Laminar and Turbulent Simulations of Several TVD Schemes in Two-Dimensions – Part I – Theory

Edisson S. G. Maciel

***Abstract*—**This work, first part of this study, describes five numerical tools to perform perfect gas simulations of the laminar and turbulent viscous flow in two-dimensions. The Van Leer, Harten, Frink, Parikh and Pirzadeh, Liou and Steffen Jr. and Radespiel and Kroll schemes, in their first- and second-order versions, are implemented to accomplish the numerical simulations. The Navier-Stokes equations, on a finite volume context and employing structured spatial discretization, are applied to solve the supersonic flow along a ramp in two-dimensions. Three turbulence models are applied to close the system, namely: Cebeci and Smith, Baldwin and Lomax and Sparlat and Allmaras. On the one hand, the second-order version of the Van Leer, Frink, Parikh and Pirzadeh, Liou and Sreffen Jr., and Radespiel and Kroll schemes is obtained from a "MUSCL" extrapolation procedure, whereas on the other hand, the second order version of the Harten scheme is obtained from the modified flux function approach. The convergence process is accelerated to the steady state condition through a spatially variable time step procedure, which has proved effective gains in terms of computational acceleration (see Maciel). The results have shown that, with the exception of the Harten scheme, all other schemes have yielded the best result in terms of the prediction of the shock angle at the ramp. Moreover, the wall pressure distribution is better predicted by the Harten scheme.

***Keywords*—**Laminar and turbulent flows, TVD algorithms, Cebeci and Smith turbulence model, Baldwin and Lomax turbulence model, Sparlat and Allmaras turbulence model.

I. Introduction

CONVENTIONAL non-upwind algorithms have been used extensively to solve a wide variety of problems ([1]). Conventional algorithms are somewhat unreliable in the sense that for every different problem (and sometimes, every different case in the same class of problems) artificial dissipation terms must be specially tuned and judicially chosen for convergence. Also, complex problems with shocks and steep compression and expansion gradients may defy solution altogether.

Upwind schemes are in general more robust but are also more involved in their derivation and application. Some upwind schemes that have been applied to the Euler equations are, for example, [2-6]. Some comments about these methods are reported below:

[2] developed a method suggesting an upwind scheme based on the flux vector splitting concept. This scheme considered the fact that the convective flux vector components could be written as flow Mach number polynomial functions, as main characteristic. Such polynomials presented the particularity of having the minor possible degree and the scheme had to satisfy seven basic properties to form such polynomials.

[3] developed a class of new finite difference schemes, explicit and with second order of spatial accuracy for calculation of weak solutions of the hyperbolic conservation laws. These highly nonlinear schemes were obtained by the application of a first order non-oscillatory scheme to an appropriately modified flux function. These second order algorithms reached high resolution, while preserving the robustness of the original scheme.

[4] proposed a new scheme, unstructured and upwind, to the solution of the Euler equations. They tested the precision and the utility of this scheme in the analysis of the inviscid flows around two airplane configurations: one of transport configuration, with turbines under the wings, and the other of high speed civil configuration. Tests were accomplished at subsonic and transonic Mach numbers with the transport airplane and at transonic and low supersonic Mach numbers with the civil airplane, yielding good results.

[5] proposed a new flux vector splitting scheme. They declared that their scheme was simple and its accuracy was equivalent and, in some cases, better than the [7] scheme accuracy in the solutions of the Euler and the Navier-Stokes equations. The scheme was robust and converged solutions were obtained so fast as the [7] scheme. The authors proposed the approximated definition of an advection Mach number at the cell face, using its neighbour cell values via associated characteristic velocities. This interface Mach number was so used to determine the upwind extrapolation of the convective quantities.

[6] emphasized that the [5] scheme had its merits of low computational complexity and low numerical diffusion as compared to other methods. They also mentioned that the original method had several deficiencies. The method yielded local pressure oscillations in the shock wave proximities, adverse mesh and flow alignment problems. In the [6] work, a

Edisson S. G. Maciel works as a post-doctorate researcher at ITA (Aeronautical Technological Institute), Aeronautical Engineering Division – Praça Marechal do Ar Eduardo Gomes, 50 – Vila das Acácias – São José dos Campos – SP – Brazil – 12228-900 (corresponding author, phone number: +55 012 99165-3565; e-mail: edisavio@edissonsavio.eng.br).

hybrid flux vector splitting scheme, which alternated between the [5] scheme and the [2] scheme, in the shock wave regions, was proposed, assuring that the resolution of strength shocks was clear and sharp.

Second order spatial accuracy can be achieved by introducing more upwind points or cells in the schemes. It has been noted that the projection stage, whereby the solution is projected in each cell face (i-1/2,j; i+1/2,j) on piecewise constant states, is the cause of the first order space accuracy of the Godunov schemes ([8]). Hence, it is sufficient to modify the first projection stage without modifying the Riemann solver, in order to generate higher spatial approximations. The state variables at the interfaces are thereby obtained from an extrapolation between neighboring cell averages. This method for the generation of second order upwind schemes based on variable extrapolation is often referred to in the literature as the MUSCL ("Monotone Upstream-centered Schemes for Conservation Laws") approach. The use of nonlinear limiters in such procedure, with the intention of restricting the amplitude of the gradients appearing in the solution, avoiding thus the formation of new extrema, allows that first order upwind schemes be transformed in TVD high resolution schemes with the appropriate definition of such nonlinear limiters, assuring monotone preserving and total variation diminishing methods.

