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# Numeric and geometric sensitivity of nozzle flow simulation

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## **Abstract**

The increasing availability of computing power and the relative ease of use of commercial CFD software bring the ability to compute supersonic nozzle flow within reach of most engineers. In order to get accurate results from the simulations certain aspects of the modeling activities and numerical procedure must be observed. In this work we point out some of the options for checking the quality of the computation with reference to analytic models. The method of constructing several types of planar converging diverging nozzles is presented and the results of the simulation are compared to the method of characteristics computation. The effects of minute changes in the geometry of the nozzle on the flow characteristics are also discussed.

## **INTRODUCTION**

Over the years there has been a considerable amount of work done trying to use CFD codes to model the flow in convergent divergent (CD) nozzles. For subsonic and transonic nozzles the flow is relatively simple and even one dimensional models are able to predict the main flow features. However, high speed supersonic nozzles ( $M_{jet} > 3$ ) introduce some complex flow physics that require more sophisticated codes [1].

Investigation of supersonic nozzle flow is important in many engineering applications such as military aircraft design, rocket launchers for missiles and spacecrafts as well as high velocity spray systems to list a few.

The three main numerical methods for computing fluid dynamics are the Finite Difference Method (FDM), Finite Volume Method (FVM) and the Finite Element Method (FEM) of which FDM is the earliest to be used while FVM is gaining popularity in recent years, due to its simple data structure that makes it easier to implement in computer codes [2].

Until the early 1990's most of these codes were used by scientists specializing in computer application and with institutes having dedicated computer hardware. The advent of desktop PC's and graphical user interface application made these codes accessible to the engineering level users [3]. While there are some codes that use high order numerical schemes, most of the commercial CFD software is based on first and second order discretization methods. Obtaining accurate results with these types of codes is possible if the necessary care is taken to avoid unphysical phenomena.

In the past it wasn't customary to conduct scientific research with the aid of commercial CFD software because of the inability of the user to familiarize himself with the code underneath the software package. Although this has not change as the code has become more complex, today most CFD software have comprehensive documentation and their widespread use has enabled many users to validate the code. In this respect the Fluent CFD software is one of the most comprehensive and extensively used in the solution of flow problems in the engineering community. Thus the question now is not whether the numerical scheme is implemented correctly in the software, but has the user setup the problem correctly to simulate the physics it is supposed to represent.

Although many works detail the results of numerical simulations of nozzle flow, very few present the precise way in which the geometry was constructed in the numerical code and the effects it has on the resulting flow [4].

## **NOZZLE FLOW**

The area-Mach number relation states that the Mach number along the nozzle depends only on the ratio between the local area and the throat area (for a specific gas, with constant specific heat ratio  $\gamma$ )

$$\left(\frac{A}{A^*}\right)^2 = \frac{1}{M^2} \left[ \frac{2}{\gamma + 1} \left( 1 + \frac{\gamma - 1}{2} M^2 \right) \right]^{(\gamma + 1)/(\gamma - 1)}$$

Where  $A^*$  is the area of the throat.

All other fluid properties (pressure, density and temperature) can be computed from isentropic relations if stagnation conditions are known.

However, this usually cannot give an indication of how the Mach numbers change in the spanwise direction as the expansion of the flow in the diverging part of the nozzle creates a non uniform profile that depends on the contour of the wall.

Expansion and compression waves can form due to discontinuities in the curvature of the wall and will propagate and reflect from opposite sides of the nozzle altering the local Mach number (Figure 1). Thus no simple analytic models can predict the flow properties inside the nozzle. However, there are certain flow features that can be modeled and serve as a benchmark to test the accuracy of the numerical simulation.

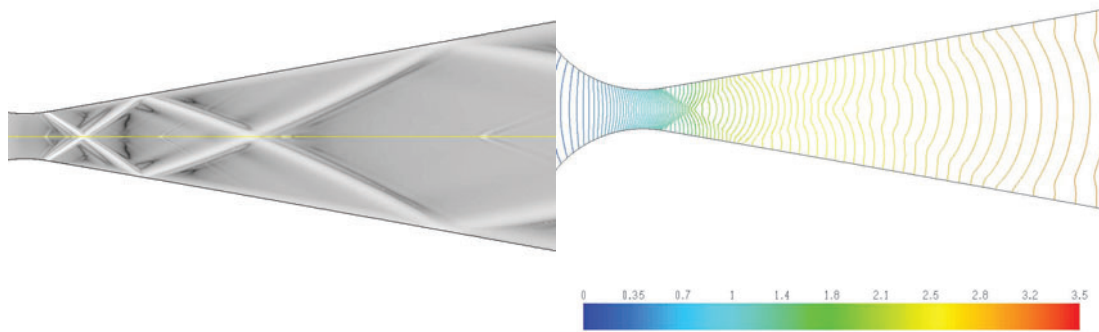


Figure 1. Numeric Shadowgraph showing expansion wave propagating in a divergent section of a conical nozzle (left). Mach number Iso-lines showing the variation in Mach number due to the expansion waves (right).

