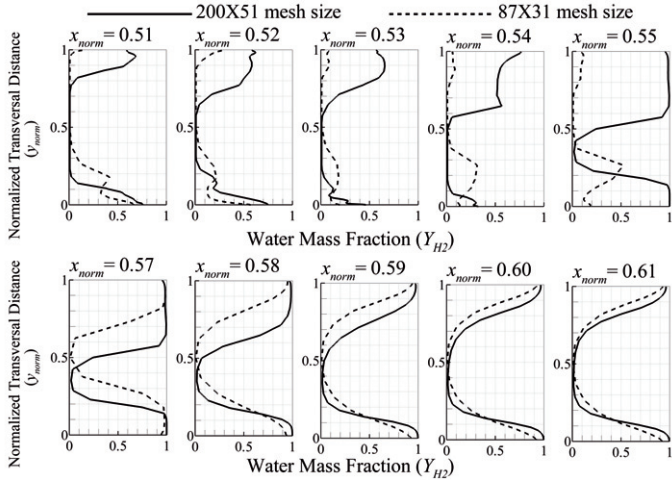


Figure 4.104: **Hydrogen mass fraction solution at different station, for the non-reacting case for mesh sizes 87×31 and 200×51**

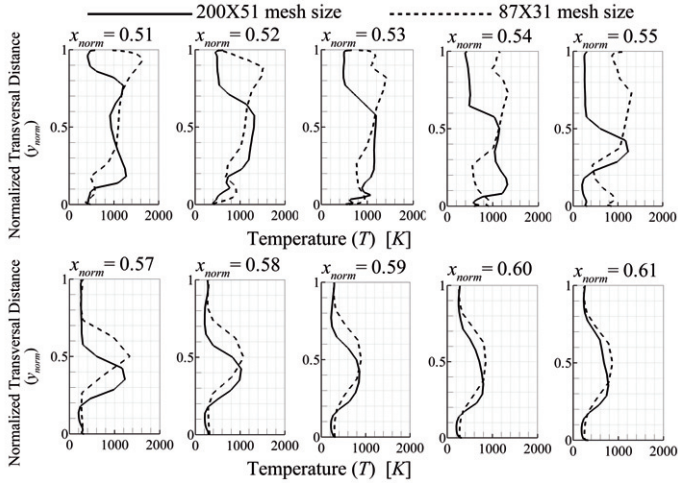


Figure 4.105: **Temperature solution at different station, for the non-reacting case for mesh sizes 87×31 and 200×51**

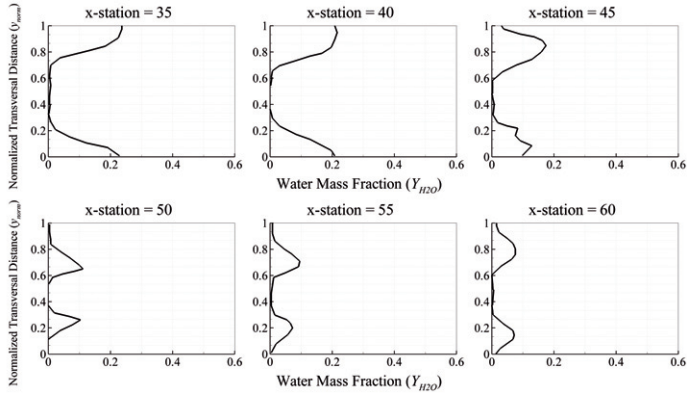


Figure 4.106: Previous solution for water mass fraction at different station, for the reacting case (ref. [13])

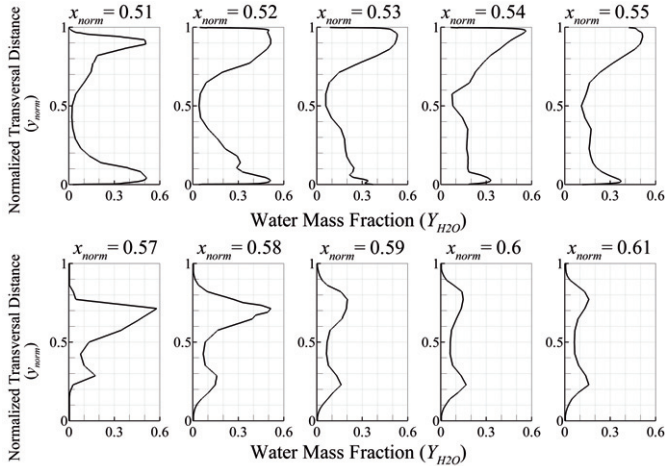


Figure 4.107: Water mass fraction solution at different station, for the reacting case for mesh size 200×51

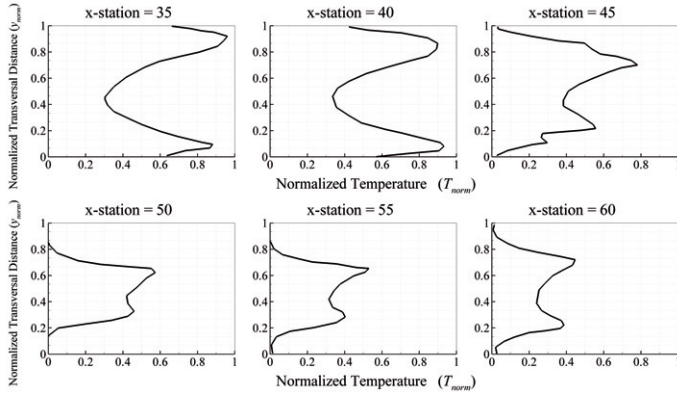


Figure 4.108: **Previous solution for normalized temperature at different station, for the reacting case (ref. [13])**

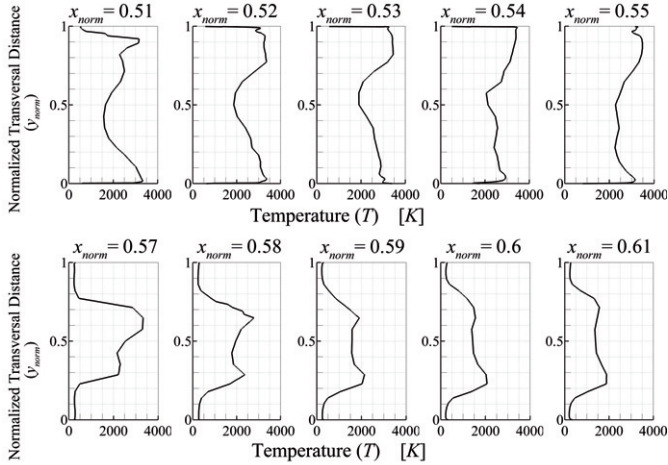


Figure 4.109: **Temperature solution at different station, for the reacting case for mesh size 200×51**

The solutions of the normalized pressure on the engine upper wall surface for the present calculations of the non-reacting flow for both mesh size, beside the reacting flow for the more refined one, are com-

pared to that calculated by Chitsomboon et al. [13]. In figure (4.110), the normalized pressure is presented along the whole engine module, where the normalized pressure for all solutions, equal to unity, at the injection zone, at 0.56 of the total length.

