Numerical simulation of two-dimensional flows with different approximation schemes for shock wave capturing

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Abstract. *Shock waves can occur inside nozzle rocket engines by different causes: relatively higher ambient pressure, nozzle geometric aspects, or even small superficial imperfections in the divergent region of the nozzle. Even if a perfect rocket nozzle could be manufactured, shock waves would appear during the transient regime, corresponding to the turning-on time interval of the rocket engine. Numerically, shock waves show a series of difficulties to be captured, since high order approximation schemes, such as the Central Differencing Scheme (CDS), can present wiggles and other numerical oscillation phenomena and low order approximation schemes, such as the Upstream Differencing Scheme (UDS), present false or numerical diffusion. In order to guarantee better numerical results for such problems, Total Variation Diminishing (TVD) schemes were developed, combining aspects of both UDS and CDS schemes. In this work, TVD, UDS and CDS schemes are compared for a two-dimensional steady flow in a rocket engine. Flow with constant properties is considered in the numerical code, implemented using the Finite Volume Method (FVM), non-starred grids, SIMPLEC pressure-velocity coupling and a suitable methodology for all speed flows. Numerical verification and validation were employed in order to certificate both the solution and the model. Richardson Repeated Extrapolations (RRE) technique were also employed as post-processing, in order to obtain more accurate numerical results. At the end of the study we conclude that (1) the model is valid and the UDS solution is verified, (2) UDS with aid of RRE had the same error magnitude as accurate schemes with shorter time, (3) this TVD procedure could not avoid completely the oscillations and (4) other analysis are needed in other improve the RRE performance with shocks.*

Keywords: *TVD, Shock wave, Repeated Richardson Extrapolations*

1 INTRODUCTION

As can be observed in various works, numerical and experimental studies of shock waves, its interactions and patterns are important subjects (Delery and Dussauge, 2009; Hagemann and Frey, 2008; Martelli et al., 2010; Mowatt and Skews, 2011). Since the Finite Volume Method has been used in many fields, and especially in Computational Fluid Dynamics, great effort has been made on the development of new high-order accuracy schemes (Ramos, 2007). In addition, for the case of convection-diffusion problems, studies were done in order to avoid numeric diffusion and false oscillation (Versteeg and Malalasekera, 2007). Among such works, many ones were the Total Variation Diminishing (TVD) schemes.

For unsteady problems TVD provided good oscillation control. In the case of steady problems, Versteeg and Malalasekera (2007) presented a procedure to use the TVD scheme. This procedure is based on deferred correction using UDS implicitly and is simple to apply, mainly in cases where UDS is present.

Besides raising the accuracy order of numerical schemes, it is also possible to use extrapolation in order to raise the solution accuracy. Numerical solutions can be improved using the extrapolation provided by Richardson (1910), or in case of multiple meshes by applying this extrapolation recursively.

Then, this work present an effort to avoid numerical oscillations, false diffusion and improve the solution accuracy by means of RRE to a two-dimensional axisymetric supersonic flow in a nozzle. Experimental data and analytical solution will be used in order to validate the model and verify the numerical solution.

2 METHODOLOGY

2.1 Mathematical model

The gas flow inside a rocket engine nozzle can be studied by a two-dimensional axisymmetric inviscid model. In this case, the mass, momentum (in axial and radial axis) and energy conservation laws and the state equation are employed:

$$\frac{\partial}{\partial z}(\rho u) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho v) = 0 \tag{1}$$

$$\frac{\partial}{\partial z}(\rho u u) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho v u) = -\frac{\partial P}{\partial z} \tag{2}$$

$$\frac{\partial}{\partial z}(\rho u v) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho v v) = -\frac{\partial P}{\partial r} \tag{3}$$

$$\frac{\partial}{\partial z}(\rho u T) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho v T) = \frac{1}{c_P}[\boldsymbol{\nabla}(p\boldsymbol{V}) - p\boldsymbol{\nabla}\boldsymbol{V}] \tag{4}$$

$$p = \rho R T \tag{5}$$

where ρ represents the density, u the velocity in the axial direction, r the radius of the nozzle, v the velocity in the radial direction, p the pressure, T the temperature, c_P the specific heat, $\boldsymbol{V}$ the velocity vector and R the gas constant.

2.2 Numerical discretization

When complex geometries need to be discretized Versteeg and Malalasekera (2007) suggest the use of non-orthogonal structured meshes. The equation and coordinate transformation process will be not shown here, more details can be seen in Maliska (2004) and Versteeg and Malalasekera (2007). Still, the variables are co-located in the mesh and we used FVM. Special treatment is given to the mass conservation equation, by the use the SIMPLEC algorithm that couple mass and momentum conservation equations. Specific details of the SIMPLEC algorithm can be found in Maliska (2004) and Versteeg and Malalasekera (2007). Because supersonic and subsonic velocities occur in a nozzle, an approach that handles with both velocity regimes needs to be used. For this, we used Marchi and Maliska (1994) methodology, suitable for flows at any speed.

