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# Numerical Simulation and Validation for High Speed Turbulent Chemically Reacting Flows

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Mohammed Kamel, Farouk Owis\*, Moumen Idres, Ali Hashem

Aerospace Engineering Department, Faculty of Engineering,  
Cairo University,  
Giza, Egypt

Email: mkamel@eng.cu.edu.eg

Email: fowis@eng.cu.edu.eg (\*Corresponding Author)

Email: midres@yahoo.com

Email: aafhashem@eng.cu.edu.eg

**Abstract** Mixing and combustion processes in 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 future 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.

**Keywords:** Scramjet Engines; Computational Fluid Dynamics; Chemically-Reacting Flows; Reynolds-Averaged Navier-Stocks; Turbulent Flows; Supersonic Combustion

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## 1 Introduction

Chemically-reacting flows are of interest across a wide range of engineering applications including supersonic combustion, space vehicle reentry, and rocket plume problems. Therefore, a great amount of effort has been focused in the areas of algorithm development and thermo-chemical modeling for these flows. An example of the important numerical simulation problems of high-speed chemically-reacting flows is the phenomenon of air-fuel mixing and flame-stabilization inside supersonic combustion ramjet engines (SCRamjets). Flame-holding

and stabilization in the supersonic flow-field are 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. In this study, we will study the first mentioned technique. A shock is induced due to the transverse sonic fuel injection into the supersonic air inlet flow, as shown in figure (1). It is one of the most efficient techniques suggested to enhance both air-fuel mixing and flame holding, as introduced by Drummond (1).

Better understanding of the flow features shown in figure(1) enables us to enhance the air-fuel mixing and flame stabilization. The air flow is decelerated by the high pressure gradient within the region of the sonic fuel injection. Then, a separation shock is formed and followed by a strong bow shock. The air diffuses into the injected fuel through the mixing layer. Examining the injection zone reveals that there is a barrel-shaped stream-tube surrounded by jet shocks. The injected fuel is accelerated to a supersonic speed and then choked at a circular plan known as *Mach Disk*. The separation shock creates a low-speed and high-temperature recirculation zone upstream the injection zone. That plays a great role in air-fuel mixing and flame holding processes.

Different features of these turbulent flows, which are generally modeled using unsteady Navier-Stokes equations, can be resolved by time-averaging approaches such as Reynolds averaged Navier-Stokes equations (RANS), or by space-averaging approaches such as Large Eddy Simulation (LES). On the other hand, Direct Numerical Simulation (DNS) considers all flow features with all the time and length scales to be resolved. Despite the shortcomings associated with the statistical representation of time-averaging RANS closures, RANS equations still show efficiency in most test cases. As, it requires much less computational effort than that required by LES or DNS approaches (4; 5). The mathematical model used in the current simulation is the unsteady Reynolds-Averaged Navier-Stokes equations (URANS). The turbulence model used is based on Boussineq's assumption, where an Baldwin-Lomax algebraic model (6) determines the eddy viscosity term. Although algebraic models are simple and robust, they give inaccurate estimations in strong flow separations (7). Therefore, their implementation needs some modifications in these flowfields.

In the coupled governing equations of chemically-reacting flows inside supersonic combustors, the order of magnitude of characteristic time of the chemical reactions is much less than that of flow residence time. The equations becomes stiff because the great gap between the time scales of the system of equations. Full implicit treatment for the governing equations for two-dimensional flows leads to solve simultaneous equations in pent-block diagonal matrix form. It is found that the iterative method of Lower-Upper Symmetric Gauss-Siedel (LUSGS) method (8) shows the fastest convergence

rates for implicit solvers. To minimize the expenses of the flow Jacobians inversion, we treat the flow fluxes explicitly, and solve the chemical source term only implicitly. This method is well-known as Chemistry-Implicit or Point-Implicit, which is first introduced by Curtiss et al. (9).

The main objective of the current study is to develop and validate an accurate computational code for the simulation of turbulent and chemically reacting flows. This work is motivated by the need to simulate the flowfields inside a typical supersonic combustion ramjet (SCRAMJET) engine. A comprehensive set of validation several test cases are presented in order to monitor the accuracy and robustness of the numerical solver, for two-dimensional chemically reacting supersonic turbulent flows, before any extension to three-dimensional flow simulations.

## 2 Mathematical Modeling

### 2.1 Governing Equations

The governing Equations are the Reynolds time averaging Navier Stocks equations. The conservative non-dimensional vector form of RANS equations for two-dimensional flow is written as follows:

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \alpha H = \frac{\partial E_v}{\partial x} + \frac{\partial F_v}{\partial y} + \alpha H_v + S(1)$$

where,  $Q$  is the vector of the conservative variables,  $E$  and  $F$  are the convective fluxes, and  $E_v$  and  $F_v$  are the diffusive fluxes. Besides,  $\alpha$  is a logical switch between planar and axisymmetric flows. In addition,  $H$  and  $H_v$  are the inviscid and viscous axisymmetric terms respectively. Finally,  $S$  represents the chemical source term:

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E_t \\ \rho Y_m \end{bmatrix}, E = \begin{bmatrix} \rho u \\ \rho u^2 + P \\ \rho uv \\ \rho H_t u \\ \rho Y_m u \end{bmatrix}, F = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + P \\ \rho H_t v \\ \rho Y_m v \end{bmatrix}, (2)$$

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

$$\alpha = \begin{cases} 0, & \text{Planar 2D Flow} \\ 1, & \text{Axisymmetric 2D Flow} \end{cases}, H = \frac{1}{y} \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 \\ \rho H_t v \\ \rho Y_m v \end{bmatrix},$$

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

$$S = [0, 0, 0, 0, \dot{\omega}_m].$$

The variables are normalized with respect to reference length, density, velocity, and temperature of the problem. (i.e.  $L_{ref}$ ,  $\rho_{ref}$ ,  $V_{ref}$ ,  $T_{ref}$ ).

### 2.1.1 Thermodynamic Model

The total mixture enthalpy ( $H_t$ ) and total internal energy ( $E_t$ ) are described as follows:

$$H_t = \frac{h_{f_{mix}}^o + \int_{T_o}^{T^*} c_{p_{mix}} d\tau + \frac{(u^2 + v^2)}{2}}{V_{ref}^2}, \quad (3)$$

$$E_t = H_t - \frac{R_{mix}(T^* - T_o)}{V_{ref}^2}$$

where:  $T^* = T.T_{ref}$ .  $h_{f_{mix}}^o$ ,  $c_{p_{mix}}$ , and  $R_{mix}$  are the mixture's heat of formation, heat coefficient at constant temperature, and gas constant, respectively. They are calculated by weighted summation of the individual species. We assume that specific heat coefficient for each species " $m$ " ( $c_{p_m}$ ) is a polynomial function in temperature ( $T$ ) as given by McBride et al. (22). The "equivalent" heat specific ratio ( $\gamma$ ) of the multi-species mixture is discussed by Shuen and Yoon (13). It is the ratio of the mixture sensible enthalpy ( $h_s$ ) to the mixture sensible internal energy ( $e_s$ ):  $\gamma = h_s/e_s = (h - h_{f_{mix}}^o)/(e - h_{f_{mix}}^o)$

### 2.1.2 Viscous Stress Tensor Modeling

$\tau_{xx_p}$  and  $\tau_{yy_p}$  are the longitudinal viscous shear stress in planar 2D coordinates.  $\tau_a$  represents the additional term for each of  $\tau_{xx}$  and  $\tau_{yy}$  in case of axisymmetric 2D flows.  $\tau_{\theta\theta}$  is the last diagonal element for axisymmetric 2D flows. ( $\tau_{xy}$ ) is the off-diagonal element in the stress tensor. These terms are expressed as follows:

$$\begin{aligned} \tau_{xx_p} &= \frac{1}{Re_{ref}} \mu \left[ \frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right], \\ \tau_{yy_p} &= \frac{1}{Re_{ref}} \mu \left[ \frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} \right], \\ \tau_{xy} &= \frac{1}{Re_{ref}} \mu \left[ \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \right], \\ \tau_a &= -\frac{2}{3} \frac{1}{Re_{ref}} \left( \frac{v}{y} \right), \\ \tau_{\theta\theta} &= \frac{1}{Re_{ref}} \mu \left[ \frac{4}{3} \frac{v}{y} - \frac{2}{3} \left( \frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) \right]. \end{aligned} \quad (4)$$