In this work several 2D nozzles with an area ratio of  $AR=8$  and a design Mach number of  $M=3.676$  are modeled using the Fluent® Version 6.3. Various aspects of the geometric modeling and numerical procedure are discussed. Although there are many possible wall contour profiles, most of them include a throat area with a circular geometry. The radius of this circular section determines the velocity profile at the throat and can be used to estimate the accuracy of the modeled flow compared to analytic computation.

## NUMERICAL METHOD

The first stage of the CD nozzle simulation starts by producing the geometry with some pre-processing application. This stage also includes meshing of the model, i.e., the computational domain, and defining its boundaries. The geometry is then transferred to the solver where the type of numerical scheme and the discretization technique are defined together with the fluid properties and the boundary conditions.

It should be stressed that even simple nozzle geometries require special attention in order to avoid unwanted effects on the flow field characteristics. The wall boundary should contain as little discontinuities as possible. Adequately fine mesh should be used in high curvature regions as the edge connecting two mesh points on the wall is treated as a straight line, thus if there is a curvature of the wall that is not resolved by enough mesh nodes the calculated flow will have a discontinuity that may lead to the development of compression or expansion wave that will propagate in the computational domain. If grid points are not spaced evenly, care should be taken not to create excessive change in cell area (or volume in case of 3D simulation) as this may create disturbances in the flow domain.

Creating a coarse grid with the meshing software and using grid adaptation in the solver to refine it

is not recommended in regions that contain curved wall boundaries. Although the grid refinement reduces the size of the cells and therefore increases the resolution, it does not change the location of the parent cell nodes (Figure 2), the resulting geometry has higher wall derivatives and may increase unphysical flow phenomena.

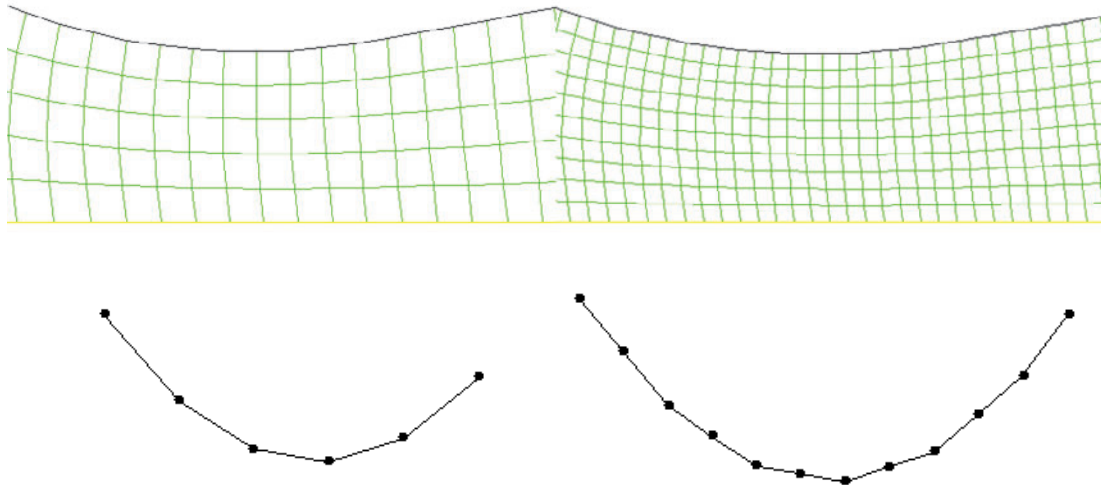


Figure 2. Grid refinement by subdividing cells; Left: Original cell size and nodes on the wall boundary, Right: Refined grid showing that the segmentation of the boundary is unchanged.