Since the mathematical model is transformed in a generalized non-orthogonal coordinate system it needs to be discretized, despite not being showed here, the transformed equations are available in a report by Marchi and Araki (2007). The properties are evaluated at the volume faces, Eq. 6 show an arbitrary property interpolated in the west face, where P represents the reference control volume, W the west volume of P, ψ the limiter function, r_{gw} the gradient ratio to the west face, α is an auxiliary constant of value 0.5 used to store the flow direction and the superscript $*$ refers to the deferred correction. In other words, these terms are solved explicitly. Equation 7 presents the gradient ratio in a positive and negative flow direction.

$$\phi_w = \phi_W(1/2 + \alpha_w) + \phi_P(1/2 - \alpha_w) + \alpha_w \psi(r_{gw}^{+-})(\phi_P^* - \phi_W^*) \tag{6}$$

$$r_{gw}^{+-} = \frac{(1/2 + \alpha_w)(\phi_W - \phi_{WW}) + (1/2 - \alpha_w)(\phi_E - \phi_P)}{\phi_P - \phi_W} \tag{7}$$

Since we are using ghost cells technique (Maliska, 2004) to apply the boundary conditions, it is observed that in the first real control volume there is no volume to evaluate the ϕ_{WW} term. Therefore, a linear interpolation is needed. With the first real volume, its respective ghost cell and the volume needed (WW) it is easy to achieve the Eq. 8, which presents the volume interpolated. Furthermore, inserting this result in a positive flow direction gradient ratio to the west face yields Eq. 9, that is the gradient ratio for the first real control volume in the case of positive direction flow. We presented only approximations to the west face, in a similar fashion the approximations to the other faces can be obtained.

$$\phi_{WW} = 2\phi_W - \phi_P \tag{8}$$

$$r_{gw}^{+} = \frac{\phi_W - \phi_{WW}}{\phi_P - \phi_W} = \frac{\phi_W - (2\phi_W - \phi_P)}{\phi_P - \phi_W} = 1 \tag{9}$$

The limiter function carry on the information about how scheme will be used, Versteeg and Malalasekera (2007) presented some of limiter functions. They also commented that UDS present false diffusion, CDS wiggles and that there is no convincing argument in favour of any TVD limiter function. Because of this, we started the study with SUPERBEE, by Roe (1965). The limiter functions used in this study are shown in Eq. 10 to 12, that are: UDS, CDS and SUPERBEE, respectively.

$$\psi = 0 \tag{10}$$

$$\psi = 1 \tag{11}$$

$$\psi(r_{gw}) = max[0, min(2r_{gw}, 1), min(r_{gw}, 2)] \tag{12}$$

2.3 Numerical verification and post-processing

In order to verify our simulation we check the apparent and effective orders of the approximations. Equations 13 and 14 show how to obtain the apparent and effective orders (Marchi, 2001), where q is the refine ratio and E is the numerical error. Subscripts 3, 2 and 1 represent solutions in thin, intermediary and coarse meshes, 32 refer to refine ratio between thin and intermediary meshes and 21 between intermediary and coarse meshes.

$$p_U = \frac{\log\left[\left(\frac{\phi_2-\phi_1}{\phi_3-\phi_2}\right)\left(\frac{q_{32}-1}{q_{21}-1}\right)\right]}{\log\left(q_{32}\right)} \tag{13}$$

$$p_E = \frac{\log\left[\frac{E(\phi_2)}{E(\phi_3)}\right]}{\log\left(q_{32}\right)} \tag{14}$$

Repeated Richardson Extrapolations were used to improve solution accuracy order, that begins with the Eq. 15 and the idea that this equation can be applied, in theory, infinitely. After that, we can write Eq. 16, that represents the RRE (Martins, 2013), where ϕ_∞ represents the extrapolated solution, the subscript g indicates the mesh level and m the extrapolation level. Superscripts p_L represent the asymptotic order and p_v the true order. The asymptotic order is the first value of the true orders, the latter can be obtained with a Taylor series expansion. More details can be seen in Marchi (2001).

$$\phi_\infty = \phi_3 + \frac{\phi_3 - \phi_2}{q^{p_L} - 1} \tag{15}$$

$$\phi_{g,m} = \phi_{g,m-1} + \frac{\phi_{g,m-1} - \phi_{g+1,m-1}}{q^{p_{v(m-1)}} - 1} \tag{16}$$

2.4 Simulation aspects

The nozzle geometry utilized in this work is same as the fifth presented in Back et al. (1965). The base mesh has 24 volumes in the axial direction and 10 in the radial direction. The mesh refinement was done with a variable refine ratio, resulting in a final mesh with 1536 volumes in the axial direction and 640 in the radial direction for UDS and TVD. The finest mesh for CDS has 384 axial and 160 radial volumes.