Second order spatial accuracy can also be obtained from the use of a modified flux function approach, as suggested by [3]. This approach consists in adopting a modified flux to be considered in the numerical flux function. A limiter is used to consider only smooth variations of the flux function. Moreover, this minmod like limiter eliminates high variations of the flux function, reducing this one to a constant behaviour between the right and left states. This approach also introduces TVD like properties into the calculation algorithm.

Computational fluid dynamics (CFD) methods have been widely used in the design of aircraft. Because of the great difficulties in experimental study, CFD demonstrates its great importance in the simulation of transonic high-angle-of-attack (AOA) flow about realistic configurations, which is dominated by extremely complex phenomena such as shock/boundary-layer interaction, massive flow separation, and complicated vortex structures. Until now, numerical prediction of such phenomena has been highly dependent on the selection of turbulence models.

There is a practical necessity in the aeronautical industry and in other fields of the capability of calculating separated turbulent compressible flows. With the available numerical methods, researches seem able to analyze several separated flows, three-dimensional in general, if an appropriated turbulence model is employed. Simple methods as the algebraic turbulence models of [9-10] supply satisfactory results with low computational cost and allow that the main features of the turbulent flow be detected.

More elaborate treatments of turbulent flow, especially involving separation, are obtained with one-equation turbulence models. Such models are cheaper than their counterpart two-equation models and a bit more expensive than the algebraic models. One such a model is the [11] one. In this model, a transport equation for the turbulent viscosity is assembled, using empiricism and arguments of dimensional analysis, Galilean invariance and selective dependence on the molecular viscosity. The equation includes a destruction term that depends on the distance to the wall, related to the one in [12] model and to one due to [13]. Unlike early one-equation models, the resulting turbulence model is local (i.e., the equation at one point does not depend on the solution at others points) and therefore compatible with grids of any structure and Navier-Stokes solvers in two- and three-dimensions. It is numerically forgiving, in terms of near-wall resolution and stiffness, and yields rapid convergence to steady state.

In 2006, [14] have presented a work that considered first-order algorithms applied to the solution of an aerospace flow problem. The [3] and [6] algorithms, both first order accurate in space, were studied. The Navier-Stokes equations written in conservative form, employing a finite volume formulation and a structured spatial discretization, in two-dimensions, were solved. The [10] turbulence algebraic model closed the problem. The steady state physical problem of the supersonic flow around a simplified version of the VLS configuration was studied. The results have demonstrated that the -Cp distribution around the geometry generated by the [3] scheme, in both solutions laminar and turbulent, was smoother than to the one obtained by the [6] scheme, presenting a minor pressure increase in the booster initial region. The lift and drag aerodynamic coefficients were minimized in the turbulent solution generated by the [3] scheme, presenting non-zero values. The [6] scheme predicted the same coefficients with values practically equal to zero to the laminar case and with small values in the turbulent case. The stagnation pressure ahead of the configuration was better predicted by the [3] scheme.

In 2008, [15] has presented a work, the second part of the study started in 2006, that considered upwind algorithms implemented with the [10] turbulence algebraic model applied to the solution of transonic and "cold gas" hypersonic problems. The [3] and [6] algorithms, both first order accurate in space, were studied. The Navier-Stokes equations written in conservative form, employing a finite volume formulation and a structured spatial discretization, in two-dimensions, were solved. The steady state physical problems of the transonic flow along a convergent-divergent nozzle and the "cold gas" hypersonic flow around a double ellipse configuration were studied. Results were compared with experimental or theoretical solutions. The results have shown good agreement between the tested algorithms. In the nozzle problem, the [3] scheme predicts a more severe shock at the throat than the [6] scheme, as well closer wall pressure distribution to experimental results, for both laminar and turbulent cases. In the double ellipse case, the [6] scheme presented more severe pressure field and better prediction of the stagnation pressure than the [3] scheme, again to both laminar and turbulent cases.

In 2010, [16] has presented a work that was the final part of the study that aimed a comparison between the turbulence models of [9-10] applied to aeronautical and aerospace problems. The [17] algorithm was used to perform the numerical experiments. The algorithm was symmetrical,

second order accurate in space and time, and the temporal integration was accomplished by a Runge-Kutta type method. The Reynolds average Navier-Stokes equations were solved, using a finite volume formulation and a structured spatial discretization, and the models of [9] and [10] were used to describe the turbulence effects in the flow properties. The physical problems of the transonic flow along a convergent-divergent nozzle and the "cold gas" hypersonic flow around a double ellipse configuration were studied. A spatially variable time step was employed to accelerate the convergence of the numerical scheme. Effective gains in terms of convergence ratio were observed with this technique, as reported in [18-19] The numerical results were compared with experimental or theoretical solutions. These results have demonstrated that the [10] model was more severe in the nozzle problem, while the [9] model was more severe in the double ellipse problem and more accurate in both examples.

This work, first part of this study, describes five numerical tools to perform perfect gas simulations of the laminar and turbulent viscous flow in two-dimensions. The [2-6] schemes, in its first- and second-order versions, are implemented to accomplish the numerical simulations. The Navier-Stokes equations, on a finite volume context and employing structured spatial discretization, are applied to solve the supersonic flow along a ramp in two-dimensions. Three turbulence models are applied to close the system, namely: [9-11]. On the one hand, the second-order version of the [2; 4-6] schemes are obtained from a "MUSCL" extrapolation procedure, whereas on the other hand, the modified flux function approach is applied in the [3] scheme for the same accuracy. The convergence process is accelerated to the steady state condition through a spatially variable time step procedure, which has proved effective gains in terms of computational acceleration (see [18-19]). The results have shown that the [2; 4-6] schemes have yielded the best results in terms of the prediction of the shock angle at the ramp. Moreover, the wall pressure distribution is better predicted by the [3] scheme.