In the following examples, 2D inviscid (Euler), density-based solver was used. The density based solver simultaneously solves the continuity, momentum and energy equations (coupled). Each equation in the coupled set of governing equations is linearized implicitly with respect to the dependent variables. The flux vector was computed with ASUM+ type scheme and a CFL (Courant-Friedrichs-Levy) number was set between 2 and 5. Pressure boundary condition for the inlet and the outlet were set. As the flow is symmetric only half of the nozzle was computed with a symmetry boundary condition along the X axis.

Since the inviscid simulation has no boundary layer length scale the flow features have no dimensional scaling factor, so in all the nozzles the throat half height was set to 1m and all other dimensions are proportional to it. The computational grid was produced by Gambit 2.4. Quad cells were used to describe the computational domain. The cells distribution was chosen so the cells at the throat section will have an aspect ratio close to 1.

## DETERMINATION OF THE SONIC LINE

In the convergent part of the nozzle the flow accelerates to sonic conditions as the area ratio,  $A/A^*$ , approaches one.

The profile of the sonic line (the spatial location where the Mach number is equal to one) at the throat isn't straight because of the wall curvature in the converging part of the nozzle and the acceleration of the flow. Using small perturbations transonic analysis it is possible to approximate the shape of the sonic line. Several researchers developed formulation for the shape of the sonic line by assuming a power series solution approximation to the perturbation velocity potential equation. Saur [5] used expansion to the 4<sup>th</sup> power leading to the shape of a parabola. Hall [6] used an expansion of inverse powers of the expansion parameter  $R$  (ratio of radius of curvature to the throat half height) to the 3<sup>rd</sup> power, this solution is limited to  $R > 1$ . Kliegel [7] modified Hall's method by using inverse powers of  $(R+1)$  thus enabling the solution for radius of curvature smaller than the throat half height. For large values of  $R$  ( $R \gg 3$ ) all these methods produce similar results [8]. Thus for the sake of simplicity only Sauer's solution is presented. Setting the throat at the symmetry line as the origin, the expression for the sonic line is:

$$x = \varepsilon - \frac{(\gamma + 1)\alpha}{2} y^2$$

Where

$$\alpha = \left[ \frac{1}{(\gamma + 1)\rho_t y_t} \right]^{1/2}; \varepsilon = \frac{(\gamma + 1)\alpha y_t^2}{6}$$

And  $\rho_t, y_t$  are the radius of curvature of the wall and the throat half height,  $\varepsilon$  is the distance between the throat location and the sonic line on the centerline.

The first case considered is a nozzle with a large radius of curvature ( $R=16$ ). The computational domain had approximately 50,000 cells. 50 cells were set across the throat of which the 10 cells near the wall boundary spaced with reducing size in the  $y$  direction. The simulation was first conducted with a first order discretization until convergence was obtained. The coordinates of the nodes having a Mach number of 1 were extracted and plotted to give the shape of the sonic line. The simulation was repeated with second order discretization with node based and cell based gradient computation. Figure 3 presents a comparison between Sauer's analytical solution and the predictions of the numerical simulations for the sonic line. As can be seen the numerical calculation show that first order discretization may not give accurate representation of the sonic line while the prediction of the second order discretization simulations is in agreement with the analytical solution.

The deviation of the results in the region close to the wall ( $Y^*=1$ ) is attributed to grid irregularity upstream of the throat. When the gradient calculation was changed to node-based, the results were in excellent agreement with the theoretical one. Using node-based gradient computation is more accurate than cell-base, especially for irregular shaped cells (skewed or distorted).