$Re_{ref}$  is the reference "Reynolds number".  $\mu$  is the summation of the molecular and turbulent eddy viscosity coefficients, i.e.  $\mu = \mu_L + \mu_T$ . The molecular viscosity coefficient is assumed to equal to the dominate Nitrogen's dynamic viscosity, which is calculated by Sutherland's equation as shown by Chitsomboon and Tiwari (17):  $\mu_L = \left[ (1.458 \times 10^{-6}) T^{* \frac{3}{2}} \right] / [T^* + 110.4]$

### 2.2 Turbulent Dynamic Viscosity Modeling

Algebraic Baldwin-Lomax turbulence model is a two-layer turbulence model; where the turbulent dynamic viscosity coefficient ( $\mu_T$ ) is calculated with one of two different sets of algebraic equations. And that depends on the distance ( $n$ ) from boundary walls, or jets centerlines.

$$\mu_T = \begin{cases} \mu_{T_{in}}, & n \leq n_{cross} \\ \mu_{T_{out}}, & n > n_{cross} \end{cases}. \quad (5)$$

( $n_{cross}$ ) is the minimum distance, at which the eddy viscosity coefficients for both the inner and outer regions, i.e. ( $\mu_{T_{in}}$  and  $\mu_{T_{out}}$ ) match. In the inner region, eddy viscosity coefficient ( $\mu_{T_{in}}$ ) is calculated in terms of the mixing length ( $l_{mix}$ ), and the vorticity vector magnitude ( $\omega$ ) as follows,

$$\begin{aligned} \mu_{T_{in}} &= \rho l_{mix}^2 \omega, \\ \omega &= \sqrt{\left[ \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right]^2}, \end{aligned} \quad (6)$$

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

$n^+$  is the wall distance in wall units. The damping factor ( $e^{-n^+/A^+}$ ) is eliminated for the cases of wakes and jets. The eddy viscosity of the outer layer ( $\mu_{T_{out}}$ ) is calculated as follows,

$$\begin{aligned} \mu_{T_{out}} &= \rho K C_{cp} F_{wake} F_{Klep}, \\ F_{wake} &= \min \left( n_{max} F_{max}, C_{wk} n_{max} \frac{u_{diff}^2}{F_{max}} \right), \\ F_{Kleb} &= \left[ 1 + 5.5 \left( \frac{n C_{Kleb}}{n_{max}} \right)^6 \right]^{-1}, \end{aligned} \quad (7)$$

where ( $u_{diff}$ ) is the difference between the maximum and minimum velocity magnitudes in the boundary layer. Besides, ( $F_{max}$ ) is the max value of the intermediate function  $F(n)$  along a certain line normal

to the wall or the centerline of the jet. This function is written as follows,

$$F(n) = \frac{1}{\kappa} l_{mix} \omega, \quad (8)$$

$$F_{max} = \max_n [F(n)], \quad n_{max} = n|_{F_{max}}.$$

As explained above,  $n_{max}$  is the normal distance ( $n$ ) at which the function ( $F$ ) reaches its global maximum value. This turbulence approach consists of six closure constants:  $A^+ = 26$ ,  $C_{cp} = 1.6$ ,  $C_{Kleb} = 0.3$ ,  $C_{wk} = 0.25$ ,  $\kappa = 0.4$ , and  $K = 0.0168$ . 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 (7), added some modifications to the previous model to eliminate the reasons leading to the model deficiency when used in separated flows. They found that  $F_{max}$  should be the *nearest local maximum* of  $F(n)$  to the wall surface, and not to be the global maximum.

### 2.3 Mass and Heat Fluxes Modeling

The diffusive mass flux of the  $m^{th}$  species in the  $x_i$  direction is notated by  $d_{mx_i}$ . And the diffusive heat flux in  $x_i$  direction is represented by  $q_{x_i}$ , where  $i = 1, 2$  and  $x_{1,2} = x, y$ . These fluxes are written as below:

$$d_{mx_i} = \frac{-1}{Re_{ref} Sc_{ref}} \left( \rho \mathcal{D}_L + \frac{\mu_T}{Sc_T} Sc_{ref} \right) \frac{\partial Y_m}{\partial x_i},$$

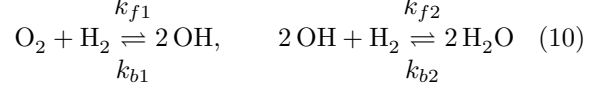
$$q_{x_i} = \frac{1}{Re_{ref}} \left[ \frac{-1}{(\gamma_{ref}-1) M_{ref}^2 Pr_{ref}} k_L \frac{\partial T}{\partial x_i} - \frac{1}{Sc_{ref}} \sum_{m=1}^{n_s} h_m \rho \mathcal{D}_L \frac{\partial Y_m}{\partial x_i} - \frac{\mu_T}{Pr_T} \frac{\partial h}{\partial x_i} \right] \quad (9)$$

$\mathcal{D}_L$  is the laminar mass diffusivity coefficient of  $m^{th}$  species into the mixture. It is set constant for all species. In addition,  $Sc_{ref}$ ,  $M_{ref}$  and  $Pr_{ref}$  are the reference “Schmidt number”, “Mach number” and “Prandtl number”, respectively. The turbulent “Schmidt number” ( $Sc_T$ ) and “Prandtl number” ( $Pr_T$ ) are set to be 0.9. Modeling of mass and heat diffusive transport coefficients (i.e.  $\mathcal{D}_L$  and  $k_L$ ) is based on assuming constant values of the laminar terms of “Prandtl number” ( $Pr_L = 0.72$ ) and “Lewis number” ( $Le = 1$ ).

### 2.4 Chemistry Modeling

Regards to the flow-chemistry modeling, we calculate the species production rates based on the laminar-chemistry assumption, where the chemical source term is evaluated based on mean flow properties. So, the flow chemistry and turbulence are

decoupled. The chemically reacting non-equilibrium system is modeled using a mechanism composed of a number of elementary reactions of finite rates. Air-Hydrogen combustion system is modeled in this study by using the two-reactions four-species mechanism suggested by Rogers and Chinitz (12):



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,

$$\dot{\omega}_m = \frac{L_{ref}}{\rho_{ref} V_{ref}} \mathcal{M}_m \sum_{r=1}^{n_r} \left[ \begin{aligned} & (\nu'_{m,r} - \nu''_{m,r}) * \\ & * \left( k_{fr} \prod_{m=1}^{n_s} \left( \frac{\rho Y_m}{\mathcal{M}_m} \right)^{\nu'_{m,r}} + \right. \\ & \left. - k_{br} \prod_{m=1}^{n_s} \left( \frac{\rho Y_m}{\mathcal{M}_m} \right)^{\nu''_{m,r}} \right) \end{aligned} \right] \quad (11)$$

where ( $\nu'$ ) and ( $\nu''$ ) 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.  $n_s$  is the total number of species in the chemical reactions mechanism. ( $k_f$ ) and ( $k_b$ ) are the chemical reaction rates in the forward and backward directions, respectively. The Arrhenius’ formula of the forward reaction rates and their pre-exponential coefficients for the two reactions are:

$$k_{f1} = \mathcal{A}_1 T^{-10} \exp \left( \frac{-4063.6485}{\mathcal{R} T^*} \right),$$

$$k_{f2} = \mathcal{A}_2 T^{-13} \exp \left( \frac{-35499.4988}{\mathcal{R} T^*} \right).$$

$$\mathcal{A}_1 = \left[ 8.917\phi + \frac{31.433}{\phi} - 28.95 \right] (10)^{44}, \quad (12)$$

$$\mathcal{A}_2 = \left[ 2 + \frac{1.333}{\phi} - 0.833\phi \right] (10)^{58}.$$

In equation (12), the units of the universal gas constant ( $\mathcal{R}$ ) is [ $kcal/kmole \ K$ ]. The units of pre-exponential coefficients are ( $m^3/kmol$ )/sec for the elementary reaction are functions of the equivalence ratio ( $\phi$ ) is the equivalence ratio, and units are .