II. Navier-Stokes equations

The flow is modeled by the Navier-Stokes equations, which express the conservation of mass and energy as well as the momentum variation of a viscous, heat conducting and compressible media, in the absence of external forces. The integral and conservative form of these equations can be represented by:

$$\frac{\partial}{\partial t}\int_V Q\,dV + \int_S \left[\left(E_e - E_v\right)n_x + \left(F_e - F_v\right)n_y\right]dS = 0\,, \qquad (1)$$

where Q is written for a Cartesian system, V is the cell volume, n_x and n_y are components of the normal unity vector to the flux face, S is the flux area, E_e and F_e are the components of the convective flux vector and E_v and F_v are the components of the diffusive flux vector. The vectors Q, E_e, F_e, E_v and F_v are represented by:

$$Q = \begin{Bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{Bmatrix},\quad E_e = \begin{Bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (e+p)u \end{Bmatrix},\quad F_e = \begin{Bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (e+p)v \end{Bmatrix},$$

$$E_v = \frac{1}{Re}\begin{Bmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xx}u + \tau_{xy}v - q_x \end{Bmatrix},\ F_v = \frac{1}{Re}\begin{Bmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ \tau_{xy}u + \tau_{yy}v - q_y \end{Bmatrix}; \quad (2)$$

The components of the viscous stress tensor are defined as:

$$\tau_{xx} = 2\mu_{effect}\,\partial u/\partial x - \frac{2}{3}\mu_{effect}\left(\partial u/\partial x + \partial v/\partial y\right),$$

$$\tau_{xy} = \mu_{effect}\left(\partial u/\partial y + \partial v/\partial x\right),$$

$$\tau_{yy} = 2\mu_{effect}\,\partial v/\partial y - \frac{2}{3}\mu_{effect}\left(\partial u/\partial x + \partial v/\partial y\right); \qquad (3)$$

and the components of the Fourier heat flux vector are defined as:

$$q_x = -\gamma\left(\mu/Prd\right)_{effect}\partial e_i/\partial x\,,\ q_y = -\gamma\left(\mu/Prd\right)_{effect}\partial e_i/\partial y\,, \qquad (4)$$

where ρ is the fluid density; u and v are the Cartesian components of velocity vector in the x and y directions, respectively; p is the static pressure; "e" is the total energy per unit volume; the τ's are the viscous stresses; q_x and q_y are the Cartesian components of the heat conduction vector (Fourier law); γ is the ratio of specific heats; μ_{effect} is the effective fluid viscosity, which is equal to the sum of the molecular viscosity with the turbulent viscosity:

$$\mu_{effect} = \mu_M + \mu_T\,; \qquad (5)$$

The $\left(\mu/Prd\right)_{effect}$ is defined as:

$$\left(\mu/Prd\right)_{effect} = \left(\mu_M/Prd_L\right) + \left(\mu_T/Prd_T\right), \qquad (6)$$

where Prd_L and Prd_T are the laminar and the turbulent Prandtl numbers, respectively, with Prd_L = 0.72 and Prd_T = 0.9; Re is the flow Reynolds number defined as:

$$Re = \rho u_{REF} l/\mu_M\,, \qquad (7)$$

where u_{REF} is a characteristic flow speed and l is a characteristic configuration length; and the internal energy is given by:

$$e_i = e/\rho - 0.5\left(u^2 + v^2\right). \qquad (8)$$

The molecular viscosity is estimated by the empiric Sutherland formula:

$$\mu_M = bT^{1/2}/(1+S/T), \quad (9)$$

where T is the absolute temperature (K), b = $1.458x10^{-6}$ Kg/(m.s.$K^{1/2}$) and S = 110.4 K, to the atmospheric air in the standard atmospheric conditions ([20]).

The Navier-Stokes equations are dimensionless in relation to the freestream density, the freestream speed of sound and the freestream molecular viscosity. The system is closed by the state equation for a perfect gas:

$$p = (\gamma - 1)\left[e - 0.5\rho(u^2 + v^2)\right], \quad (10)$$

considering the ideal gas hypothesis. The total enthalpy is determined by:

$$H = (e + p)/\rho . \quad (11)$$

III. TVD Algoritmos

The description of the convective algorithms of [2-6] is presented in [21-31] and the reader is encouraged to read these papers to become familiar with the numerical schemes. Moreover, the second order spatial accuracy, which incorporates TVD and high resolution properties, is described in [21-22] and in [27-31]. Hereafter, this paper will present the viscous formulation of all numerical schemes.

The numerical flux vector is defined for the [3] scheme, for instance, considering the (i+1/2,j) interface:

$$F^l_{i+1/2,j} = \left(E^l_{e_{i+1/2,j}} - E^l_{v_{i+1/2,j}}\right)n_x + \left(F^l_{e_{i+1/2,j}} - F^l_{v_{i+1/2,j}}\right)n_y + 0.5D^l_{Harten}, \quad (12)$$

where: l varies from 1 to 4 (two-dimensional space) and D_{Harten} is the Harten's dissipation function, defined in [21-22] and in [25-26]. The Euler vectors are defined by the convective contributions of the numerical schemes.