It is important to notice that the previous solution of the reacting case, is almost matching with the non-reacting solution of the same mesh size (87×31). However, the solutions of more refined meshes predict higher values of wall normalized pressure, for both reacting and non-reacting cases. The solution of the reacting of 200×51 -sized mesh, predicts that the wall pressure exceeds the injection pressure, in the flow choking regimes, located upstream the injection ports. However, there is approximate matching between all solution downstream in the expansion zone.

High variation in the results in the injection upstream recirculation zone, may refer to the high unsteadiness of the flowfield in this regime, and to the great grid-sensitivity of the solution of this complicated turbulent flow.

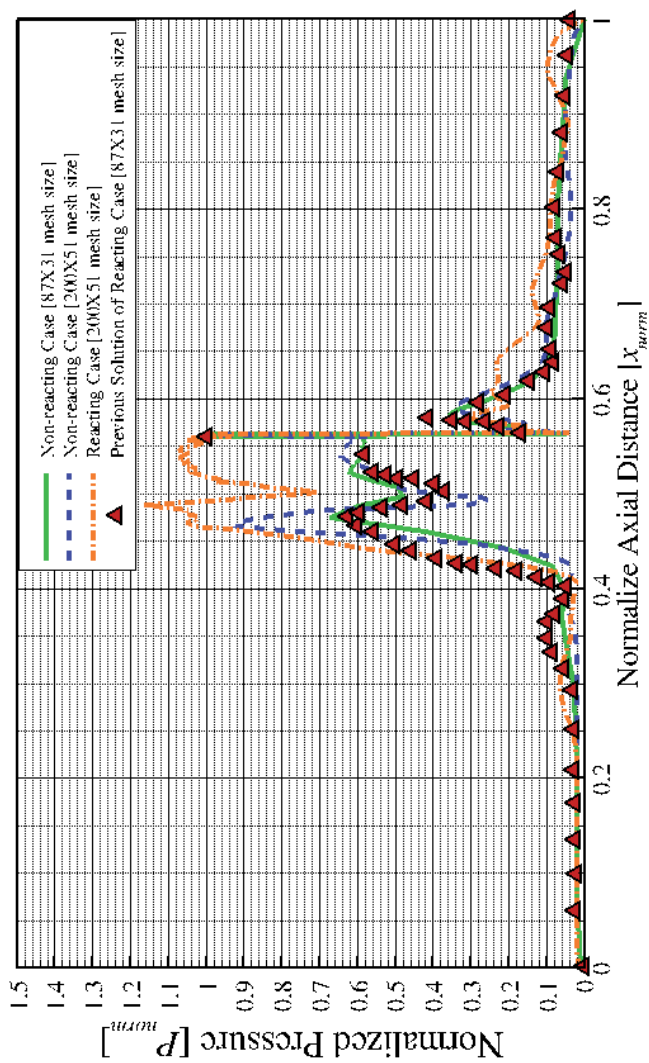


Figure 4.110: Normalized pressure solution on the upper wall, compared to the previous solution (ref.[13])

Chapter 5

Conclusion

It will be focused here on the most important remarks and comments about the mathematical modeling, numerical treatment and computational results for different test cases.

First of all, the main target of this study is to construct a numerical code capable of resolving the chemically reacting turbulent flows inside scramjet engine, and to investigate the mixing and flame-stabilization processes applying fuel transverse sonic injection, in order to be a future tool for parametric design analysis for scramjet engine development. The mathematical model is governed by unsteady Reynolds-Averaged Navier-Stocks equations (RANS). Separate time-space discretizations are employed. Finite-volume volume second-order Roe's scheme is applied for spatial discretization. Total variation diminishing are achieved by using minmode limiter, which is characterized by stable performance. Integration in time by second order accurate Runge-Kutta two step method, applying Point-implicit scheme, which solves only the chemical source term implicitly. So, the stiffness of the chemical source term is removed, without the need to solve all terms implicitly, and to invert huge matrices. Turbulence modeling is based on Boussinesq's assumption, and applies Baldwin-Lomax algebraic model.

The code is evaluated with different several test cases, to explore its coding bugs and deficiencies, and to improve its computation. The numerical code show excellent results for laminar and turbulent air flow over flat plate, where the numerical solutions for velocity profile and wall shear stress matches with well-known analytical equations concerned with these problem.

The code capability of solving reacting flows is tested by two problems for different boundary conditions. The first problem is the inviscid chemically reacting flow of premixed H_2 -air flow, through the divergent part of two-dimensional axisymmetric sine-nozzle. The problem is solved for two different back pressures. The numerical solution of complete expansion and over-expansion cases are close to the previous quasi one-dimensional flow of ref. [21] and [30] respectively. The second chemically reacting problem is turbulent premixed H_2 -air flow inside a two-dimensional ramped duct. The problem is solved for two different inlet static temperatures; below and above the ignition threshold of H_2 -air combustion. It is found that the formed shock wave has a role in combustion excitation, and sustainability. That clarifies the potential of shock induced combustion, to be an efficient flame-stabilization technique in engines of high speed internal flow. Also, a noticeable closure between the present calculations between ref. [14] and [66], for inlet temperatures of 900 [K] and 1200 [K], respectively.

Rogers and Chinitz semi-global two chemical reaction model for Hydrogen-air combustion, was the simplest chemical mechanism after the global one-reaction model. It present great result for high speed reacting flows. [48] However, the reaction forward-direction rates are greatly overestimated within the shock-induced combustion regimes. That results in the formation discrete peaks in Hydroxyl mass fraction across the shock wave, where the intensity and numbers of its nonphysical peaks are greatly sensitive on the grid resolution.

The code is examined to resolve the complicated flowfield accompanying the sonic transverse injection of Helium, into supersonic air flow. The present solution is verified by the previous results of Kraemer and Rogers experiment. The solution of the wall pressure upstream and downstream the injection almost coincides with the experimental results, while the solution of the pressure along an axial station, is has smoother variation, compared to the previous results.

In spite of its stable performance, minmode limiter shows modest resolution of sharp strong shocks because of its diffusive effect as previously mentioned in ref. [32]. Also, because it is a discontinuous slope limiter, it is recommended not to apply it in problems of continuous local maxima and minima in the flow field, as it would result in formation of nonphysical smooth peaks, beside the resolved physical flow variables peaks, as discussed before in the problem of over-expansion inside axisymmetric nozzle.

After this set of test cases, sufficient experience is gained to start in solving turbulent chemically reacting flows inside scramjet engines. First non-reacting case is solved for turbulent flow inside single strut scramjet engine introduced by Drummond and Weidner [22]. Then reacting case is solved starting from the non-reacting case solution. It is shown that the problem is high sensitive to the mesh resolution, especially in the recirculation zone upstream the injection ports, for both non-reacting and reacting cases. That is refereed to the high unsteadiness of the flowfield in this domain.