### 2.5 Numerical Treatment

To simplify the discretized equations for structured meshes, it is recommended that all domain cells have equal unit spacing. So, we transform the governing equations from the physical ( $x - y$ ) domain to the generalized ( $\xi - \eta$ ) domain, where the variables are denoted by (—). And, The spatial steps between

grid points are unity ( $\Delta\xi = \Delta\eta = 1$ ). The equations are solved by nodal-centered finite-volume scheme, where the mesh nodes represent the centroids of the control volumes. The fluxes are modeled at the cell faces: The discrete integral vector form of the governing equation in the computational domain for an individual cell is formulated as follows,

$$\begin{aligned} \frac{\bar{Q}_{i,j}^{n+1} - \bar{Q}_{i,j}^n}{\Delta t} = & -\frac{\bar{E}_{i+\frac{1}{2},j}^n - \bar{E}_{i-\frac{1}{2},j}^n}{\Delta\xi} - \frac{\bar{F}_{i,j+\frac{1}{2}}^n - \bar{F}_{i,j-\frac{1}{2}}^n}{\Delta\eta} \\ & + \frac{\bar{E}_{vi+\frac{1}{2},j}^n - \bar{E}_{vi-\frac{1}{2},j}^n}{\Delta\xi} + \frac{\bar{F}_{vi,j+\frac{1}{2}}^n - \bar{F}_{vi,j-\frac{1}{2}}^n}{\Delta\eta} \\ & - \alpha \bar{H}_{i,j}^n + \alpha \bar{H}_{vi,j}^n + \bar{S}_{i,j}^{n+1} \end{aligned} \quad (13)$$

In equation (13),  $\bar{E}_{i\pm\frac{1}{2},j}$  and  $\bar{F}_{i,j\pm\frac{1}{2}}$  are the convective fluxes at the cell faces in  $\xi$ -direction and  $\eta$ -direction, respectively. Roe's Flux-difference splitting scheme is used to estimate these fluxes. We use the extended version of Roe's scheme for chemically and thermally nonequilibrium multidimensional-flows presented by Walters et al. (11). The spatial accuracy of the flux-difference splitting scheme depends on the number of the surrounding mesh nodes whose flow properties are used to calculate the right and left sides fluxes at the cell interface (21). The solver applies Monotone Upstream-centered Schemes for Conservative Laws (MUSCL), where Total variation diminishing (TVD) are achieved by using minmode slope non-linear limiter. The utilized limiter overrides the numerical oscillations formed around the flow discontinuities caused by the dispersive nature of second order schemes, and saves the monotonicity of the solution to match the physical one. The diffusive fluxes  $\bar{E}_{vi\pm\frac{1}{2},j}$  and  $\bar{F}_{vi,j\pm\frac{1}{2}}$  are determined using central differencing.

The chemical source term ( $\bar{S}_{i,j}$ ) in equation (13) is the only term that is treated implicitly in the right hand side to solve the stiffness problem. Time linearization of second temporal accuracy is implemented to the chemical source term as shown the following equation, where ( $\bar{H}_{i,j}$ ) is the chemical source Jacobian in the computational domain. By treating the source term implicitly, the time step taken in integration is no longer restricted by the chemical characteristic time. Applying point-implicit scheme leads to solve mono-block diagonal matrix for the system of equations. We simplify the

chemical Jacobian by assuming that source term is only dependent on the species concentrations:

$$\begin{aligned} \bar{S}_{i,j}^{n+1} &= \bar{S}_{i,j}^n + \left(\frac{\partial \bar{S}}{\partial \bar{Q}}\right)_{i,j} \left(\frac{\partial \bar{Q}}{\partial t}\right)_{i,j} \Delta t + \mathcal{O}\Delta t^2 \\ &= \bar{S}_{i,j}^n + \bar{H}_{i,j} \left(\bar{Q}_{i,j}^{n+1} - \bar{Q}_{i,j}^n\right) + \mathcal{O}\Delta t^2 \end{aligned} \quad (14)$$

Although the chemical source term is solved implicitly, the value of the CFL (Courant-Friedrichs-Lewy) number ( $\sigma$ ) should not exceed unity, due to the explicit treatment of the other flow terms. CFL number relates the integration time step and maximum convective flow Jacobian for turbulent reacting flows (14; 18). Runge-Kutta two-step second order temporal accurate is used in the current study for the time integration. The global minimum time step is used in the first iterations to ensure the solution stability. After that, the computational iterations use the time step based on the local flow variable to accelerate the solution convergence.

### 3 Results

#### 3.1 Viscous Air Flows over a Flat Plate

Viscous air flows over a flat plate with a zero angle of attack is first presented to evaluate the ability of the code to predict accurately viscous and turbulent momentum fluxes. The reference length is taken to be the plate length, which is unity ( $L_{ref} = 1$  [m]). The inlet Mach Number  $M_{in}$  is set to be 0.4. The problem is considered to be single-species flows (i.e.  $n_s = 1$ ). Besides, the air transport coefficients are assumed to be constants, i.e.  $\mu_L = 15 \times 10^{-6}$  [N.sec/m<sup>2</sup>] and  $k_L = 20 \times 10^{-3}$  [W/m.K].

##### 3.1.1 Laminar Flow Test Case

For the case of laminar air flow over a flat plate, Reynolds number is taken less than the transition limit ( $Re_{ref} = 4.3 \times 10^5$ ). The inlet flow variables are selected as follows:  $P_{in} = 4000$  [Pa],  $\rho_{in} = 0.04$  [kg/m<sup>3</sup>],  $u_{in} = 150$  [m/sec], and  $v_{in} = 0$  [m/sec]. The laminar flow is resolved using two mesh sizes  $51 \times 55$  and  $101 \times 55$ . The numerical solutions of streamwise velocity and wall skin friction ( $c_f$ ) equations is compared to the analytical solutions of Blasius laminar boundary-layer. The results of the velocity profiles at different stations match with that derived by Blasius equation, as shown in figure(2). In figure (3). the numerical calculations overestimate the local friction coefficient, especially near the leading edge. As the number of the streamwise mesh nodes increases, the results become very close to the analytical solution.

### 3.1.2 Turbulent Flow Test Case

For this problem, inlet Reynolds number is set as ( $Re = 5.4 \times 10^6$ ). The inlet conditions for turbulent flow case are:  $P_{in} = 50000$  [Pa],  $\rho_{in} = 0.5$  [kg/m<sup>3</sup>],  $u_{in} = 150$  [m/sec], and  $v_{in} = 0$  [m/sec]. The velocity profiles are plotted in wall units in figure(4). The numerical solutions at different stations coincides with the velocity profile of the analytical solution of the law of the wall. Also, the local skin friction coefficient for turbulent flow is compared to the solutions of the one fifth power law ( $c_f = 0.058/Re_x^{1/5}$ ) and White's law ( $c_f = 0.455/[\ln(0.06 Re_x)]^2$ ) as shown in figure (5). It is observed that the "fully turbulent log-law zone" increases downstream, as the boundary layer thickness increases and the friction velocity decreases in the downstream direction. In addition, It is clear that the local friction coefficient ( $c_f$ ) is overestimated by the numerical solver, especially at the leading edge.

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

The numerical code is used to solve inviscid premixed hydrogen-air chemically reacting flows with and without shocks. This case will validate the modeling of convective flow fluxes and chemical source terms. As shown in figure(6), the mixture equivalence ratio  $\phi$  is 0.29841. The other inlet conditions are given as follows:  $T_{in} = 1884.3$  [K],  $P_{in} = 0.8026 \times 10^5$  [Pa],  $u_{in} = 1245$  [m/sec] and  $v_{in} = 0$  [m/sec]. The length of the axisymmetric nozzle is considered to be 2 meters. The nozzle radius is a sinusoidal function of the streamwise as follows,  $r = 0.125L [1 + \sin(\frac{\pi x}{2L})]$ . Only half of the axisymmetric 2D domain is solved, where a symmetry condition is applied at the nozzle centerline. The nozzle walls is assumed to be adiabatic.