The viscous vectors are calculated with the gradients of the conserved and primitive variables keeping constant in each volume and the application of the Green's theorem to change from a volume integral to a surface integral.

The time integration is performed by a time splitting method, for the [2-3; 5-6] schemes, which divides the integration in two parts, each one associated with a spatial coordinate direction. Therefore, to the ξ direction, one has:

$$\Delta Q^*_{i,j} = -\frac{\Delta t_{i,j}}{V_{i,j}}\left(F^n_{i+1/2,j} - F^n_{i-1/2,j}\right); \quad Q^*_{i,j} = Q^n_{i,j} + \Delta Q^*_{i,j}; \quad (13)$$

and to the η direction, one has:

$$\Delta Q^{n+1}_{i,j} = -\frac{\Delta t_{i,j}}{V_{i,j}}\left(F^*_{i,j+1/2} - F^*_{i,j-1/2}\right); \; Q^{n+1}_{i,j} = Q^*_{i,j} + \Delta Q^{n+1}_{i,j} . \quad (14)$$

The [4] scheme uses a Runge-Kutta time steeping method to perform time integration. This Runge-Kutta method is a five step one. Details in [30-31].

IV. Turbulence Models

A. Turbulence Model of Cebeci and Smith

The problem of the turbulent simulation is in the calculation of the Reynolds stress. Expressions involving velocity fluctuations, originating from the average process, represent six new unknowns. However, the number of equations keeps the same and the system is not closed. The modeling function is to develop approximations to these correlations. To the calculation of the turbulent viscosity according to the [9] model, the boundary layer is divided in internal and external.

Initially, the (ν_w) kinematic viscosity at wall and the ($\tau_{xy,w}$) shear stress at wall are calculated. After that, the (δ) boundary layer thickness, the (δ_{LM}) linear momentum thickness and the (Vt_{BL}) boundary layer tangential velocity are calculated. So, the (N) normal distance from the wall to the studied cell is calculated. The N^+ term is obtained from:

$$N^+ = \sqrt{Re}\sqrt{\tau_{xy,w}/\rho_w}\; N/\nu_w , \quad (15)$$

where ρ_w is the wall density. The van Driest damping factor is calculated by:

$$D = 1 - e^{(-N^+\sqrt{\rho/\rho_w}\,\mu_w/\mu/A^+)}, \quad (16)$$

with $A^+ = 26$ and μ_w is the wall molecular viscosity. After that, the (dVt/dN) normal to the wall gradient of the tangential velocity is calculated and the internal turbulent viscosity is given by:

$$\mu_{Ti} = Re\,\rho(\kappa N D)^2\, dVt/dN , \quad (17)$$

where κ is the von Kárman constant, which has the value 0.4. The intermittent function of Klebanoff is calculated to the external viscosity by:

$$g_{Kleb}(N) = \left[1 + 5.5(N/\delta)^6\right]^{-1}. \quad (18)$$

With it, the external turbulent viscosity is calculated by:

$$\mu_{Te} = Re(0.0168)\rho Vt_{BL}\delta_{LM} g_{Kleb} . \quad (19)$$

Finally, the turbulent viscosity is chosen from the internal and the external viscosities: $\mu_T = MIN(\mu_{Ti}, \mu_{Te})$.

B. Turbulence Model of Baldwin and Lomax

To the calculation of the turbulent viscosity according to the [10] model, the boundary layer is again divided in internal and external. In the internal layer,

$$\mu_{Ti} = \rho l^2_{mix}\|\omega\| \quad \text{and} \quad l_{mix} = \kappa N\left(1 - e^{-N^+/A^+_0}\right). \quad (20)$$

In the external layer,

$$\mu_{Te} = \rho\alpha C_{cp} F_{wake} F_{Kleb}(N; N_{max}/C_{Kleb}), \quad (21)$$

with:

$$F_{wake} = MIN\left[N_{max} F_{max}; C_{wk} N_{max} U_{dif}^2 / F_{max}\right],$$
$$F_{max} = 1/\kappa\left[\underset{N}{MAX}\left(l_{mix}\|\omega\|\right)\right]. \quad (22)$$

Hence, N_{max} is the value of N where $l_{mix}\|\omega\|$ reached its maximum value and l_{mix} is the Prandtl mixture length. The constant values are: $\kappa = 0.4$, $\alpha = 0.0168$, $A_0^+ = 26$, $C_{cp} = 1.6$, $C_{Kleb} = 0.3$ and $C_{wk} = 1$. F_{Kleb} is the intermittent function of Klebanoff given by:

$$F_{Kleb}(N) = \left[1 + 5.5\left(C_{Kleb} N / N_{max}\right)^6\right]^{-1}, \quad (23)$$

$\|\omega\|$ is the magnitude of the vortex vector and U_{dif} is the maximum velocity value in the boundary layer case. To free shear layers,

$$U_{dif} = \left(\sqrt{u^2 + v^2 + w^2}\right)_{max} - \left(\sqrt{u^2 + v^2 + w^2}\right)_{N=N_{max}}. \quad (24)$$

C. Turbulence Model of Sparlat and Allmaras

The purpose of the [11] one-equation model was overcome the algebraic model limitations and, at the same time, to avoid the difficulties in the implementation of the two-equation models or the Reynolds stress equations. This model employs a transport turbulent viscosity to solve the turbulence scaling. Such model takes naturally into account the turbulence and diffusion histories, which improves its accuracy.