Grid sensitivity analysis cannot be carried out as the reacting case of the most refined utilized mesh takes about two months in running time. As personal computational units are only utilized without parallel computations

It is required in the future research to employ parallel computations on

more powerful computational units, to solve the problem of the long running time. It is suggested to employ fully implicit treatment, to minimize the solution iterations. More sophisticated H_2 -oxygen chemical mechanism is required to improve the solution accuracy at temperatures around the ignition threshold, which is approximately equals to 1000 [K]. Also, more advanced turbulence modeling is required in jets and free shear layers. It is required to fulfill TVD conditions using other sloper limiter capable of resolving sharp discontinuities and to resolve continual peaks with high degree of accuracy. And it is required in the same time to ensure that of its stable performance in the solution convergence history.

Appendix A

Flow Variables Non-dimensionalization

The non-dimensionalization reference values are selected from the characteristic flow variables of the studied test case. The reference length (L_{ref}) is considered as a longest dimension of the problem geometry. Besides, the reference values of velocity, density and temperature (i.e. V_{ref} , ρ_{ref} , and T_{ref}) are taken to be the velocity magnitude, and the stagnant density and temperature respectively, at the main flow inlet. Also, we set the reference values of transport coefficient, i.e. (μ_{ref} , k_{ref} , and $\mathcal{D}_{ref}$) and thermodynamic properties (i.e. R_{ref} , cp_{ref} , and γ_{ref}) are equal to those of the mixture at the main flow inlet. If the dimensional flow variables are notated with the superscript (*), the dimensionless variables will be given as follows:

$$\begin{aligned} x &= \frac{x^*}{L_{ref}} & y &= \frac{y^*}{L_{ref}} & t &= \frac{t^*}{L_{ref}/V_{ref}} & \rho &= \frac{\rho^*}{\rho_{ref}} & T &= \frac{T^*}{T_{ref}} \\ u &= \frac{u^*}{V_{ref}} & v &= \frac{v^*}{V_{ref}} & P &= \frac{P^*}{\rho_{ref}V_{ref}^2} & e &= \frac{e^*}{V_{ref}^2} & h &= \frac{h^*}{V_{ref}^2} \\ E_t &= \frac{E_t^*}{V_{ref}^2} & H_t &= \frac{H_t^*}{V_{ref}^2} & \mu &= \frac{\mu^*}{\mu_{ref}} & k &= \frac{k^*}{k_{ref}} & \mathcal{D} &= \frac{\mathcal{D}^*}{\mathcal{D}_{ref}} \end{aligned} \tag{A.1}$$

The studied test case can be characterized by a group of dimensionless variables derived from the test case reference values. These di-

mensionless variables are represented in Reynolds Number (Re_{ref}), Prandtl Number (Pr_{ref}), Schmidt Number (Sc_{ref}), and Mach Number ($\mathbf{M}_{ref}$):

$$\begin{aligned} Re_{ref} &= \frac{\rho_{ref} V_{ref} L_{ref}}{\mu_{ref}}, & Pr_{ref} &= \frac{\mu_{ref} c p_{ref}}{k_{ref}}, \\ Sc_{ref} &= \frac{\mu_{ref}}{\rho_{ref} \mathcal{D}_{ref}}, & \mathbf{M}_{ref} &= \frac{V_{ref}}{\sqrt{\gamma_{ref} R_{ref} T_{ref}}}. \end{aligned} \quad (\text{A.2})$$

Appendix B

Reynolds Averaged Navier-Stocks Equations

B.1 Flow Variables Treatment

In turbulent flow models based on time-averaging approach, each flow variable is considered to be composed of two components. The first is the time-averaged term. While, the other is corresponding to the random fluctuations of the flow variable magnitude.

The conventional variable decomposition, is to considered a variable f is consisting of two components: time averaged one which is expressed as follows:

$$\bar{f} = \frac{1}{\Delta t} \int_t^{t+\Delta t} f \, dt. \quad (\text{B.1})$$

Δt is the time interval which is much longer than the turbulent fluctuation time intervals, and smaller than the flow characteristic time. According to equation (B.1), the flow variable f is decomposed as follows:

$$f = \bar{f} + f'. \quad (\text{B.2})$$

We can conclude that the time averaging of fluctuations term f' is equal to zero:

$$\overline{f'} = \frac{1}{\Delta t} \int_t^{t+\Delta t} f' dt = 0. \quad (\text{B.3})$$

The second method of decomposition, which is weight-based on the time averaging, which is known as ‘‘Favre’’’s averaging, divides variable f into two components as follows:

$$f = \tilde{f} + f''. \quad (\text{B.4})$$

where the weight-based time averaged term $\tilde{f}$ is written as follows:

$$\tilde{f} = \frac{1}{\rho} \left(\frac{1}{\Delta t} \int_t^{t+\Delta t} \rho f dt \right) = \frac{\overline{\rho f}}{\bar{\rho}}. \quad (\text{B.5})$$

Here, the time averaging of the fluctuations term f'' will not equal to zero. But its weight-base averaging vanishes:

$$\overline{f''} = \frac{1}{\Delta t} \int_t^{t+\Delta t} f'' dt \neq 0. \quad (\text{B.6})$$

$$\overline{\rho f''} = \frac{1}{\Delta t} \int_t^{t+\Delta t} \rho f'' dt = 0. \quad (\text{B.7})$$

From above equation we can conclude the following relations, to be used in the derivation of RANS equations:

$$\begin{aligned} \overline{f_1 \pm f_2} &= \overline{f_1} \pm \overline{f_2}, & \overline{f_1 \times f_2} &\neq \overline{f_1} \times \overline{f_2}, & \overline{\tilde{f}_1 f_2''} &= \tilde{f}_1 \overline{f_2''} \neq 0, \\ \overline{\tilde{f}_1 f_2'} &= \tilde{f}_1 \overline{f_2'} = 0, & \overline{f_1' f_2'} &\neq 0, & \overline{f_1'' f_2''} &\neq 0, \\ \overline{f_1' f_2''} &\neq 0, & \overline{\rho f_1} &= \bar{\rho} \tilde{f}_1. \end{aligned} \quad (\text{B.8})$$

To minimize the number of terms in the averaged equation, some approximation are taken, where some terms of very small order of magnitude compared to the other terms in the equations, as follows:

- The spatial derivative of the fluctuation term

$$\frac{\partial \overline{f_1''}}{\partial x_i} \ll \frac{\partial \overline{f_1}}{\partial x_i}. \quad (\text{B.9})$$

- The time-averaging of three fluctuations terms

$$\overline{f_1'' f_2'' f_3''} \ll \overline{f_1 f_2'' f_3''}. \quad (\text{B.10})$$

The conventional kind of decomposition is applied for density and pressure. But, on the other hand, the rest of the flow variables is decomposed using Favre's definition. The flow variable decomposition is written in the following form:

$$\begin{aligned} \rho &= \bar{\rho} + \rho', \quad P = \bar{P} + P', \quad T = \tilde{T} + T'', \quad u = \tilde{u} + u'', \quad v = \tilde{v} + v', \\ e &= \tilde{e} + e'', \quad h = \tilde{h} + h'', \quad H_t = \tilde{H}_t + H_t'', \quad E_t = \tilde{E}_t + E_t'', \quad Y_m = \tilde{Y}_m + Y_m''. \end{aligned} \quad (\text{B.11})$$

Besides, the mixture diffusive transport coefficients fluctuations are neglected; each time-averaged transport coefficient is the same to that in the case of the laminar flow:

$$\bar{\mu} = \mu_L, \quad \bar{k} = k_L, \quad \bar{\mathcal{D}} = \mathcal{D}_L. \quad (\text{B.12})$$

B.2 Derivation of Reynolds Averaged Navier-Stocks Equations for Planar 2D Flows

Time-averaged Navier-Stocks equations are presented here for planar 2D flows, which is the case of all the studied test cases in this thesis, which are concerned with turbulent flows. This derivation can be extended to derive the governing equations form in the case of 2D axisymmetric internal flows.