#### 3.2.1 Complete Expansion Test Case

The used mesh size in this case is  $(41 \times 11)$ . The numerical solution is presented and compared with the quasi one dimensional flow solution introduced by Drummond et al. (14) in figures (9-12). It is clear that the rapid rate of formation of the main product (i.e water) occurs approximately in one tenth of the nozzle length. Also, figure (9) illustrates steep rise in the Hydroxyl mass fraction ( $Y_{OH}$ ) at the inlet. That is because its characteristic time of formation is of order  $10^{-11}$  seconds. The species concentrations do not seem to be significantly changed in the

remaining part of the nozzle. That means the chemical equilibrium model could be enough to simulate this test case, which represents a typical 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 (12) and (11) show a rise in pressure and temperature. The temperature is raised just after an abrupt increase in OH mass fraction.

It is clear that there is semi-coincidence between the present and previous results for species mass fractions in figures (9)-(10). It is concluded that the chemical reactions rates is slightly higher at the nozzle centerline than that at the nozzle wall. However, it is observed that there is no significant change in the species concentration in the radial direction. In figure (11), the averaged solution of pressure matches with the quasi 1D solution (14). Also, it is shown that the maximum value of pressure is 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 as shown in figure (11). The 1D calculations of Drummond et al. (14) overestimates temperature along nozzle, as presented in figure (12). That is because of the difference in the calculations of the specific heat coefficient ( $c_p$ ) for the different species. The specific heat coefficients are calculated in the current work using fifth order polynomial functions given by McBride et al. (22). On the other hand, Drummond et al. (14) calculated them using linear functions.

#### 3.2.2 Over-Expansion Test Case

Imposing atmospheric back pressure, i.e ( $P_{out} = 101325$  [Pa]), forms a normal shock wave inside the nozzle. The used mesh size is  $(41 \times 11)$ . In figures(9-12)The present cross-sectional averaged solution are compared with the previous calculations of Grossman and Cinnella (10). The Hydroxyl sudden rise takes place in the region just after the flow inlet as shown in figure (9). This implies that the numerical results of Hydroxyl concentration, is greatly dependent on the mesh size, especially at the regions of combustion initiation. The shock wave contributes in accelerating the rate formation of Hydroxyl-group, while the water mass fraction ( $Y_{H_2O}$ ) seems to be unaffected except at the wall

surface. That indicates that water reaches its chemical equilibrium, and it is no longer sensitive to the static temperature increase provided by the normal shock wave. It is shown that variables discontinuity at the normal shock is not sharp, even though second order spatial accurate scheme is applied. That is because of two reasons: the first reason is the diffusive effect of minmode limiter. In addition, the normal shock wave takes the shape of the spherical shell as shown in figure(8). So, the location of flow discontinuity varies in the radial direction. It is observed that the averaged solution matches with the general trend of the 1D flow. We found that the flow discontinuity at the centerline is the closet to the shock wave of the previous calculation.

### 3.3 Turbulent Chemically Reacting Flows in a Ramped Duct

The numerical code is also used to solve turbulent premixed Hydrogen-air supersonic flow in a 2D ramped duct shown in figure (17). The duct walls are assumed to be adiabatic. The incoming flow is premixed hydrogen-air at stoichiometric ratio. The problem is solved for two different inlet temperatures (900 [K] and 1200 [K] ); below and above the ignition threshold which is equal to 1000 [K]. The other inlet conditions are described as follows:  $P_{in} = 101325 [Pa]$  and  $M_{in} = 4.0$ . For each of the two cases, three different mesh sizes will be utilized:  $31 \times 51$ ,  $61 \times 51$  and  $91 \times 51$ . The horizontal mesh lines are clustered near the lower and upper duct walls.

#### 3.3.1 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]). In figure(18), the variation of specific heat ratio show the zone of reaction initiation zones. The temperature rises after the oblique shock wave and in the viscous layers near upper and lower wall surfaces, to become high enough for combustion initiation. The formed oblique shock is considered as *detonation wave*, as it is responsible in the reaction excitation and sustainability. Figures (19)-(22) present the numerical solutions at the normal distance of 0.13 [cm] from the wall compared to the previous solutions of Chitsomboon et al. (19), and Shuen and Yoon (13). The present solutions are unsensitive to grid resolution. Also, there is qualitative and quantitative agreement between the current results and the previous solution of Chitsomboon et al. (19). In addition, the present solutions give

smooth rise in pressure across shock, due to the diffusive effect of TVD scheme. There is a good agreement between the current estimation of the temperature and the published results (19). It is clear 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. This is due to the poor estimation of Rogers and Chinitz model (12) as discussed by Chitsomboon et al. (17).

#### 3.3.2 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. That is shown in the gradual variation in the mixture specific heat ratio before the oblique shock and its steep change after it, as shown in figure(23). Figures (24)-(27) present the numerical solutions for three meshes a distance of 0.13 [cm] from the lower wall. The results are compared with the previous results of Yee and Shinn (24) and that of Shuen and Yoon (13). There is a sudden rise in Hydroxyl concentration at the duct inlet. The results of OH concentrations are greatly sensitive to the grid resolution at the duct inlet. However, there is a good agreement between the present solution and that of Yee and Shinn (24). In figure (26), the pressure solution of Shuen and Yoon (13) has non-physical oscillations after the shock. The present results and the results of Yee and Shinn (24) have no oscillation, due to the diffusive effect of the TVD schemes. In figure (27), there is about 20 % variation between the present solution and that of Shuen and Yoon (13). We conclude that the pressure and temperature are overestimated by Shuen and Yoon (13), 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. (19) in the first case, and that of Yee and Shinn (24) in the second one.

### 3.4 Sonic Transverse Helium Injection into Supersonic Air Flows

Before we simulate the air-Hydrogen mixing and combustion inside a supersonic combustor using transverse fuel sonic injection technique, we solve here the 2D problem of non-reacting case of Helium sonic transverse injection into supersonic air stream. This case will examine the code ability to capture the complicated flow features previously discussed and shown in figure(1). Helium

is injected at supersonic speed from a 2D slot of width  $0.0559 [cm]$  at  $x = x_o = 0.178 [m]$ , as shown in figure(28). The conditions of inlet air and injected Helium are as follows:  $M_{in_{air}} = 2.9$ ,  $T_{in_{air}} = 108.0 [K]$ ,  $P_{in_{air}} = 0.0663 [MPa]$ ,  $M_{in_{He}} = 1.0$ ,  $T_{in_{He}} = 217 [K]$  and  $P_{in_{He}} = 1.24 [MPa]$ . Air is assumed to be completely homogenous and it is assumed here as a single species. Therefore, a two species model of air and Helium is used in the simulation. The thermodynamic properties of both air and Helium are assumed to be constants.

In figure (29) indicates that a recirculation zones are formed around the perpendicularly injected Helium stream. These low-speed zones have a significant role in the mixing process of air and Helium. In addition, the separation shock prevents the transverse flow from being swept by the supersonic air stream. One of the most characteristic phenomena of transverse sonic injection is the acceleration of the injected gas inside a barrel-shaped stream tube. The injected gas is usually surrounded with bow shocks and then the gas is decelerated to sonic speed again at the Mach disk. The current simulation succeeded to capture this complicated system of flow features discussed the introduction. The effect of transverse sonic injection on flame holding and mixing is presented in figures (32) and (31). The contours of temperature ( $T$ ) presented in figure (32) shows the effect of the front recirculation zone on flame holding. High values of the static temperature is sustained in the vorticity region due to the separation shock. Also, the mixing process expressed in terms of the Helium mass fraction distribution is shown in figure (31), where the main mixing process is carried out in the front recirculation zone. In addition, He-air mixing takes place by the diffusion of He-transfer through the mixing free shear layer.