The transport equation to the work turbulent kinematic viscosity is described by:

$$\frac{D\tilde{\nu}}{Dt} = c_{b1}\tilde{S}\tilde{\nu} + \frac{1}{\sigma}\left[\nabla \bullet \left((\nu + \tilde{\nu})\nabla\tilde{\nu}\right) + c_{b2}(\nabla\tilde{\nu})^2\right] - c_{w1} f_w(r)\left(\frac{\tilde{\nu}}{N}\right)^2. \quad (25)$$

In this equation, the first term of the right-hand-side is the production contribution to the work kinematic viscosity; the second term is the viscosity diffusion; and the last term is the destruction of the work kinematic viscosity. The turbulent viscosity is defined by:

$$\mu_T = \rho\tilde{\nu} f_{v1}. \quad (26)$$

With the purpose of assuring that $\tilde{\nu}$ becomes equal to $K \times N \times \sqrt{\tau_{xy,w}/\rho_w}$ in the logarithmic layer and in the viscous sub-layer, the f_{v1} damping function is defined by:

$$f_{v1} = \frac{\lambda^3}{\lambda^3 + {c_{v1}}^3} \quad (27)$$

as function of the $\lambda = \tilde{\nu}/\nu$ variable. The $\tilde{S}$ function, representing the deformation work of the mean flow, is determined as follows:

$$\tilde{S} = \left|\frac{\partial u}{\partial y}\right| + \left[\frac{\tilde{\nu}}{(\kappa N)^2} f_{v2}\right], \quad (28)$$

in which f_{v2} has the following expression:

$$f_{v2} = 1 - \frac{\lambda}{1 + \lambda f_{v1}}. \quad (29)$$

The destruction term should disappear at the external region of the boundary layer. [11] purpose the following function to reproduce such behavior:

$$f_w(r) = g\left[\frac{1 + {c_{w3}}^6}{g^6 + {c_{w3}}^6}\right]^{1/6}, \; g = r + c_{w2}\left(r^6 - r\right), \; r = \frac{\tilde{\nu}}{(\kappa N)^2 \tilde{S}}, \quad (30)$$

with the r argument and the f_w function reaching the value 1.0 at the logarithmic layer and decreasing at the external region. The g function is merely a limiter to prevent f_w high values. The [11] model constants are:

$$c_{b1} = 0{,}1355, \; c_{b2} = 0{,}622, \; c_{w2} = 0{,}3, \; c_{v1} = 7{,}1;$$
$$\sigma = 2/3, \; c_{w3} = 2{,}0, \; c_{w1} = \frac{c_{b1}}{\kappa^2} + \frac{(1 + c_{b2})}{\sigma}. \quad (31)$$

The [11] model is marched in time using a LU-SGS ("Lower-Upper Factorization – Symmetrical Gauss-Seidel") implicit method. Details of the implicit implementation in two-dimensions are found in [11]. The extension to three-dimensions is straightforward.

In this work, the term referent to the diffusion of the work kinematic viscosity was not implemented. The studied model considers only the production and dissipation terms of the work kinematic viscosity.

V. Spatially Variable Time Step

The basic idea of the spatially variable time step procedure consists in keeping constant the CFL number in all calculation domain, allowing, hence, the use of appropriated time steps to each specific mesh region during the convergence process. In this work, a convective + diffusive option of spatially variable time step calculated at each iteration was studied and is described below:

To a viscous simulation and according to the work of [32], it is possible to write:

$$\Delta t_i = \left(\frac{CFL(\Delta t_c \Delta t_v)}{\Delta t_c + \Delta t_v}\right)_{i,j}, \quad (32)$$

with Δt_c being the convective time step and Δt_v being the viscous time step. These quantities are defined as:

$$(\Delta t_c)_{i,j} = \frac{V_{i,j}}{(\lambda_c)_{i,j}},\ (\lambda_c)_{i,j} = \max\left(\lambda^{max}_{i,j-1/2}, \lambda^{max}_{i+1/2,j}, \lambda^{max}_{i,j+1/2}, \lambda^{max}_{i-1/2,j}\right),$$

$$\lambda^{max}_{int} = \left(\left|u_{int} n_x + v_{int} n_y\right| + a_{int}\right) S_{int}; \quad (33)$$

$$(\Delta t_v)_{i,j} = K_v \frac{V_{i,j}}{(\lambda_v)_{i,j}},\ (p1)_{i,j} = \frac{\gamma^{3/2} M_\infty}{(Re\, Pr\, d_L) V_{i,j}},$$

$$(p2)_{i,j} = \frac{\mu_{i,j-1/2}}{\rho_{i,j-1/2}} S^2_{i,j-1/2} + \frac{\mu_{i+1/2,j}}{\rho_{i+1/2,j}} S^2_{i+1/2,j} + \frac{\mu_{i,j+1/2}}{\rho_{i,j+1/2}} S^2_{i,j+1/2} + \frac{\mu_{i-1/2,j}}{\rho_{i-1/2,j}} S^2_{i-1/2,j};$$

$$(\lambda_v)_{i,j} = (p1 \times p2)_{i,j}, \quad (34)$$

where interface properties are calculated by arithmetical average, M_∞ is the freestream Mach number, μ is the fluid molecular viscosity and K_v is equal to 0.25, as recommended by [32].