The derivation of “Reynolds-Averaged Navier-Stocks” equations (RANS), starts from the “Unsteady Navier-Stocks”, which can be expresses in

the thermally-equilibrium, chemically-nonequilibrium, planar 2D coordinates as follows:

• **Mixture Mass Continuity Equation**

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) = 0. \quad (\text{B.13})$$

• **Momentum Equation in x -direction**

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2 + P) + \frac{\partial}{\partial y}(\rho uv) = \frac{\partial}{\partial x}(\tau_{xx_L}) + \frac{\partial}{\partial y}(\tau_{xy_L}). \quad (\text{B.14})$$

• **Momentum Equation in y -direction**

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho vu) + \frac{\partial}{\partial y}(\rho v^2 + P) = \frac{\partial}{\partial x}(\tau_{xy_L}) + \frac{\partial}{\partial y}(\tau_{yy_L}). \quad (\text{B.15})$$

• **Mixture Energy Equation**

$$\begin{aligned} \frac{\partial}{\partial t}(\rho E_t) + \frac{\partial}{\partial x}(\rho H_t u) + \frac{\partial}{\partial y}(\rho H_t v) = \\ = \frac{\partial}{\partial x}(\tau_{xx_L} u + \tau_{xy_L} v - q_{x_L}) + \frac{\partial}{\partial y}(\tau_{xy_L} u + \tau_{yy_L} v - q_{y_L}). \end{aligned} \quad (\text{B.16})$$

• **Individual Species Mass Continuity Equation**

$$\frac{\partial}{\partial t}(\rho Y_m) + \frac{\partial}{\partial x}(\rho Y_m u) + \frac{\partial}{\partial y}(\rho Y_m v) = \dot{\omega}_m - \frac{\partial}{\partial x}(d_{mx_L}) - \frac{\partial}{\partial y}(d_{my_L}). \quad (\text{B.17})$$

Derivation of the time-averaged form of the governing equation can be achieved by decomposing the flow variables in equations (B.13)-(B.17), as explained in section B.1, followed by time-averaging the entire equations.

B.2.1 Reynolds Averaged Continuity Equation for Planar 2D Flow

After flow variables decomposition in equation (B.13), The mixture mass continuity equations becomes, :

$$\frac{\partial}{\partial t}[(\bar{\rho} + \rho')] + \frac{\partial}{\partial x}[(\bar{\rho} + \rho')(\tilde{u} + u'')] + \frac{\partial}{\partial y}[(\bar{\rho} + \rho')(\tilde{v} + v'')] = 0. \quad (\text{B.18})$$

Then, the entire equation is time-averaged, regarding the relations of (B.8). The Reynolds averaged continuity equation is expressed as follows:

$$\frac{\partial}{\partial t} (\bar{\rho}) + \frac{\partial}{\partial x} (\bar{\rho}\tilde{u}) + \frac{\partial}{\partial y} (\bar{\rho}\tilde{v}) = 0. \quad (\text{B.19})$$

B.2.2 Reynolds Averaged Momentum Equations for Planar 2D Flow

After the flow variables decomposition, we can rewrite the momentum equations in x and y directions, by referring to equations and . The momentum equation for planar 2D flow will be in the following form:

$$\begin{aligned} \frac{\partial}{\partial t} [(\bar{\rho} + \rho') (\tilde{u} + u'')] + \frac{\partial}{\partial x} [(\bar{\rho} + \rho') (\tilde{u} + u'')^2 + (\bar{P} + P')] + \\ + \frac{\partial}{\partial y} [(\bar{\rho} + \rho') (\tilde{u} + u'') (\tilde{v} + v'')] = \frac{\partial}{\partial x} (\tau_{xx_L}) + \frac{\partial}{\partial y} (\tau_{xy_L}). \end{aligned} \quad (\text{B.20})$$

And the momentum equation in y -direction, in planar 2D domain, is rewritten after decomposition as follows:

$$\begin{aligned} \frac{\partial}{\partial t} [(\bar{\rho} + \rho') (\tilde{v} + v'')] + \frac{\partial}{\partial x} [(\bar{\rho} + \rho') (\tilde{v} + v'') (\tilde{u} + u'')] + \\ + \frac{\partial}{\partial y} [(\bar{\rho} + \rho') (\tilde{v} + v'')^2 + (\bar{P} + P')] = \frac{\partial}{\partial x} (\tau_{xy_L}) + \frac{\partial}{\partial y} (\tau_{yy_L}). \end{aligned} \quad (\text{B.21})$$

Each of the viscous stress tensor components (i.e. τ_{xx_L} , τ_{yy_L} , and τ_{xy_L}), is divided into two sets of spatial derivatives: The first is composed of the derivatives of the time-averaged velocity magnitudes, while other is of derivatives of fluctuated velocity components magnitudes.

$$\begin{aligned} \tau_{xx_L} &= \mu_L \left\{ \left[\frac{4}{3} \frac{\partial \tilde{u}}{\partial x} - \frac{2}{3} \frac{\partial \tilde{v}}{\partial y} \right] + \left[\frac{4}{3} \frac{\partial u''}{\partial x} - \frac{2}{3} \frac{\partial v''}{\partial y} \right] \right\}, \\ \tau_{yy_L} &= \mu_L \left\{ \left[\frac{4}{3} \frac{\partial \tilde{v}}{\partial y} - \frac{2}{3} \frac{\partial \tilde{u}}{\partial x} \right] + \left[\frac{4}{3} \frac{\partial v''}{\partial y} - \frac{2}{3} \frac{\partial u''}{\partial x} \right] \right\}, \\ \tau_{xy_L} &= \mu_L \left\{ \left[\frac{\partial \tilde{u}}{\partial y} + \frac{\partial \tilde{v}}{\partial x} \right] + \left[\frac{\partial u''}{\partial y} + \frac{\partial v''}{\partial x} \right] \right\}. \end{aligned} \quad (\text{B.22})$$