The injection pressure is taken to be about 20 times the air inlet flow pressure to decelerate the supersonic air flow upstream the injection zone. Raising the injection pressure strengthens the formed shock system surrounding the injection regime and improves the injected gas penetration into the main stream. The current numerical results are compared with the previous calculations of Shuen and Yoon (13) and with the experimental results of Kraemer, G.O, and Rogers, R.C., which are reported by Drummond and Weidner (15). The comparison is presented for the pressure distribution at the lower wall around the injection zone at  $x = 216 [mm]$  from the duct inlet. There is a good agreement

between the current results and the experimental results as shown in figure (30).

### 3.5 Mixing and Combustion Processes in Single-Strut Scramjet Engines

Non-reacting and reacting turbulent flow field in a 2D single strut scramjet engine model problem are simulated in this study to investigate the effect of the transverse sonic fuel injection on the scramjet engine performance. The configuration of the problem is described in figure (33) as introduced by Drummond and Weidner (15). The engine length is  $0.78 [m]$ , while its width at the inlet is  $0.15 [m]$ . The middle fuel injection strut is  $0.258 [m]$  long and it is centered around the module minimum cross-section, which is located at  $0.378 [m]$  from the inlet leading edge. The half inclination angles of the injection-strut walls are  $7.1$  degrees. This geometry is a 2D 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 located at  $0.06 [m]$  downstream from the minimum cross-section. The injection slot's width is  $0.1 [cm]$  such that the overall equivalence ratio of air- hydrogen mixture is one. The inlet conditions of both air and Hydrogen are given as follows:  $M_{in_{air}} = 5.03$ ,  $T_{in_{air}} = 335.0 [K]$ ,  $P_{in_{air}} = 3546.0 [Pa]$ ,  $T_{in_{H_2}} = 246.0 [K]$  and  $P_{in_{H_2}} = 254824.0 [Pa]$ . Only the upper half of the scramjet model is considered in the simulation and symmetrical boundary conditions are applied at the engine centerline. Meshes of sizes  $87 \times 31$  and  $200 \times 51$ , are employed. The grid lines are clustered near the wall surface and around the vertical line ( $x = x_o = 0.378 [m]$ ) at which Hydrogen is injected from the lower wall.

The results of the normalized pressure on the engine upper wall surface are compared with the calculations of Chitsomboon et al. (18). The normalized axial distance and pressure is given as follow:

$$x_{norm} = \frac{x - x_{\text{intake leading edge}}}{x_{\text{intake leading edge}} - x_{\text{nozzle trailing edge}}}, \quad (15)$$

$$P_{norm} = \frac{P - P_{\text{air inlet}}}{P_{H_2 \text{ injection}} - P_{\text{air inlet}}}$$

In figure (34), the normalized pressure is presented along the whole engine module, where the normalized pressure for all solutions equal to unity at the injection zone. The previous solution of the reacting case agrees with the non-reacting solution of the

same mesh size ( $87 \times 31$ ). The estimated upstream normal shocks strength increases as the mesh resolution increases. Also the current numerical solver predicts higher wall pressure upstream the injection zone. That is due to the hydrogen propagation in the upstream direction with the aid of flow recirculation, and its reaction with incoming air just at the engine wall boundary layer, and after the oblique shock formed at the engine strut.

The non-reacting and reacting test cases are compared with each other in figures(35) and (36). Both have the same mesh of  $200 \times 51$ . The mach number distribution is shown, and show the effect of the air-hydrogen combustion in the thermal shocking of the flow close to the injection zone inside the engine. The sizes of bubbles upstream the injectors obviously increase in the reacting cases. That indicates the significance of the choice of the injection's pressure, location, and orientation. And it shows its strong effect on the overall performance of the scramjet engine.

## 4 Conclusion

An accurate numerical solver is developed to simulate turbulent chemically-reacting flows inside supersonic combustors. The Reynolds average Navier-Stokes equations are solved numerically on a structured finite volume grid using zero equation turbulence model. The stiffness because of the chemical characteristic time is resolved by chemical implicit time integration. The convective fluxes are discretized using the second order Roe scheme. And, the diffusive fluxes are discretized using central differencing. A two-step second order accurate Runge-Kutta is used for the time integration of the governing equations. This research presents the a comprehensive set of validation test cases which evaluates the solver capability of capturing different features of the two-dimensional turbulent chemically reacting flows, and supersonic combustion and mixing. It is clear that small time formation of intermediate Hydroxyl group increases the mesh sensitivity of the solution. The results show good agreement with the published data of these cases. And, that proves the developed solver is a efficient and accurate tool to simulate chemically-reacting supersonic turbulent flows. The simulation of the single strut scramjet engine test case shows the importance of the sonic fuel injection configuration parameters to optimize the overall engine performance. And that

could be a candidate parametric study to apply the developed numerical solver in the future.

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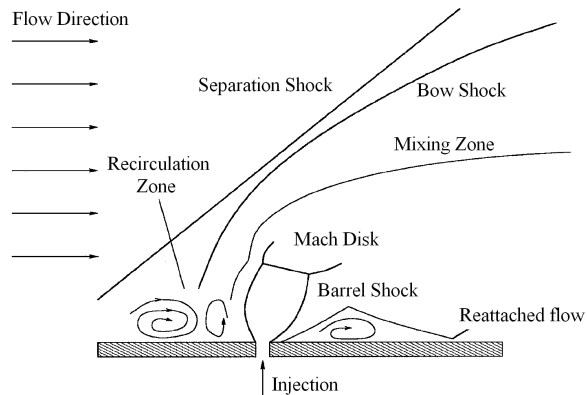


Figure 1 Flow features in sonic transverse injection to supersonic flow stream

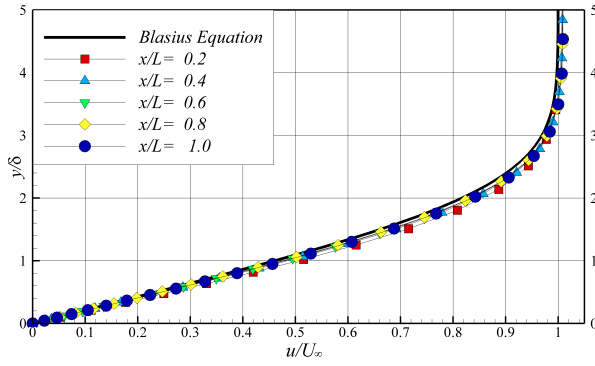


Figure 2 Velocity profile for laminar flow solved by Blasius equations versus numerical solution at different stations

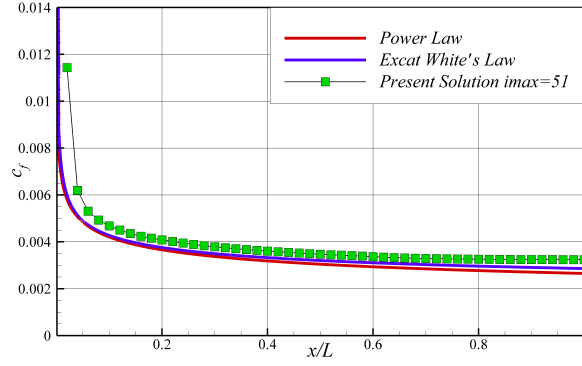


Figure 5 Turbulent local skin friction coefficient over a flat plate of the numerical solver, and the analytical solutions of Power and White's laws

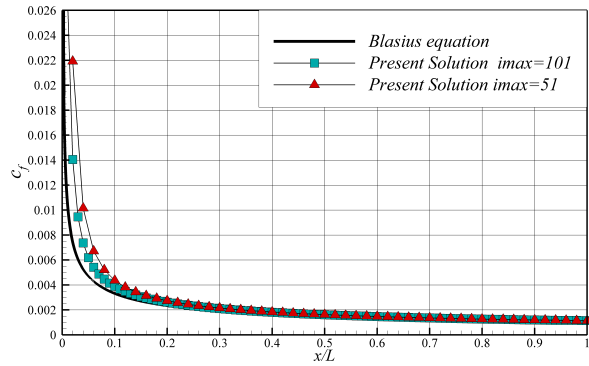


Figure 3 Local skin friction coefficient of laminar flows using Blasius equation and numerical solver for two mesh sizes