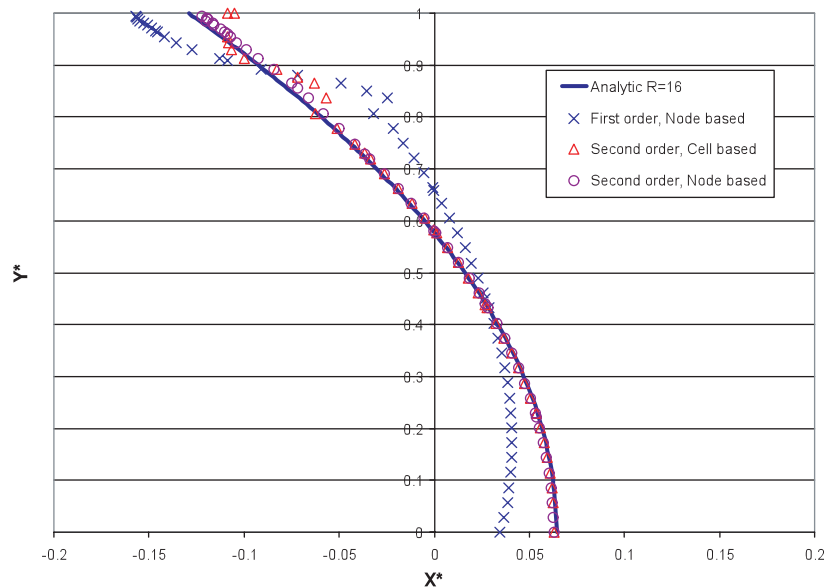


Figure 3. Comparison of sonic line location at the throat of a converging diverging nozzle with  $R=16$ ,  $X$  and  $Y$  are nondimensionalized by the throat height; Solid line- Analytic result based on Sauer's method, Markers- First and Second order results from CFD computations.

Another nozzle was constructed with  $R=6$ . The throat was divided into 40 equal size cell segments; the resulting circular section was approximated by a polygon with an edge angle equal to  $0.5^\circ$  (compared to  $0.1^\circ$  in the previous case). In this simulation both the first and the second order discretizations failed to compute the sonic line near the wall, but the second order gave better results near the symmetry line. Increasing the number of cells across the throat to 60 and 120 (edge angle of  $0.3^\circ$  and  $0.1^\circ$ ) did not improve the results (Figure 4).



Since both the first and the second order simulations predicted similar results near the wall, it is possible that the discrepancy of the results near the wall is due to the Sauer computation and not the numerical simulation. The transonic solution assumes that the throat geometry solely determines the sonic line, some evidence suggests that as  $R$  decreases the upstream nozzle geometry begins to influence the flow [9].

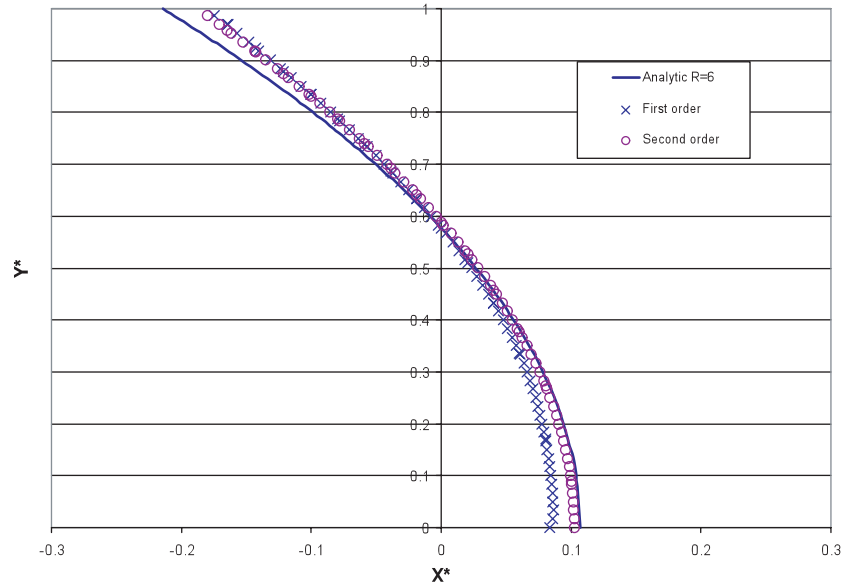


Figure 4. Comparison of sonic line location at the throat of a converging-diverging nozzle with  $R=6$ ; Solid line- Analytic result based on Sauer's method, Markers- First and Second order results from CFD computation.

## PRESERVATION OF ISENTROPIC CONDITIONS

If there are no shocks in the nozzle and the flow is modeled as inviscid and adiabatic with an ideal gas, then the flow should be isentropic.

One way to test this is by checking the stagnation (i.e., the total) pressure in the converging and diverging parts of the nozzle. Figure 5 presents the normalized total pressure along the axis of symmetry as predicted by the first and the second order discretization simulations. It can be seen that when using first order discretization there is a 13% reduction of the total pressure when the flow passes the throat (Figure 5) although the stagnation temperature remains constant throughout the nozzle. Improving the grid and refining it reduces the pressure loss but does not cancel this abnormality. When using second order discretization the variation in total pressure was reduced to less than 0.2%.