After time-averaging the whole momentum equations, and elimination of the zero-valued and low order of magnitude terms, the momentum

equation in x -direction can be written as follows:

$$\begin{aligned} \frac{\partial}{\partial t} (\overline{\rho u}) + \frac{\partial}{\partial x} (\overline{\rho u^2} + \overline{P}) + \frac{\partial}{\partial y} (\overline{\rho u v}) &= \frac{\partial}{\partial x} (\overline{\tau_{xx_L}} - \overline{\rho u''^2}) + \frac{\partial}{\partial y} (\overline{\tau_{xy_L}} - \overline{\rho u'' v''}) \\ &= \frac{\partial}{\partial x} (\overline{\tau_{xx_L}} + \overline{\tau_{xx_T}}) + \frac{\partial}{\partial y} (\overline{\tau_{xy_L}} + \overline{\tau_{xy_T}}). \end{aligned} \quad (\text{B.23})$$

And the final form of the time-averaged momentum equation in y -direction is reformulated in the following form:

$$\begin{aligned} \frac{\partial}{\partial t} (\overline{\rho v}) + \frac{\partial}{\partial x} (\overline{\rho u v}) + \frac{\partial}{\partial y} (\overline{\rho v^2} + \overline{P}) &= \frac{\partial}{\partial x} (\overline{\tau_{xy_L}} - \overline{\rho u'' v''}) + \frac{\partial}{\partial y} (\overline{\tau_{yy_L}} - \overline{\rho v''^2}) \\ &= \frac{\partial}{\partial x} (\overline{\tau_{xy_L}} + \overline{\tau_{xy_T}}) + \frac{\partial}{\partial y} (\overline{\tau_{yy_L}} + \overline{\tau_{yy_T}}) \end{aligned} \quad (\text{B.24})$$

$\overline{\rho u''^2}$, $\overline{\rho v''^2}$, and $\overline{\rho u'' v''}$ are considered the elements of the turbulent stress tensor ($\overline{\tau_{ij_T}}$), which is also known as “Reynolds stress tensor”. More detailed explanation for its modeling will be introduced in section **B.2.5**.

On the other side, the averaged derivatives of the velocity fluctuations in the averaged viscous stresses (i.e. $\overline{\tau_{xx_L}}$, $\overline{\tau_{yy_L}}$, and $\overline{\tau_{xy_L}}$), are neglected to the other terms according to equation (B.9), and the time averaged shear stresses can be written as follows:

$$\begin{aligned} \overline{\tau_{xx_L}} &\approx \mu_L \left[\frac{4}{3} \frac{\partial \tilde{u}}{\partial x} - \frac{2}{3} \frac{\partial \tilde{v}}{\partial y} \right], \\ \overline{\tau_{yy_L}} &\approx \mu_L \left[\frac{4}{3} \frac{\partial \tilde{v}}{\partial y} - \frac{2}{3} \frac{\partial \tilde{u}}{\partial x} \right], \\ \overline{\tau_{xy_L}} &\approx \mu_L \left[\frac{\partial \tilde{u}}{\partial y} + \frac{\partial \tilde{v}}{\partial x} \right]. \end{aligned} \quad (\text{B.25})$$

B.2.3 Reynolds Averaged Energy Equation for Planar 2D Flow

By flow variable decomposition in equation (B.16), we can rewrite the energy equation in the following form:

$$\begin{aligned}
 & \frac{\partial}{\partial t} \left[(\bar{\rho} + \rho') \left(\widetilde{E}_t + E_t'' \right) \right] + \frac{\partial}{\partial x} \left[(\bar{\rho} + \rho') \left(\widetilde{H}_t + H_t'' \right) (\widetilde{u} + u'') \right] + \\
 & + \frac{\partial}{\partial y} \left[(\bar{\rho} + \rho') \left(\widetilde{H}_t + H_t'' \right) (\widetilde{v} + v'') \right] = \\
 & = \frac{\partial}{\partial x} \left[\tau_{xx} (\widetilde{u} + u'') + \tau_{xy_L} (\widetilde{v} + v'') - q_{x_L} \right] + \\
 & + \frac{\partial}{\partial y} \left[\tau_{xy} (\widetilde{u} + u'') + \tau_{yy_L} (\widetilde{v} + v'') - q_{y_L} \right].
 \end{aligned} \tag{B.26}$$

Also, each of the diffusive heat fluxes (i.e. q_{x_L} and q_{y_L}) can be broken down into time-averaged and fluctuations terms, as follows:

$$\begin{aligned}
 q_{x_L} &= -k_L \frac{\partial}{\partial x} \left(\widetilde{T} + T'' \right) - \sum_{m=1}^{n_s} \left(\widetilde{h}_m + h_m'' \right) (\bar{\rho} + \rho'') \mathcal{D}_L \frac{\partial}{\partial x} \left(\widetilde{Y}_m + Y_m'' \right). \\
 q_{y_L} &= -k_L \frac{\partial}{\partial y} \left(\widetilde{T} + T'' \right) - \sum_{m=1}^{n_s} \left(\widetilde{h}_m + h_m'' \right) (\bar{\rho} + \rho'') \mathcal{D}_L \frac{\partial}{\partial y} \left(\widetilde{Y}_m + Y_m'' \right).
 \end{aligned} \tag{B.27}$$

By time-averaging of equation (B.26), and deleting the zero-valued time-averaged terms according to the rules presented in section B.1.

Reynolds averaged energy equation for planar 2D domain yields:

$$\begin{aligned}
 & \frac{\partial}{\partial t} \left(\bar{\rho} \widetilde{E}_t \right) + \frac{\partial}{\partial x} \left(\bar{\rho} \widetilde{H}_t \widetilde{u} \right) + \frac{\partial}{\partial y} \left(\bar{\rho} \widetilde{H}_t \widetilde{v} \right) = \\
 & = \frac{\partial}{\partial x} \left(\overline{\tau_{xx_L}} \widetilde{u} + \overline{\tau_{xy_L}} \widetilde{v} - \overline{q_{x_L}} - \overline{\rho H_t'' u''} \right) + \frac{\partial}{\partial y} \left(\overline{\tau_{xy_L}} \widetilde{u} + \overline{\tau_{yy_L}} \widetilde{v} - \overline{q_{y_L}} - \overline{\rho H_t'' v''} \right).
 \end{aligned} \tag{B.28}$$

The fluctuations terms can be cancelled in time averaged diffusive heat fluxes (i.e. $\overline{q_{x_L}}$ and $\overline{q_{y_L}}$) as follows:

$$\begin{aligned}
 \overline{q_{x_L}} &= -k_L \frac{\partial \widetilde{T}}{\partial x} - \sum_{m=1}^{n_s} \widetilde{h}_m \bar{\rho} \mathcal{D}_L \frac{\partial \widetilde{Y}_m}{\partial x}. \\
 \overline{q_{y_L}} &= -k_L \frac{\partial \widetilde{T}}{\partial y} - \sum_{m=1}^{n_s} \widetilde{h}_m \bar{\rho} \mathcal{D}_L \frac{\partial \widetilde{Y}_m}{\partial y}.
 \end{aligned} \tag{B.29}$$

B.2.4 Reynolds Averaged Individual Species Continuity Equation in Planar Two Dimensional Coordinates