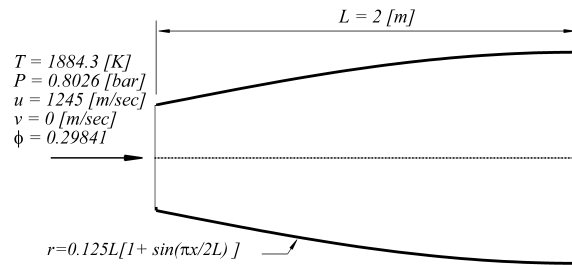


Figure 6 Schematic diagram for the inviscid chemically reacting hydrogen-air flow in axisymmetric nozzle

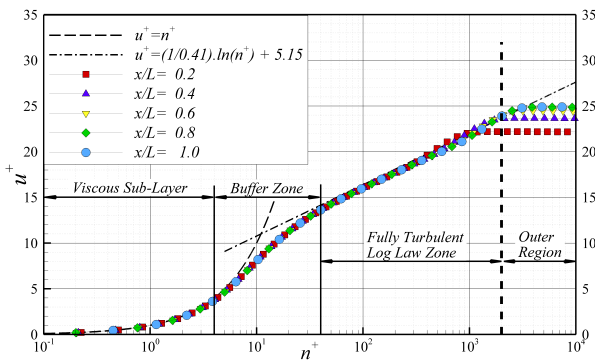


Figure 4 Turbulent velocity profiles for the analytical solution and numerical results at different stations

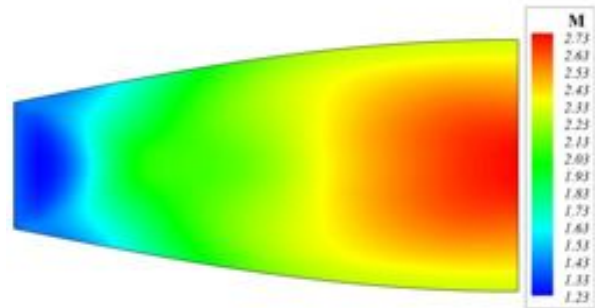


Figure 7 Contours of Mach Number for the complete expansion case)

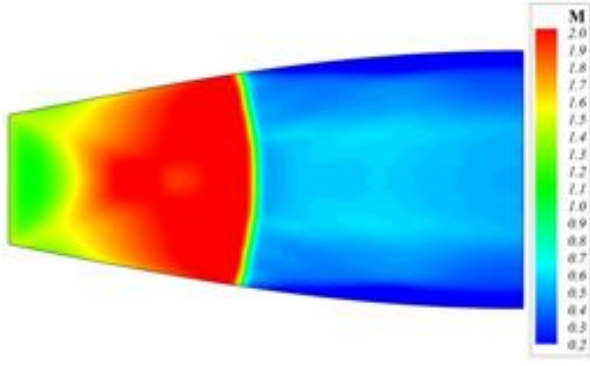


Figure 8 Contours of Mach Number for the over expansion case)

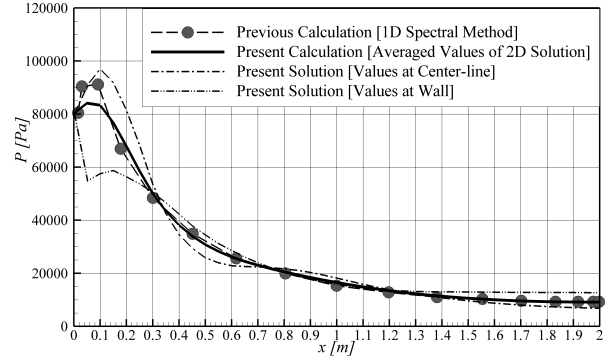


Figure 11 Present solution compared to previous calculations (14) for pressure ( $P$ )

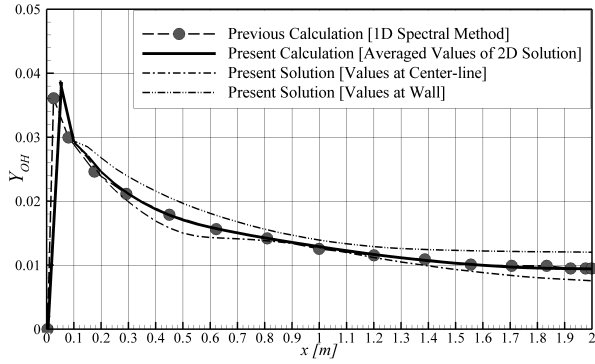


Figure 9 Present solution compared to previous calculations (14) for Hydroxyl mass fraction ( $Y_{OH}$ )

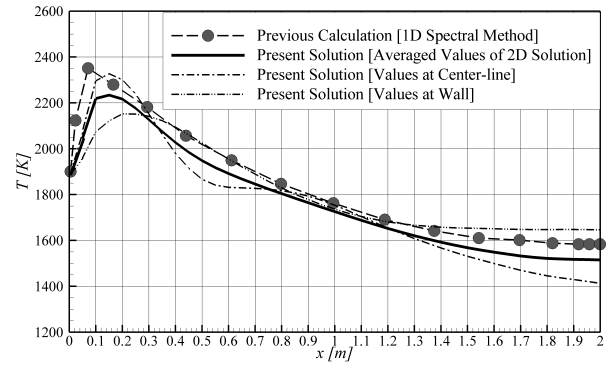


Figure 12 Present solution compared to previous calculations (14) for temperature ( $T$ )

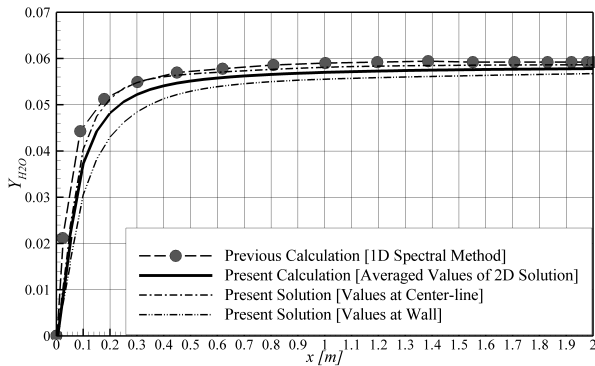


Figure 10 Present solution compared to previous calculations (14) for water mass fraction ( $Y_{H_2O}$ )

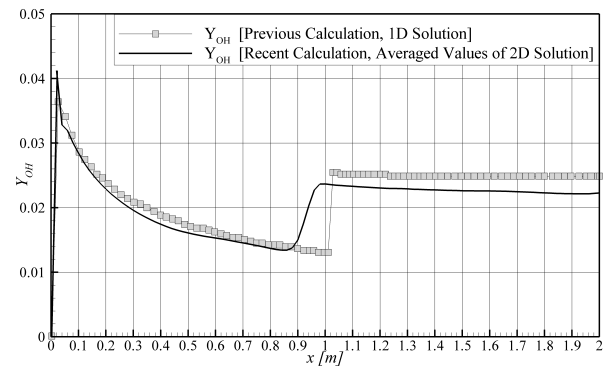


Figure 13 Present solution compared to previous calculations (10) for Hydroxyl mass fraction ( $Y_{OH}$ )

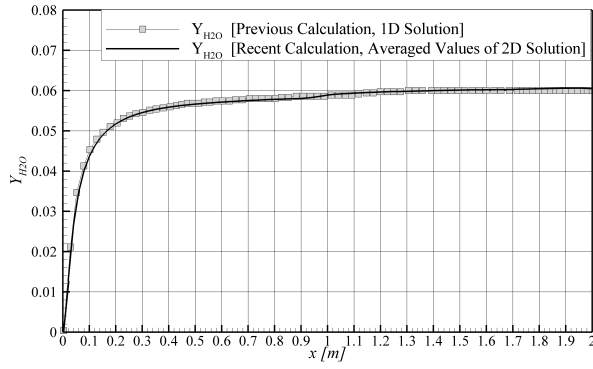


Figure 14 Present solution compared to previous calculations (10) for water mass fraction ( $Y_{OH}$ )