When comparing other flow properties at the nozzle exit such as static pressure, density and Mach number between first and second order computations the differences are less than 2%. This may seem a minor discrepancy but as the jet emerges from the nozzle it interacts with the ambient pressure by creating an oblique shock or an expansion fan depending on whether the flow is overexpanded or underexpanded. The ratio of the jet stagnation pressure to the ambient determines the properties of this interaction and may be affected by it. This problem is typical of all nozzles modeled.

## MODELING OF A MINIMUM LENGTH NOZZLE

In order to produce uniform supersonic flow from a converging-diverging nozzle the nozzle should have a certain wall contour. Normal nozzle design has an expansion region after the throat that accelerates the flow, followed by a straitening region which produces a uniform and parallel flow at the nozzle exit. A simplified way of designing the nozzle contour by the method of characteristics (MoC) is done by constructing a minimum length nozzle [6]. This type of nozzle has its expansion region reduced to a point at the throat, creating a centered expansion fan followed by a straitening section designed to cancel the characteristics at the wall. The method used in this study was presented by Anderson[10] (Figure 6). In this calculation it is assumed that the sonic line is straight. The wall points derived from this computation were used to construct the nozzle geometry in Fluent.

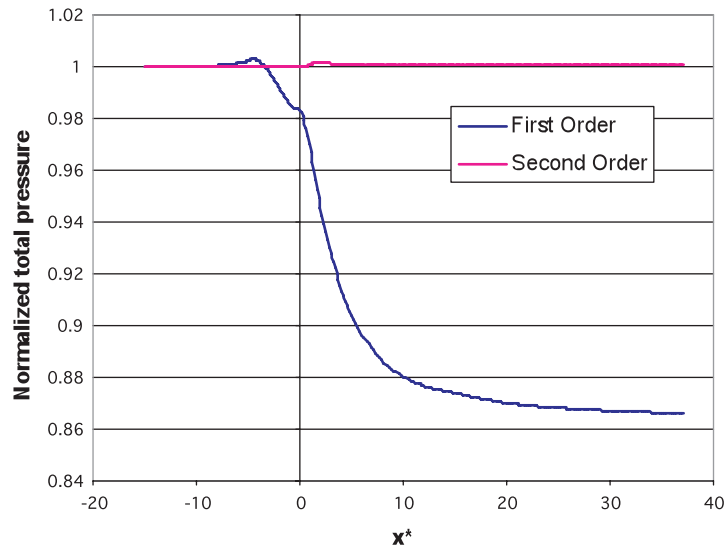


Figure 5. Variation of total pressure on the line of symmetry of a CD nozzle showing the unphysical decrease in the total pressure when using a first order solver.

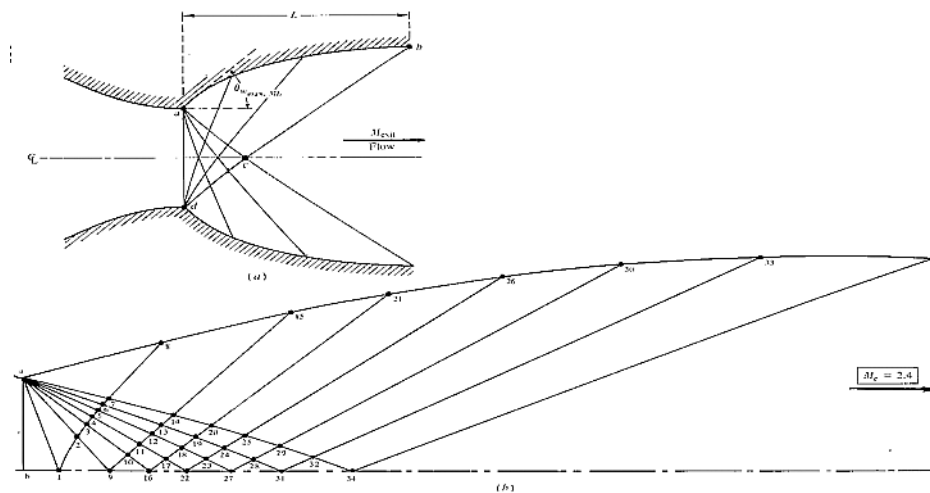


Figure 6. Minimum Length Nozzle structure (top) and layout of computational points for the method of characteristics (from Anderson).