VI. Initial and Boundary Conditions

A. Initial Condition

Freestream values, at all grid cells, are adopted for all flow properties as initial condition, as suggested by [17] and [33]. Therefore, the vector of conserved variables is defined as:

$$Q_{i,j} = \left\{1 \quad M_\infty \cos\alpha \quad M_\infty \sin\alpha \quad \frac{1}{\gamma(\gamma-1)} + 0.5 M^2_\infty\right\}^T. \quad (35)$$

B. Boundary Conditions

The boundary conditions are basically of three types: solid wall, entrance, and exit. These conditions are implemented in ghost cells.

Wall Condition. Considering the viscous case, it imposes the non-permeability and non-slip wall conditions. Therefore, the tangent velocity component of the ghost volume at wall has the same magnitude as the respective velocity component of its real neighbor cell, but opposite signal. In the same way, the normal velocity component of the ghost volume at wall is equal in value, but opposite in signal, to the respective velocity component of its real neighbor cell. These procedures lead to the following expressions to u_{ghost} and v_{ghost}:

$$u_{ghost} = -u_{real} \quad \text{and} \quad v_{ghost} = -v_{real} \quad (36)$$

The pressure gradient normal to the wall is assumed to be equal to zero, following a boundary-layer like condition. The same hypothesis is applied to the temperature gradient normal to the wall, considering adiabatic wall. The ghost volume density and pressure are extrapolated from the respective values of the real neighbor volume (zero order extrapolation), with these two conditions. The total energy is obtained by the state equation of a perfect gas.

Entrance Condition. The entrance condition considers subsonic and supersonic flow. They are detailed below:

(a) Subsonic flow: Three properties are specified and one extrapolated. This approach is based on information propagation analysis along characteristic directions in the calculation domain (see [33]). In other words, for subsonic flow, three characteristic propagate information pointing into the computational domain. Thus three flow properties must be fixed at the inlet plane. Just one characteristic line allows information to travel upstream. So, one flow variable must be extrapolated from the grid interior to the inlet boundary. The pressure was the extrapolated variable from the real neighbor volumes, for the studied problem. Density and velocity components adopted values of freestream flow.
(b) Supersonic flow: In this case no information travels upstream; therefore all variables are fixed with their freestream values.

Exit Condition. Again, two flow situations are analyzed. They are detailed below:

(a) Subsonic flow: Three characteristic propagate information outward the computational domain. Hence, the associated variables should be extrapolated from interior information. The characteristic direction associated to the "(q_{normal}-a)" velocity should be specified because it points inward to the computational domain (see [33]). In this case, the ghost volume pressure is specified from its initial value. Density, and velocity components are extrapolated. The total energy is obtained from the state equation of a perfect gas.
(b) Supersonic flow: All variables are extrapolated from interior grid cells, as no flow information can make its way upstream. In other words, nothing can be fixed.

VII. Conclusions

This work, first part of this study, describes five numerical tools to perform perfect gas simulations of the laminar and turbulent viscous flow in two-dimensions. The [2-6] schemes, in its first- and second-order versions, are implemented to accomplish the numerical simulations. The Navier-Stokes equations, on a finite volume context and employing structured spatial discretization, are applied to solve the supersonic flow along a ramp in two-dimensions. Three turbulence models are applied to close the system, namely: [9-11]. On the one hand, the second-order version of the [2; 4-6] schemes are obtained from a "MUSCL" extrapolation procedure, whereas on the other hand, the modified flux function approach is applied in the [3] scheme for the same accuracy. The convergence process is accelerated to the steady state condition through a spatially variable time step procedure, which has proved effective gains in terms of computational acceleration (see [18-19]). The results have shown that the [2; 4-6] schemes have yielded the best results in terms of the prediction of the shock angle at the ramp. Moreover, the wall pressure distribution is also better predicted by the [3] scheme.

It is important to emphasize that the study of the present turbulence models aims a verification of their potentialities to

be used in re-entry flows in Earth and entry flows in Mars, to perform turbulent reactive simulations on the future. Some references to the reader become familiar with such line of research of the present author are: [34-38].

REFERENCES

[1] P. Kutler, "Computation of Three-Dimensional, Inviscid Supersonic Flows", Lecture Notes in Physics, Vol. 41, 1975, pp. 287-374.

[2] B. Van Leer, "Flux-Vector Splitting for the Euler Equations", Proceedings of the 8th International Conference on Numerical Methods in Fluid Dynamics, E. Krause, Editor, Lecture Notes in Physics, Vol. 170, 1982, pp. 507-512, Springer-Verlag, Berlin.

[3] A. Harten, "High Resolution Schemes for Hyperbolic Conservation Laws", Journal of Computational Physics, Vol. 49, 1983, pp. 357-393.

[4] N. T. Frink, P. Parikh, and S. Pirzadeh, "Aerodynamic Analysis of Complex Configurations Using Unstructured Grids", AIAA 91-3292-CP, 1991.

[5] M. Liou, and C. J. Steffen Jr., "A New Flux Splitting Scheme", Journal of Computational Physics, Vol. 107, 1993, pp. 23-39.

[6] R. Radespiel, and N. Kroll, "Accurate Flux Vector Splitting for Shocks and Shear Layers", Journal of Computational Physics, Vol. 121, 1995, pp. 66-78.

[7] P. L. Roe, "Approximate Riemann Solvers, Parameter Vectors, and Difference Schemes", Journal of Computational Physics, Vol. 43, 1981, pp. 357-372.

[8] C. Hirsch, "Numerical Computation of Internal and External Flows – Computational Methods for Inviscid and Viscous Flows", John Wiley & Sons Ltd, 691p., 1991.