Finally, the variables decomposition in equation (B.17) for the m^{th} species takes the following form:

$$\begin{aligned} \frac{\partial}{\partial t} \left[(\bar{\rho} + \rho') \left(\widetilde{Y}_m + Y_m'' \right) \right] + \frac{\partial}{\partial x} \left[(\bar{\rho} + \rho') \left(\widetilde{Y}_m + Y_m'' \right) (\widetilde{u} + u'') \right] + \\ + \frac{\partial}{\partial y} \left[(\bar{\rho} + \rho') \left(\widetilde{Y}_m + Y_m'' \right) (\widetilde{v} + v'') \right] = \dot{\omega}_m - \frac{\partial}{\partial x} \left(d_{mx_L} \right) - \frac{\partial}{\partial y} \left(d_{my_L} \right). \end{aligned} \quad (\text{B.30})$$

The diffusive mass flux in x and y directions can be written as follows:

$$\begin{aligned} d_{mx_L} &= -(\bar{\rho} + \rho') \mathcal{D}_L \frac{\partial}{\partial x} \left(\widetilde{Y}_m + Y_m'' \right). \\ d_{my_L} &= -(\bar{\rho} + \rho') \mathcal{D}_L \frac{\partial}{\partial y} \left(\widetilde{Y}_m + Y_m'' \right). \end{aligned} \quad (\text{B.31})$$

The time-averaged form of equation (B.18) will be written as:

$$\begin{aligned} \frac{\partial}{\partial t} \left(\overline{\rho \widetilde{Y}_m} \right) + \frac{\partial}{\partial x} \left(\overline{\rho \widetilde{Y}_m \widetilde{u}} \right) + \frac{\partial}{\partial y} \left(\overline{\rho \widetilde{Y}_m \widetilde{v}} \right) = \\ = \overline{\dot{\omega}_m} - \frac{\partial}{\partial x} \left(\overline{d_{mx_L}} + \overline{\rho Y_m'' u''} \right) - \frac{\partial}{\partial y} \left(\overline{d_{my_L}} + \overline{\rho Y_m'' v''} \right). \end{aligned} \quad (\text{B.32})$$

The time averaged mass diffusive fluxes can be approximated to be:

$$\begin{aligned} \overline{d_{mx_L}} &= -\bar{\rho} \mathcal{D}_L \frac{\partial \widetilde{Y}_m}{\partial x}, \\ \overline{d_{my_L}} &= -\bar{\rho} \mathcal{D}_L \frac{\partial \widetilde{Y}_m}{\partial y}. \end{aligned} \quad (\text{B.33})$$

B.2.5 Modeling of Reynolds Stresses

Boussinesq [7] suggested reformulation of Reynolds stresses “or turbulent shearing stresses” in terms of the spatial gradients of the time-averaged velocities, in addition to turbulent eddy coefficient (μ_T), which represents the turbulence effects on momentum transfer. By neglecting the turbulent kinetic energy, the Reynolds stress tensor

can be written in index notation as follows:

$$\overline{\rho u_i'' u_j''} = \mu_T \left[\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial \tilde{u}_k}{\partial x_k} \right] \quad (\text{B.34})$$

Thus, the Reynolds stress tensor elements in Cartesian 2D coordinates are written as follows:

$$\begin{aligned} \overline{\rho u''^2} &= \overline{\tau_{xx_T}} = \mu_T \left[\frac{4}{3} \frac{\partial \tilde{u}}{\partial x} - \frac{2}{3} \frac{\partial \tilde{v}}{\partial y} \right], \\ \overline{\rho v''^2} &= \overline{\tau_{yy_T}} = \mu_T \left[\frac{4}{3} \frac{\partial \tilde{v}}{\partial y} - \frac{2}{3} \frac{\partial \tilde{u}}{\partial x} \right], \\ \overline{\rho u'' v''} &= \overline{\tau_{xy_T}} = \mu_T \left[\frac{\partial \tilde{u}}{\partial y} + \frac{\partial \tilde{v}}{\partial x} \right]. \end{aligned} \quad (\text{B.35})$$

B.2.6 Modeling of the Total Heat and Mass Fluxes for Turbulent Flows

As shown in equation (B.28) and (B.32), we have other extra terms representing the turbulence effects on heat and mass transfer. These extra terms are simply represented in the turbulent heat flux vector $(\overline{\rho H_t'' u_i''})$, and the turbulent mass flux vector $(\overline{\rho Y_m'' u_i''})$.

The fluctuations term of the total enthalpy is the difference between the total enthalpy and the weighted time-averaged total enthalpy, which consists of three terms: the weighted averaged mixture enthalpy $(\tilde{h})$, the weighted averaged kinetic energy $(\frac{1}{2} \tilde{u}_k \tilde{u}_k)$, and finally the turbulent kinetic energy $(\frac{1}{2} \overline{u_k'' u_k''})$, which is not considered in this study because of applying an algebraic approach to model turbulent eddy coefficient. The fluctuations in total enthalpy magnitude can be written down in index notation as follows:

$$\begin{aligned} H_t'' &= H_t - \tilde{H}_t \\ &= \left[\left(\tilde{h} + h'' \right) + \frac{1}{2} (\tilde{u}_k + u_k'') (\tilde{u}_k + u_k'') \right] - \left[\tilde{h} + \frac{1}{2} \tilde{u}_k \tilde{u}_k \right] \\ &= h'' + u_k'' \tilde{u}_k + \frac{1}{2} u_k'' u_k''. \end{aligned}$$

So, the turbulent heat flux ($\overline{\rho H_t'' u_i''}$) is expressed as follows:

$$\begin{aligned}\overline{\rho H_t'' u_i''} &= \overline{\rho h'' u_i''} + \overline{\rho u_i'' u_k''} \tilde{u}_k + \overline{\rho u_i'' u_k''} \tilde{u}_k \\ &= \overline{\rho h'' u_i''} + \overline{\rho u_i'' u_k''} \tilde{u}_k.\end{aligned}\quad (\text{B.36})$$

As shown in equation (B.36), we eliminate the time averaged term for the product of three fluctuated variables, according to the assumption set in appendix **B**. Thus, from equations (B.34) and (B.36), we can write the turbulent heat flux for 2D coordinates as follows:

$$\begin{aligned}\overline{\rho H_t'' u''} &= \overline{\rho h'' u''} + \overline{\tau_{xx_T}} \tilde{u} + \overline{\tau_{xy_T}} \tilde{v}. \\ \overline{\rho H_t'' v''} &= \overline{\rho h'' v''} + \overline{\tau_{xy_T}} \tilde{u} + \overline{\tau_{yy_T}} \tilde{v}.\end{aligned}\quad (\text{B.37})$$

It is suggested model the turbulent terms ($\overline{\rho h'' u''}$) and ($\overline{\rho h'' v''}$) in terms of the spatial derivatives of weighed time-averaged specific enthalpy and the dynamic turbulent viscosity (μ_T), where the Prandtl number for turbulent terms (Pr_T) is suggested to be constant:

$$\begin{aligned}\overline{\rho h'' u''} &= \overline{q_{x_T}} = -\frac{\mu_T}{Pr_T} \frac{\partial \tilde{h}}{\partial x}, \\ \overline{\rho h'' v''} &= \overline{q_{y_T}} = -\frac{\mu_T}{Pr_T} \frac{\partial \tilde{h}}{\partial y}.\end{aligned}\quad (\text{B.38})$$