In order to minimize the effects of the sonic line curvature, the converging part of the nozzle was designed with a large radius of curvature, but due to inaccurate representation of the arc that was used to construct the converging part; the throat was offset upstream in relation to the point where the expansion fan starts. The deviation was less than 0.5% of the throat height, but as a result the sonic line moved back to the position of the actual throat (Figure 7).

As a result the Mach number at the point of expansion was increased to  $M=1.3$  with a highly non-linear distribution across the throat (Figure 8).

Comparison between the predictions of the numerical simulations and the MoC computation shows that the resulting Mach number at the nozzle exit is lower than the designed Mach number by about 5%. The distribution of Mach numbers along the symmetry line are in reasonable agreement with the MoC computation and the second order discretization gives better results than the first order.

After correcting the geometry of the nozzle throat to represent the conditions of the MoC calculation the resulting Mach number distribution across the throat was relatively close to sonic conditions and the distribution along the nozzle symmetry line was in excellent agreement with the MoC calculation (Figure 9).

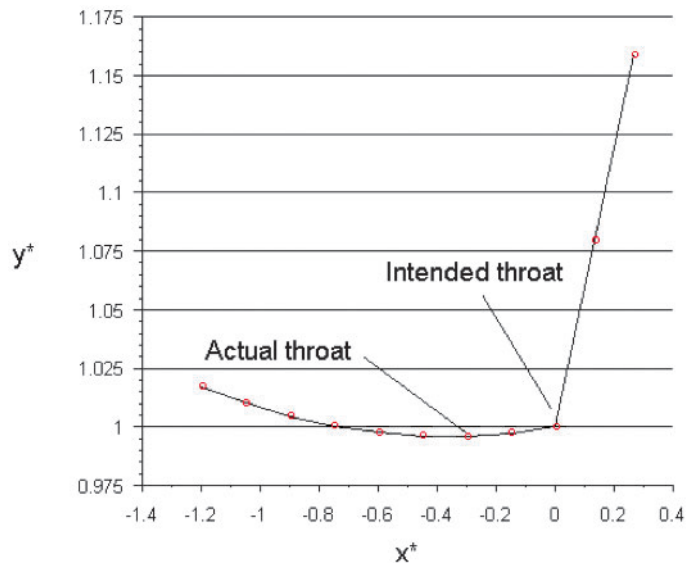


Figure 7. Boundary nodes in the CFD model showing the location of the intended and actual throat.

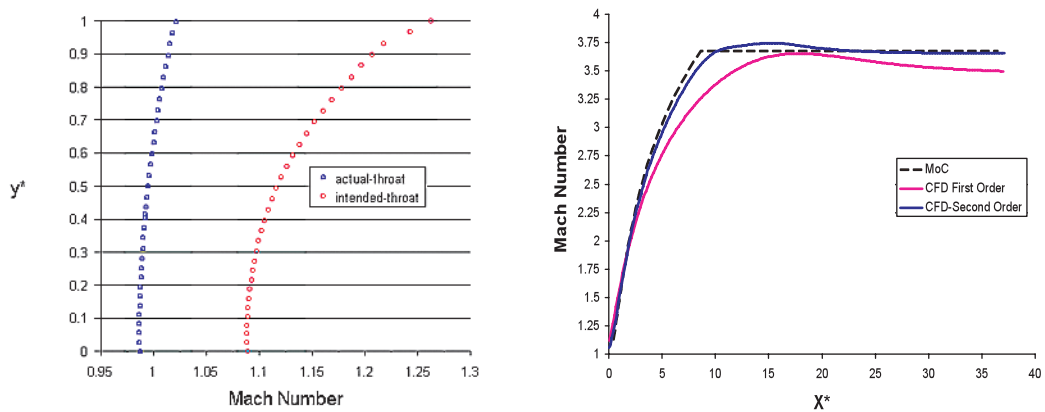


Figure 8. Mach number distribution across the nozzle at the location of the intended and actual throat (Left); Mach number distribution along the nozzle at the symmetry line; Dashed line - MoC, Solid line - CFD (Right).