[9] T. Cebeci, and A. M. O. Smith, "A Finite-Difference Method for Calculating Compressible Laminar and Turbulent Boundary Layers", Journal of Basic Engineering, Trans. ASME, Series B, Vol. 92, No. 3, 1970, pp. 523-535.

[10] B. D. Baldwin, and H. Lomax, "Thin Layer Approximation and Algebraic Model for Separated Turbulent Flows", AIAA Paper 78-257, 1978.

[11] P. R. Sparlat, and S. R. Allmaras, "A One-Equation Turbulence Model for Aerodynamic Flows", AIAA Paper 92-0439, 1992.

[12] Secundov, Smirnova, Kozlov, Gulyaev, "One-Equation Eddy Viscosity Model" (Modified L. S. J. Kovasznay Model), Short Summary of the Equations, Personal Communication, 1990.

[13] J. C. R. Hunt, "Turbulence Structure in Thermal Convection and Shear-Free Boundary Layers", J. Fluid Mech., Vol. 138, 1984, pp. 161-184.

[14] E. S. G. Maciel, and N. G. C. R. Fico Jr., "High Resolution Algorithms Coupled with the Baldwin and Lomax Model Applied to a Turbulent Flow Problem", Proceedings of the 5th Spring School of Transition and Turbulence (V EPTT), Rio de Janeiro, RJ, Brazil, 2006. [available in CD-ROM]

[15] E. S. G. Maciel, "First Order Upwind Algorithms Coupled with the Baldwin and Lomax Model Applied to Turbulent Flow Problems – Part II", Proceedings of the V National Congress of Mechanical Engineering (V CONEM), Salvador, BA, Brazil, 2008. [available in CD-ROM]

[16] E. S. G. Maciel, "Comparison Between the Cebeci and Smith and the Baldwin and Lomax Turbulence Models – Final Results", Proceedings of the VI National Congress of Mechanical Engineering (VI CONEM), Campina Grande, PB, Brazil, 2010. [available in CD-ROM]

[17] A. Jameson, and D. J. Mavriplis, "Finite Volume Solution of the Two-Dimensional Euler Equations on a Regular Triangular Mesh", AIAA Journal, Vol. 24, No. 4, 1986, pp. 611-618.

[18] E. S. G. Maciel, "Analysis of Convergence Acceleration Techniques Used in Unstructured Algorithms in the Solution of Aeronautical Problems – Part I", Proceedings of the XVIII International Congress of Mechanical Engineering (XVIII COBEM), Ouro Preto, MG, Brazil, 2005. [available in CD-ROM]

[19] E. S. G., Maciel, "Analysis of Convergence Acceleration Techniques Used in Unstructured Algorithms in the Solution of Aerospace Problems – Part II", Proceedings of the XII Brazilian Congress of Thermal Engineering and Sciences (XII ENCIT), Belo Horizonte, MG, Brazil, 2008. [available in CD-ROM]

[20] R. W. Fox, and A. T. McDonald, "Introdução à Mecânica dos Fluidos", Ed. Guanabara Koogan, Rio de Janeiro, RJ, Brazil, 632p., 1988

[21] E. S. G. Maciel, "Comparison Among Predictor-Corrector, Simmetrical and TVD Upwind Schemes in the Solution of the Euler Equations in Two-Dimensions – Theory", Proceedings of the 19th International Congress of Mechanical Engineering (XIX COBEM), Brasília, DF, Brazil, 2007. [available in CD-ROM]

[22] E. S. G. Maciel, "Comparison Among Predictor-Corrector, Simmetrical and TVD Upwind Schemes in the Solution of the Euler Equations in Two-Dimensions – Results", Proceedings of the 19th International Congress of Mechanical Engineering (XIX COBEM), Brasília, DF, Brazil, 2007. [available in CD-ROM]

[23] E. S. G. Maciel, "Comparison Among the First Order Upwind Algorithms of Roe, of Steger and Warming, of Van Leer and of Chakravarthy and Osher in the Solution of the Euler Equations in 2D – Theory", Proceedings of the VIII Symposium of Computational Mechanics (VIII SIMMEC), Belo Horizonte, MG, Brazil, 2008. [available in CD-ROM]

[24] E. S. G. Maciel, "Comparison Among the First Order Upwind Algorithms of Roe, of Steger and Warming, of Van Leer and of Chakravarthy and Osher in the Solution of the Euler Equations in 2D – Results", Proceedings of the VIII Symposium of Computational Mechanics (VIII SIMMEC), Belo Horizonte, MG, Brazil, 2008. [available in CD-ROM]

[25] E. S. G. Maciel, "Comparação entre Algoritmos de Separação de Vetores de Fluxo e de Diferenças de Fluxo de Primeira Ordem na Solução das Equações de Euler em Duas Dimensões – Teoria", Proceedings of the Primer Congreso Argentino Ingeniería (I CAIM), Bahía Blanca, Argentina, 2008. [available in CD-ROM]

[26] E. S. G. Maciel, "Comparação entre Algoritmos de Separação de Vetores de Fluxo e de Diferenças de Fluxo de Primeira Ordem na Solução das Equações de Euler em Duas Dimensões – Resultados Finais", Proceedings of the Primer Congreso Argentino Ingeniería (I CAIM), Bahía Blanca, Argentina, 2008. [available in CD-ROM]