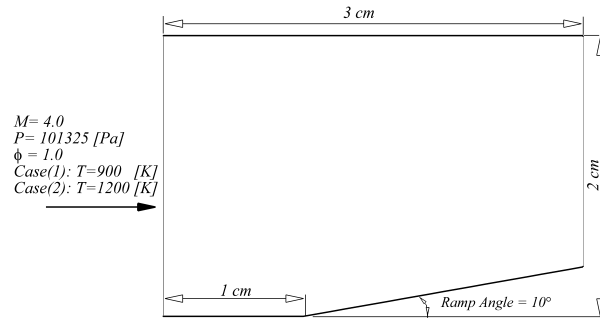


Figure 17 Schematic diagram of Hydrogen-air flow in 2D ramped duct

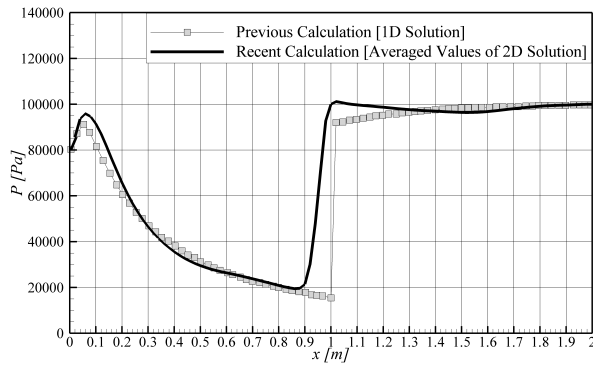


Figure 15 Present solution compared to previous calculations (10) for pressure ( $P$ )

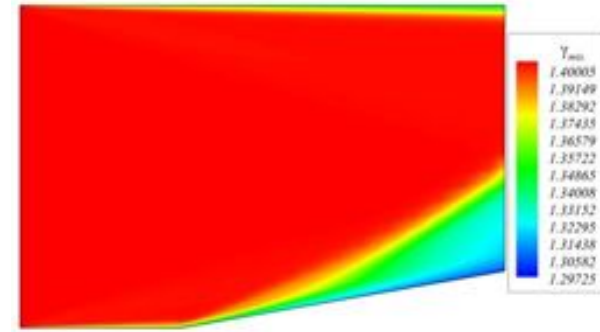


Figure 18 Specific heat ratio contours for the case  $T_{in} = 900$  [K]

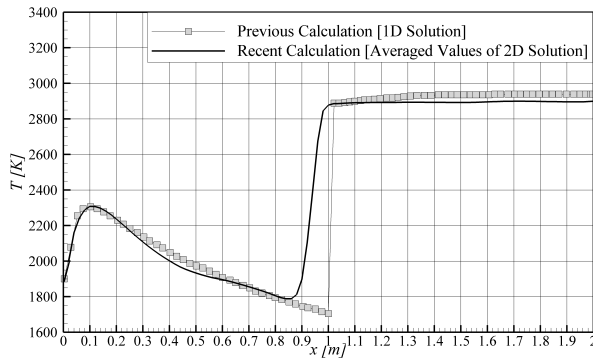


Figure 16 Present solution compared to previous calculations (10) for temperature ( $T$ )

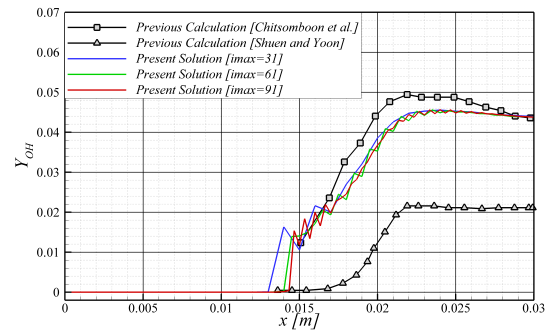


Figure 19 Present solution compared to previous calculations (19; 13) for OH mass fraction at 0.13 cm from the lower wall

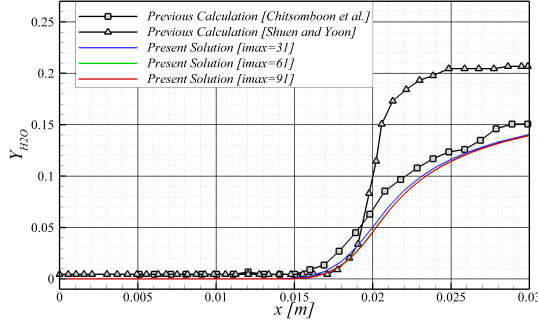


Figure 20 Present solution compared to previous calculations (19; 13) for  $\text{H}_2\text{O}$  mass fraction at 0.13 cm from the lower wall, for the case  $T_{in} = 900$  [K]

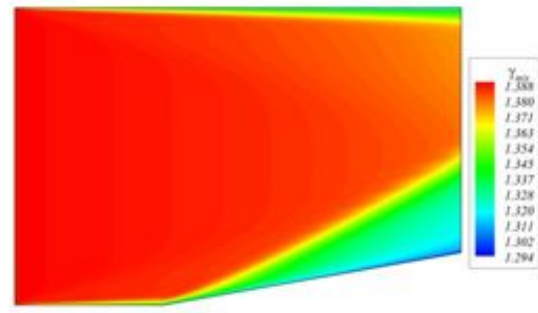


Figure 23 Specific heat ratio contours for the case  $T_{in} = 1200$  [K]

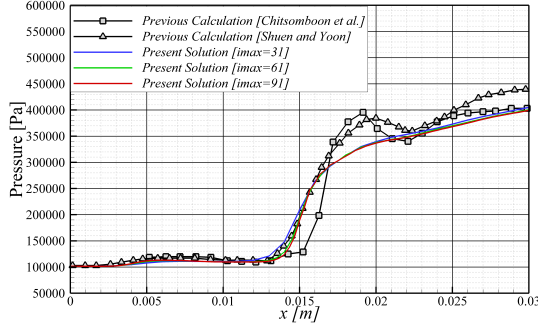


Figure 21 Present solution compared to previous calculations (19; 13) for pressure at 0.13 cm from the lower wall, for the case  $T_{in} = 900$  [K]

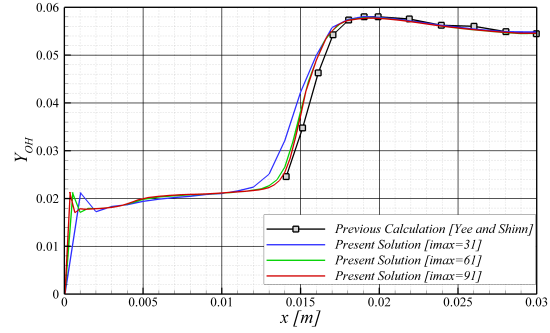


Figure 24 Present solution compared to previous calculations (24) for OH mass fraction at 0.13 cm from the lower wall, for the case  $T_{in} = 1200$  [K]

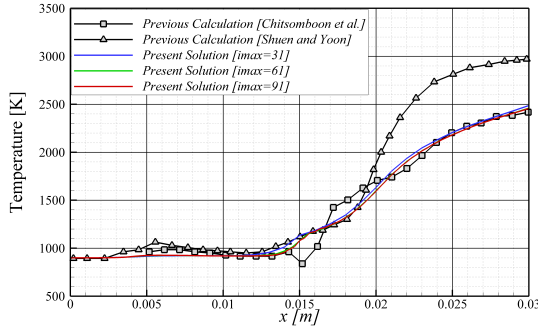


Figure 22 Present solution compared to previous calculations (19; 13) for temperature at 0.13 cm from the lower wall, for the case  $T_{in} = 900$  [K]