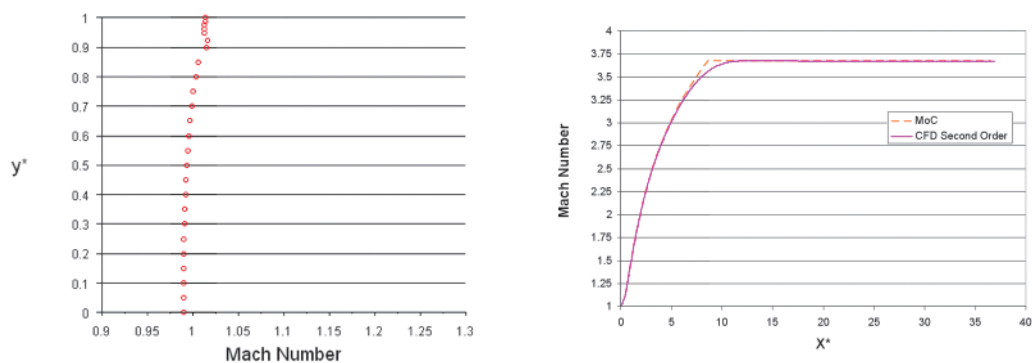


Figure 9. Mach number distribution across the nozzle at the throat (Left); Mach number distribution along the nozzle at the symmetry line; Dashed line - MoC, Solid line - CFD (Right).

## MODELING OF IDEAL NOZZLES

Sivells [11] developed a computational code based on the method of characteristics in order to design axisymmetric and planar nozzles for use in wind tunnels. The requirement for uniform flow in the test section at specified Mach number, while considering viscosity and heat transfer conditions, requires a set of computational methods. The nozzle is divided into several regions and the solution in each region is stitched to the others.

The throat region is calculated using the small perturbations transonic solution for irrotational flow. Then the upstream and downstream limits of the radial flow region are computed along with the final characteristic bounding the uniform flow area. Next, a network of characteristics is built from these boundaries and the wall of the nozzle is determined by comparing the mass flow through the throat to the integrated flow along each characteristic (Figure 10). The code allows imposing specific Mach numbers at the beginning and the end of the radial flow region as well as setting the Mach number distribution along the centerline. The last part of the code computes the turbulent boundary layer on the nozzle wall and adds a correction factor to the inviscid wall ordinate.

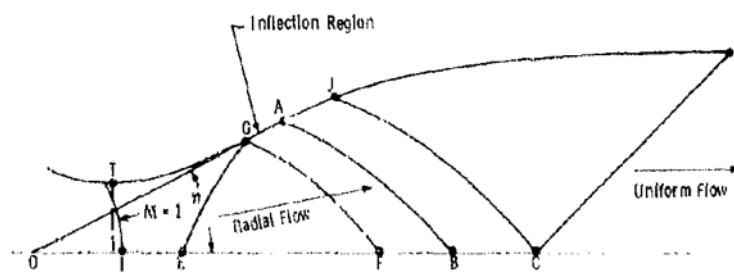


Figure 10. Defining points for calculating the contour of an ideal nozzle; D - source of radial flow, I - Sonic line, G - inflection point (from Sivells [11]).

The entered parameters to the code included the gas properties, radius of curvature of the throat (16), exit Mach number (3.676) and various parameters for the number of points on each characteristic. No restrictions were set for the Mach number distribution and the inflection point. The resulting nozzle has a rapid expansion and a short length.

After computing the nozzle geometry using Sivells code the calculated points along the wall were used to produce a curve for building the model in Fluent by using spline interpolation. Due to the small number of points used in the inflection region the shape of the curve was slightly distorted. The maximum offset in geometry of the wall was 2% of the local Y value (Figure 11).