[27] E. S. G. Maciel, "Extension of the Steger and Warming and Radespiel and Kroll Algorithms to Second Order Accuracy and Implicit Formulation Applied to the Euler Equations in Two-Dimension – Theory", Proceedings of the VI National Congress of Mechanical Engineering (VI CONEM), Campina Grande, Paraiba, Brazil, 2010. [available in CD-ROM]

[28] E. S. G. Maciel, "Extension of the Steger and Warming and Radespiel and Kroll Algorithms to Second Order Accuracy and Implicit Formulation Applied to the Euler Equations in Two-Dimension – Results", Proceedings of the VI National Congress of Mechanical Engineering (VI CONEM), Campina Grande, Paraiba, Brazil, 2010. [available in CD-ROM]

[29] E. S. G. Maciel, "Extension of the Roe and Van Leer Algorithms to Second Order Accuracy Applied to the Euler Equations in Two-Dimensions", Proceedings of the 12th Pan-American Congress of Applied Mechanics (XII PACAM), Port of Spain, Trinidad, 2012. [available in CD-ROM]

[30] E. S. G. Maciel, "Extension of the Frink, Parikh and Pirzadeh and Liou and Steffen Jr. Algorithms to Second Order Accuracy and Implicit Formulations Applied to the Euler Equations in Two-Dimensions – Theory", Proceedings of the VII National Congress of Mechanical Engineering (VII CONEM), São Luis do Maranhão, Maranhão, Brazil, 2012. [available in CD-ROM]

[31] E. S. G. Maciel, "Extension of the Frink, Parikh and Pirzadeh and Liou and Steffen Jr. Algorithms to Second Order Accuracy and Implicit Formulations Applied to the Euler Equations in Two-Dimensions – Results", Proceedings of the VII National Congress of Mechanical Engineering (VII CONEM), São Luis do Maranhão, Maranhão, Brazil, 2012. [available in CD-ROM]

[32] D. J. Mavriplis, and A. Jameson, "Multigrid Solution of the Navier-Stokes Equations on Triangular Meshes", AIAA Journal, Vol. 28, No. 8, 1990, pp. 1415-1425.

[33] E. S. G. Maciel, "Simulação Numérica de Escoamentos Supersônicos e Hipersônicos Utilizando Técnicas de Dinâmica dos Fluidos Computacional", Doctoral Thesis, ITA, CTA, São José dos Campos, SP, Brazil, 2002.

[34] E. S. G. Maciel, and A. P. Pimenta, "Thermochemical Non-Equilibrium Reentry Flows in Two-Dimensions – Part I", WSEAS TRANSACTIONS ON MATHEMATICS, Vol. 11, Issue 6, June, 2012, pp. 520-545.
[35] E. S. G. Maciel, and A. P. Pimenta, "Thermochemical Non-Equilibrium Reentry Flows in Two-Dimensions: Seven Species Model – Part I", WSEAS TRANSACTIONS ON APPLIED AND THEORETICAL MECHANICS, Vol. 7, Issue 4, October, 2012, pp. 311-337.
[36] E. S. G. Maciel, and A. P. Pimenta, "Thermochemical Non-Equilibrium Reentry Flows in Two-Dimensions – Part II", WSEAS TRANSACTIONS ON MATHEMATICS, Vol. 11, Issue 11, November, 2012, pp. 977-1005.
[37] E. S. G. Maciel, and A. P. Pimenta, "Thermochemical Non-Equilibrium Entry Flows in Mars in Two-Dimensions – Part I", WSEAS TRANSACTIONS ON APPLIED AND THEORETICAL MECHANICS, Vol. 8, Issue 1, January, 2013, pp. 26-54.
[38] E. S. G. Maciel, and A. P. Pimenta, "Thermochemical Non-Equilibrium Reentry Flows in Two-Dimensions: Seven Species Model – Part II", WSEAS TRANSACTIONS ON APPLIED AND THEORETICAL MECHANICS, Vol. 8, Issue 1, January, 2013, pp. 55-83.

Edisson S. G. Maciel (F'14), born in 1969, february, 25, in Recife, Pernambuco. He is a Mechanical Engineering undergraduated by UFPE in 1992, in Recife, PE, Brazil; Mester degree in Thermal Engineering by UFPE in 1995, in Recife, PE, Brazil; Doctor degree in Aeronautical Engineering by ITA in 2002, in São José dos Campos, SP, Brazil; and Post-Doctor degree in Aeronautical Engineering by ITA in 2009, in São José dos Campos, SP, Brazil.

Actually, he is doing a new post-doctorate curse in Aerospace Engineering at ITA. The last researches are based on thermochemical non-equilibrium reentry simulations in Earth and thermochemical non-equilibrium entry simulations in Mars. They are: Maciel, E. S. G., and Pimenta, A. P., "Thermochemical Non-Equilibrium Reentry Flows in Two-Dimensions – Part I', WSEAS Transactions on Mathematics, Vol. 11, Issue 6, June, pp. 520-545, 2012; Maciel, E. S. G., and Pimenta, A. P., "Thermochemical Non-Equilibrium Entry Flows in Mars in Two-Dimensions – Part I', WSEAS Transactions on Applied and Theoretical Mechanics, Vol. 8, Issue 1, January, pp. 26-54, 2013; and he has three published books, the first one being: Maciel, E. S. G., "Aplicações de Algoritmos Preditor-Corretor e TVD na Solução das Equações de Euler e de Navier-Stokes em Duas Dimensões", Recife, PE, Editor UFPE, 2013. He is interested in the Magnetogasdynamic field with applications to fluid dynamics and in the use of ENO algorithms.