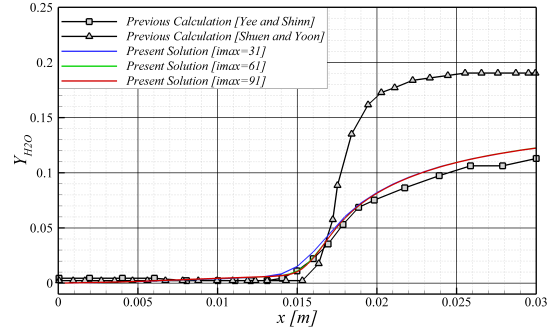


Figure 25 Present solution compared to previous calculations (24; 13) for  $\text{H}_2\text{O}$  mass fraction at 0.13 cm from the lower wall, for the case  $T_{in} = 1200$  [K]

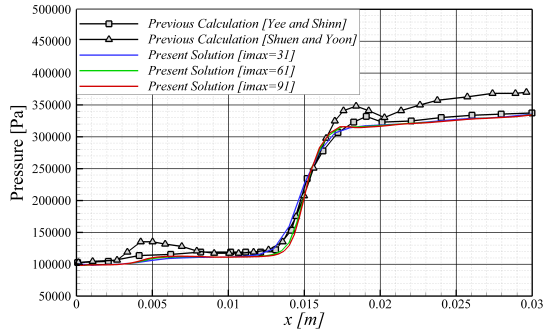


Figure 26 Present solution compared to previous calculations (24; 13) for pressure at 0.13 cm from the lower wall, for the case  $T_{in} = 1200$  [K]

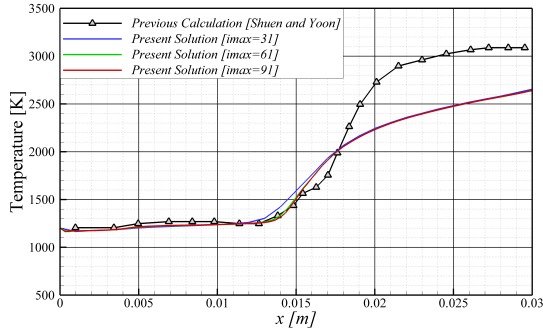


Figure 27 Present solution compared to previous calculations (13) for temperature at 0.13 cm from the lower wall, for the case  $T_{in} = 1200$  [K]

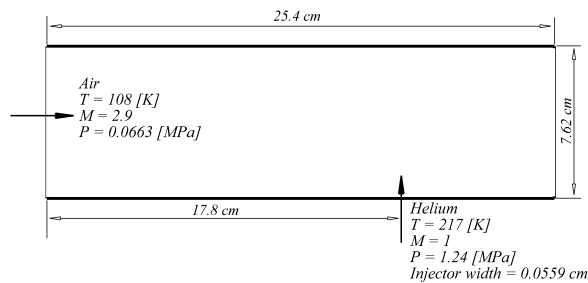


Figure 28 Schematic diagram of Helium sonic transverse injection into supersonic air flow

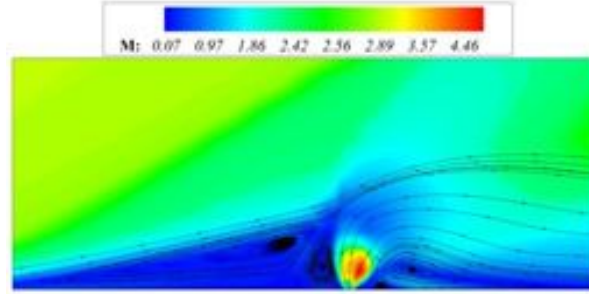


Figure 29 Detailed view around the injection zone, showing the contours of the Mach number (M), showing the formed recirculation zones

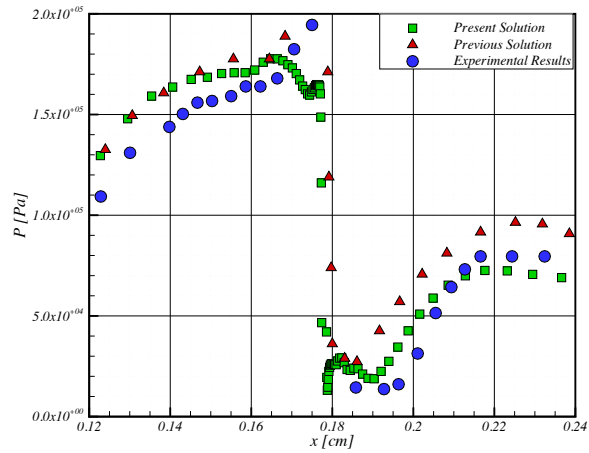


Figure 30 The solution of pressure at the lower wall around injector, compared to experimental results and previous calculations (ref. (13))

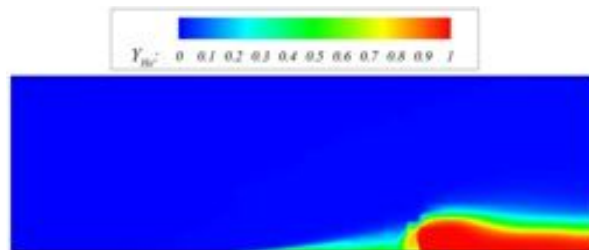


Figure 31 Helium mass fraction ( $Y_{He}$ ) contours for the test case of Helium sonic transverse injection]

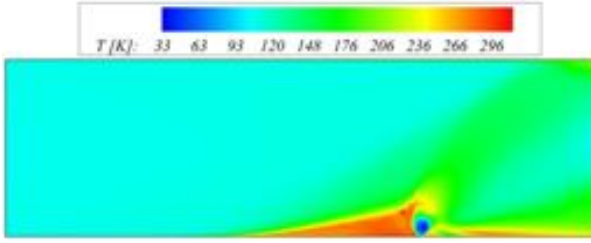


Figure 32 Temperature ( $T$ ) contours for the test case of Helium sonic transverse injection]

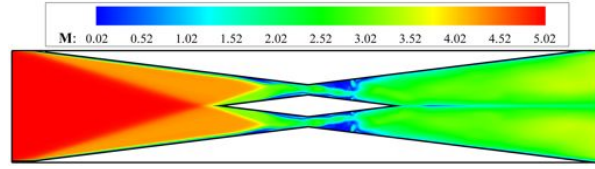


Figure 35 Mach number ( $M$ ) contours of the non-reacting case solution, for mesh size  $200 \times 51$

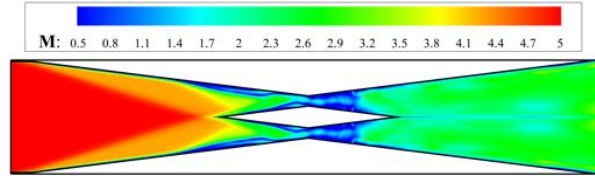


Figure 36 Mach number ( $M$ ) contours of the reacting case solution, for mesh size  $200 \times 51$

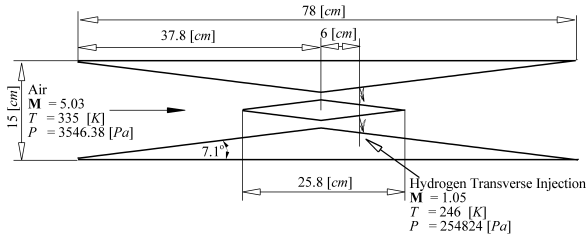


Figure 33 Schematic diagram of Helium sonic transverse injection into supersonic air flow

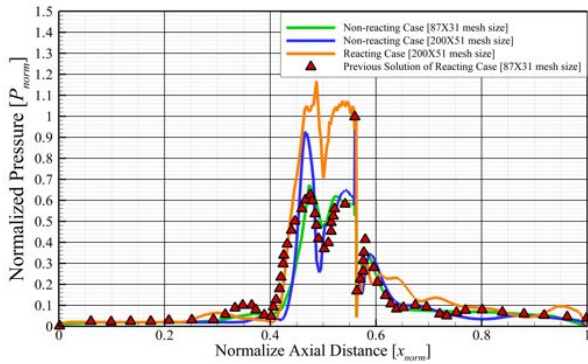


Figure 34 Normalized pressure solution on the upper wall, compared to the previous solution (ref.(18))