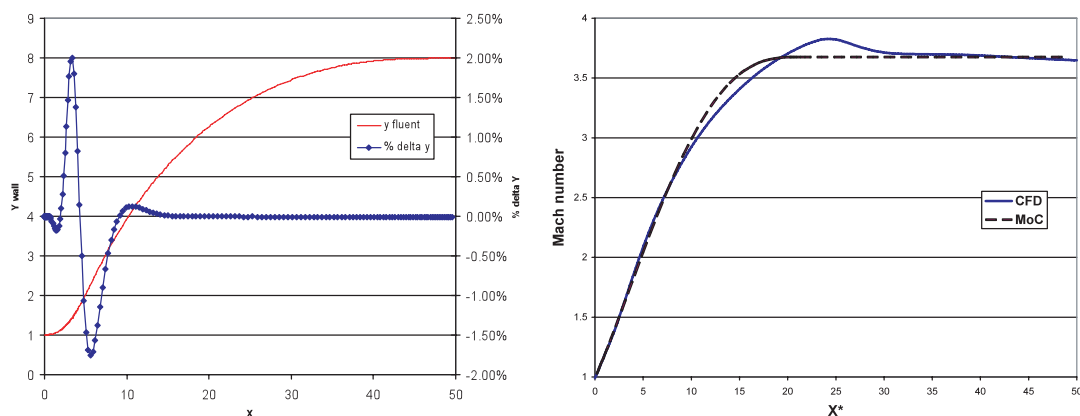


Figure 11. Deviation between wall contour calculated from MoC to geometry used in Fluent simulation; Solid line - nozzle wall, Marker line - % deviation between MoC and CFD (Left). Mach number distribution along symmetry line; Dashed line - MoC, Solid line - CFD (Right).

As a result of this deviation a weak disturbance emanated from the inflection region on the wall and propagated towards the symmetry of the nozzle, reflecting from it towards the nozzle outlet. This produced a 4% increase in Mach number at  $X=25$  compared to the design Mach number followed by a gradual decrease from that point downstream. At the nozzle exit plane the Mach number was somewhat non-uniform. Small geometric changes in the throat and expansion regions of the nozzle were found to cause significant changes in the performance of high-Mach number wind-tunnel nozzles [12].

After increasing the number of points on the wall near the inflection region and rebuilding the geometry, the error in the wall contour was reduced to less than 0.025%.

The resulting flow simulation showed improved flow uniformity and excellent agreement with the MoC calculation (Figure 12).

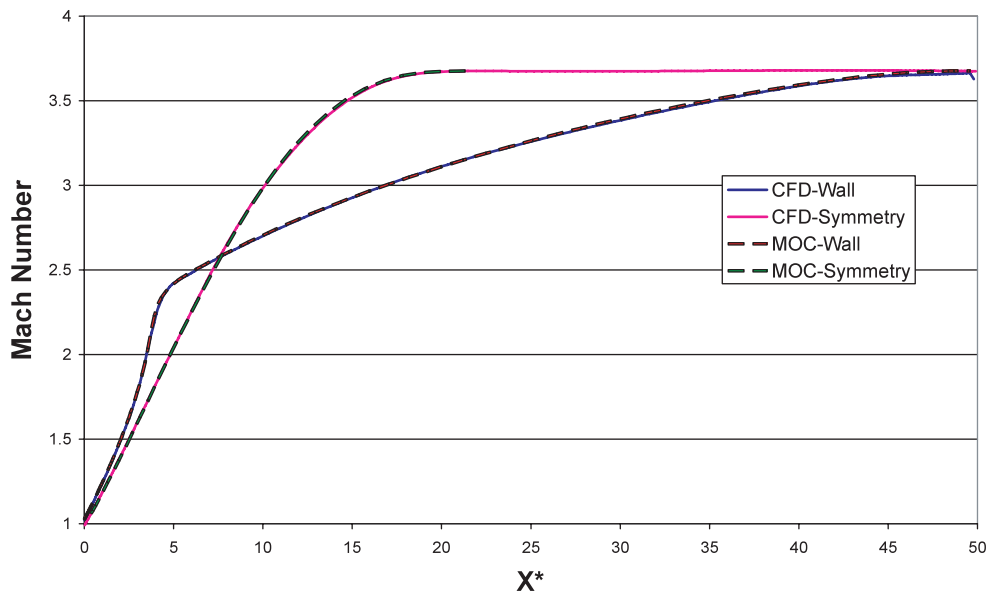


Figure 12. Mach number distribution along symmetry line after fixing the geometry; Dashed line - MoC, Solid line - CFD.

## CONCLUSION

Nozzle flow simulation can be as simple as solving one-dimensional flow equations or as complex as using high order numerical schemes on parallel computer clusters. For the engineering level, today's commercial CFD software offer a convenient way of acquiring accurate flow properties from supersonic converging-diverging nozzles provided that certain specific elements of the model are observed. Special attention must be given to the geometric building of the computational domain. Determination of the exact placement of nodes on the boundary representing the wall of the nozzle is critical and even small displacement of the nodes in the region of the throat and expansion area may result in formation of a disturbance that will propagate in the computational domain and affect the flow characteristics.

Fine resolution of the wall nodes is needed to accurately represent the curvature of the throat section and cannot be done by producing a coarse grid and then using mesh adaptation features while using the solver.

First order discretization should only be used to start the computational procedure and as a way of accelerating convergence, but for accurate results second order or higher is essential.

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