In like manner, the turbulent mass flux ($\overline{\rho Y_m'' u''}$) of the m^{th} species, can be expressed in terms of the spatial gradients of its weighted time-averaged mass fraction and dynamic turbulent viscosity, assuming the turbulent Schmidt number (Sc_T) is constant as recommended in several references:

$$\begin{aligned}\overline{\rho Y_m'' u''} &= \overline{d_{mx_T}} = -\frac{\mu_T}{Sc_T} \frac{\partial \tilde{Y}_m}{\partial x}, \\ \overline{\rho Y_m'' v''} &= \overline{d_{my_T}} = -\frac{\mu_T}{Sc_T} \frac{\partial \tilde{Y}_m}{\partial y}.\end{aligned}\quad (\text{B.39})$$

Appendix C

Basic Equations of Fluid Dynamics in Orthogonal Curvilinear Coordinates

As mentioned in reference [59], we can derive the Navier-Stokes equations for a general orthogonal curvilinear coordinate system by using some transformation equations relating between the orthogonal curvilinear coordinates (x_1, x_2, x_3) , and the Cartesian coordinates (x, y, z) , as:

$$x_1 = x_1(x, y, z), \quad x_2 = x_2(x, y, z), \quad x_3 = x_3(x, y, z). \quad (\text{C.1})$$

And the infinitesimal length in the domain can be expressed in terms of the both coordinates systems as:

$$(ds)^2 = (dx)^2 + (dy)^2 + (dz)^2 = (h_1 dx_1)^2 + (h_2 dx_2)^2 + (h_3 dx_3)^2 \quad (\text{C.2})$$

where:

$$\begin{aligned}
(h_1)^2 &= \left(\frac{\partial x}{\partial x_1} \right)^2 + \left(\frac{\partial y}{\partial x_1} \right)^2 + \left(\frac{\partial z}{\partial x_1} \right)^2 \\
(h_2)^2 &= \left(\frac{\partial x}{\partial x_2} \right)^2 + \left(\frac{\partial y}{\partial x_2} \right)^2 + \left(\frac{\partial z}{\partial x_2} \right)^2 \\
(h_3)^2 &= \left(\frac{\partial x}{\partial x_3} \right)^2 + \left(\frac{\partial y}{\partial x_3} \right)^2 + \left(\frac{\partial z}{\partial x_3} \right)^2 .
\end{aligned} \tag{C.3}$$

Some basics to write the fluid dynamics fundamental equations in any orthogonal coordinate system, are presented below:

C.1 Gradient of a Scalar Quantity

The gradient of a scalar quantity in orthogonal curvilinear coordinates is written as follows:

$$\vec{\nabla} f = \frac{1}{h_1} \frac{\partial f}{\partial x_1} \vec{i}_1 + \frac{1}{h_2} \frac{\partial f}{\partial x_2} \vec{i}_2 + \frac{1}{h_3} \frac{\partial f}{\partial x_3} \vec{i}_3 . \tag{C.4}$$

C.2 Laplacian Operator of a Scalar Quantity in Orthogonal Curvilinear Coordinates

For as scalar quantity f , its Laplacian Operator can be in terms of its spatial derivatives as follows:

$$\nabla^2 f = \frac{1}{h_1 h_2 h_3} \left(\frac{\partial}{\partial x_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial f}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left(\frac{h_1 h_3}{h_2} \frac{\partial f}{\partial x_2} \right) + \frac{\partial}{\partial x_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial f}{\partial x_3} \right) \right) . \tag{C.5}$$

C.3 Divergence of a Vector

Divergence of a Vector in Orthogonal Curvilinear Coordinates is expressed by the following equation:

$$\vec{\nabla} \cdot \vec{A} = \frac{1}{h_1 h_2 h_3} \left(\frac{\partial}{\partial x_1} (h_2 h_3 A_1) + \frac{\partial}{\partial x_2} (h_1 h_3 A_2) + \frac{\partial}{\partial x_3} (h_1 h_2 A_3) \right). \quad (\text{C.6})$$

C.4 Shear Stress Tensor

Shear Stress Tensor in orthogonal curvilinear coordinates is written as:

$$\begin{aligned} \tau_{x_1 x_1} &= \frac{2}{3} \mu (2e_{x_1 x_1} - e_{x_2 x_2} - e_{x_3 x_3}), \\ \tau_{x_2 x_2} &= \frac{2}{3} \mu (2e_{x_2 x_2} - e_{x_1 x_1} - e_{x_3 x_3}), \\ \tau_{x_3 x_3} &= \frac{2}{3} \mu (2e_{x_3 x_3} - e_{x_1 x_1} - e_{x_2 x_2}), \\ \tau_{x_1 x_2} &= \frac{2}{3} \mu e_{x_1 x_2}, \quad \tau_{x_2 x_3} = \frac{2}{3} \mu e_{x_2 x_3}, \quad \tau_{x_1 x_3} = \frac{2}{3} \mu e_{x_1 x_3}. \end{aligned} \quad (\text{C.7})$$

where:

$$\begin{aligned}
e_{x_1x_1} &= \frac{1}{h_1} \frac{\partial u_1}{\partial x_1} + \frac{u_2}{h_1 h_2} \frac{\partial h_1}{\partial x_2} + \frac{u_3}{h_1 h_3} \frac{\partial h_1}{\partial x_3}, \\
e_{x_2x_2} &= \frac{1}{h_2} \frac{\partial u_2}{\partial x_2} + \frac{u_1}{h_2 h_1} \frac{\partial h_2}{\partial x_1} + \frac{u_3}{h_2 h_3} \frac{\partial h_2}{\partial x_3}, \\
e_{x_3x_3} &= \frac{1}{h_3} \frac{\partial u_3}{\partial x_3} + \frac{u_1}{h_3 h_1} \frac{\partial h_3}{\partial x_1} + \frac{u_2}{h_3 h_2} \frac{\partial h_3}{\partial x_2}, \\
e_{x_1x_2} &= \frac{h_2}{h_1} \frac{\partial}{\partial x_1} \left(\frac{u_2}{h_2} \right) + \frac{h_1}{h_2} \frac{\partial}{\partial x_2} \left(\frac{u_1}{h_1} \right), \\
e_{x_2x_3} &= \frac{h_3}{h_2} \frac{\partial}{\partial x_2} \left(\frac{u_3}{h_3} \right) + \frac{h_2}{h_3} \frac{\partial}{\partial x_3} \left(\frac{u_2}{h_2} \right), \\
e_{x_1x_3} &= \frac{h_3}{h_1} \frac{\partial}{\partial x_1} \left(\frac{u_3}{h_3} \right) + \frac{h_1}{h_3} \frac{\partial}{\partial x_3} \left(\frac{u_1}{h_1} \right).
\end{aligned} \tag{C.8}$$

C.5 Gradient of the Shear Stress Tensor

The component of the gradient of the shear stress tensor in any orthogonal curvilinear coordinates, can be written as follows:

- $\vec{\nabla} \cdot [\tau]$ component in the x_1 direction

$$\begin{aligned}
\vec{\nabla} \cdot [\tau] \cdot \vec{i}_1 &= \\
&= \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial x_1} (h_2 h_3 \tau_{x_1 x_1}) + \frac{\partial}{\partial x_2} (h_1 h_3 \tau_{x_1 x_2}) + \frac{\partial}{\partial x_3} (h_1 h_2 \tau_{x_1 x_3}) \right] + \\
&+ \tau_{x_1 x_2} \frac{1}{h_1 h_2} \frac{\partial h_1}{\partial x_2} + \tau_{x_1 x_3} \frac{1}{h_1 h_3} \frac{\partial h_1}{\partial x_3} - \tau_{x_2 x_2} \frac{1}{h_1 h_2} \frac{\partial h_2}{\partial x_1} - \tau_{x_3 x_3} \frac{1}{h_1 h_3} \frac{\partial h_3}{\partial x_1}
\end{aligned} \tag{C.9}$$

- $\vec{\nabla} \cdot [\tau]$ component in the x_2 direction

$$\begin{aligned} \vec{\nabla} \cdot [\tau] \cdot \vec{i}_2 &= \\ &= \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial x_1} (h_2 h_3 \tau_{x_1 x_2}) + \frac{\partial}{\partial x_2} (h_1 h_3 \tau_{x_2 x_2}) + \frac{\partial}{\partial x_3} (h_1 h_2 \tau_{x_2 x_3}) \right] + \\ &+ \tau_{x_2 x_3} \frac{1}{h_2 h_3} \frac{\partial h_2}{\partial x_3} + \tau_{x_1 x_2} \frac{1}{h_1 h_2} \frac{\partial h_2}{\partial x_1} - \tau_{x_3 x_3} \frac{1}{h_2 h_3} \frac{\partial h_3}{\partial x_2} - \tau_{x_1 x_1} \frac{1}{h_2 h_1} \frac{\partial h_1}{\partial x_2} \end{aligned} \quad (\text{C.10})$$

- $\vec{\nabla} \cdot [\tau]$ component in the x_3 direction

$$\begin{aligned} \vec{\nabla} \cdot [\tau] \cdot \vec{i}_3 &= \\ &= \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial x_1} (h_2 h_3 \tau_{x_1 x_3}) + \frac{\partial}{\partial x_2} (h_1 h_3 \tau_{x_2 x_3}) + \frac{\partial}{\partial x_3} (h_1 h_2 \tau_{x_3 x_3}) \right] + \\ &+ \tau_{x_1 x_3} \frac{1}{h_1 h_3} \frac{\partial h_3}{\partial x_1} + \tau_{x_2 x_3} \frac{1}{h_2 h_3} \frac{\partial h_3}{\partial x_1} - \tau_{x_1 x_1} \frac{1}{h_1 h_3} \frac{\partial h_1}{\partial x_3} - \tau_{x_2 x_2} \frac{1}{h_2 h_3} \frac{\partial h_2}{\partial x_3} \end{aligned} \quad (\text{C.11})$$

C.6 The Transformation Functions from Cartesian to Planar 2-D and Axisymmetric Coordinates

In the two dimensional and axisymmetric coordinates, the axes (x_1, x_2, x_3) are defined in terms of the cartesian coordinates as follows:

$$x_1 = x, \quad x_2 = y, \quad x_3 = \theta^\alpha. \quad (\text{C.12})$$

$$\alpha = \begin{cases} 0, & \text{for Two Dimensional Flow.} \\ 1, & \text{for Axisymmetric Flow.} \end{cases} \quad (\text{C.13})$$

We have to mention that the above definition for the axisymmetric axes, is valid only if for internal flows without any immersed body (e.g. axisymmetric nozzles). This makes the utilized equations becomes much more simplified than that when the more general case

is used. Also, it is sufficient for the recently studied test cases. The transformation coefficients for this case are:

$$h_1 = 1, \quad h_2 = 1, \quad h_3 = y^\alpha. \quad (\text{C.14})$$

And the velocities are written as:

$$u_1 = u, \quad u_2 = v, \quad u_3 = \alpha w. \quad (\text{C.15})$$

To satisfy the axisymmetric condition, any property variation along the rotating angle around the flow axis is equal to zero:

$$\frac{\partial f}{\partial \theta} = 0. \quad (\text{C.16})$$

Appendix D

Thermodynamic Properties for Different Species

The specific heat coefficient $c_p [J/kg.K]$ of different species (O_2 , H_2O , H_2 , OH , N_2), and their enthalpies are calculated as polynomials of fifth order as a function of temperature $T[K]$ as presented in the following equations:

$$\begin{aligned} c_{p_m} &= a_{1_m} + a_{2_m}T + a_{3_m}T^2 + a_{4_m}T^3 + a_{5_m}T^4 \left[\frac{J}{kgK} \right] & (D.1) \\ h_m &= h_{f_m}^o + a_{1_m}T + \frac{1}{2}a_{2_m}T^2 + \frac{1}{3}a_{3_m}T^3 + \frac{1}{4}a_{4_m}T^4 + \frac{1}{5}a_{5_m}T^5 \left[\frac{J}{kg} \right] & (D.2) \end{aligned}$$

Where the polynomial coefficients and the heat of formation are given in table **D.1** according to McBride et al. [43].

Species Name	a_1 [J/kgK]	a_2 [J/kgK^2]
O ₂	9.5122068815×10^2	$1.7314050440 \times 10^{-1}$
H ₂ O	1.2365684095×10^3	1.3733629147
H ₂	1.2192656305×10^4	3.4364159708
OH	1.3883483970×10^3	$5.415507055 \times 10^{-1}$
N ₂	8.7678667013×10^2	$4.1480463533 \times 10^{-1}$
Species Name	a_3 [J/kgK^3]	a_4 [J/kgK^4]
O ₂	$-3.66746062920 \times 10^{-5}$	$5.37318477325 \times 10^{-9}$
H ₂ O	$-3.57417115973 \times 10^{-4}$	$4.36204855594 \times 10^{-8}$
H ₂	$-6.08631107179 \times 10^{-4}$	$6.40633717453 \times 10^{-8}$
OH	$-1.4375035792 \times 10^{-4}$	$2.05722370687 \times 10^{-8}$
N ₂	$-1.46285221244 \times 10^{-4}$	$2.33402971301 \times 10^{-8}$
Species Name	a_5 [J/kgK^5]	h_f^o [J/kg]
O ₂	$-3.37551156405 \times 10^{-14}$	-316204.9196
H ₂ O	$-1.97192667978 \times 10^{-12}$	-13804792.4445
H ₂	$-2.86353222493 \times 10^{-12}$	-3380116.9531
OH	$-1.18442053849 \times 10^{-13}$	1928948.65241
N ₂	$-1.36819647016 \times 10^{-13}$	-274363.2506

Table D.1: Coefficient of the fifth order polynomial of $c_p[J/kgK]$ as a function of $T[K]$ of different species and their heat of formation at $0^\circ[K]$

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