Since we want to compare the numerical results with experimental data, it is necessary to use the same parameters originally used by Back et al. (1965). The pressure utilized was $1725.07\ MPa$ and temperature of $833.33\ K$. The numerical study was conducted using specific gas constant of $286.90\ J/kgK$ and specific heat ratio of 1.40. The flow is considered to be not disturbed in the entrance and locally parabolic in the exit. The conditions for the upper boundary were zero pressure gradient. Finally, the lower boundary is a symmetry line. More detailed information about the application of the boundary conditions can be observed in the report by Marchi and Araki (2007).

3 NUMERICAL RESULTS

Table 1 presents simulation aspects for the schemes used, due to great oscillation problems the CDS had diverged since mesh 7. Table 2 shows the absolute numerical errors of the discharge coefficient with and without RRE for the schemes in respective mesh. The discharge coefficient is a ratio between the numerical solution and one-dimensional analytical mass flow rate (Araki, 2007). Kliegel and Levine (1969) presented a method to evaluate the analytical discharge coefficient based on the nozzle geometry. This method were used in this work to evaluate the analytical discharge coefficient.

Table 1: Simulation aspects

Mesh	Mean size in z $[m]$	Volumes axial x radial	Refine ratio	Simulation processing time UDS	CDS	TVD
1	7.71E-03	24x10	-	0.06 $[s]$	0.89 $[s]$	0.41 $[s]$
2	3.85E-03	48x20	2.0	0.19 $[s]$	7.02 $[s]$	1.52 $[s]$
3	1.93E-03	96x40	2.0	0.98 $[s]$	1.83 $[min]$	13.0 $[s]$
4	9.64E-04	192x80	2.0	20.245 $[s]$	19.3 $[min]$	5.14 $[min]$
5	6.42E-04	288x120	1.5	1.51 $[min]$	1.54 $[h]$	15.5 $[min]$
6	4.82E-04	384x160	1.3	6.82 $[min]$	4.42 $[h]$	43.9 $[min]$
7	3.21E-04	576x240	1.5	29.3 $[min]$	-	4.81 $[h]$
8	2.41E-04	768x320	1.3	1.11 $[h]$	-	15.4 $[h]$
9	1.61E-04	1152x480	1.5	6.22 $[h]$	-	9.68 $[days]$
10	1.20E-04	1536x640	1.3	16.6 $[h]$	-	12.6 $[days]$

Note: - not obtained or unavailable

It is clear from Tab. 1 that the UDS solutions required the smallest processing time, followed by TVD and CDS. Now, from Tab. 2 we see that UDS reached the same error magnitude than CDS and TVD at mesh 7 with RRE. Since the post-processing time to use RRE is small, the time requirement imposed by the UDS is smaller than CDS and TVD to achieve the same error magnitude. Furthermore, the RRE could not reach the optimal performance as expected, despite reducing the error in some cases.

Figure 1 shows the pressure distribution on the wall due to experimental data from Back et al. (1965) and UDS, CDS and TVD numerical solutions. Recalling that CDS had diverged since mesh 7, the Fig. 1 and 2 to 4 show the numerical solution in the thinnest possible mesh.

The numerical solutions are close to the experimental data, except in the high gradient region were the maximum estimated error to UDS was 9.12 $\%$ and to TVD 9.20 $\%$. Since the maximum experimental error was 5 $\%$, the estimated error is reasonable.

Figures 2 to 4 shows Mach number isolines for the finest meshes. In such figures, we see an oblique shock wave, same as observed by Back et al. (1966), and oscillations produced by CDS and TVD. One can note that CDS oscillations appears before and after the shock wave and its reflection, while TVD oscillations appears only after. This TVD procedure could not avoid oscillations, despite of blocking them to propagate upstream to the entire flow.

Table 2: Numerical errors to the discharge coefficient with and without RRE

	Without RRE			With RRE		
Mesh size $[m]$	UDS	CDS	TVD	UDS	CDS	TVD
7.71E-03	9.38E-02	2.93E-02	5.01E-02	-	-	-
3.85E-03	6.07E-02	5.69E-03	1.68E-02	2.79E-02	1.82E-02	1.67E-02
1.93E-03	3.25E-02	1.53E-03	7.94E-04	3.49E-03	2.58E-03	1.47E-02
9.64E-04	1.76E-02	8.98E-04	6.24E-04	2.84E-03	1.03E-03	8.60E-03
6.42E-04	1.18E-02	7.14E-04	4.63E-04	4.26E-03	1.62E-04	5.30E-03
4.82E-04	8.90E-03	5.72E-04	4.27E-04	3.82E-03	9.60E-04	5.16E-03
3.21E-04	5.95E-03	-	3.08E-04	5.01E-04	-	1.92E-03
2.41E-04	4.41E-03	-	2.93E-04	2.62E-03	-	3.80E-03
1.61E-04	2.85E-03	-	2.90E-04	6.56E-04	-	7.79E-04
1.20E-04	2.08E-03	-	2.77E-04	2.80E-04	-	2.44E-04

Note: - not obtained or unavailable

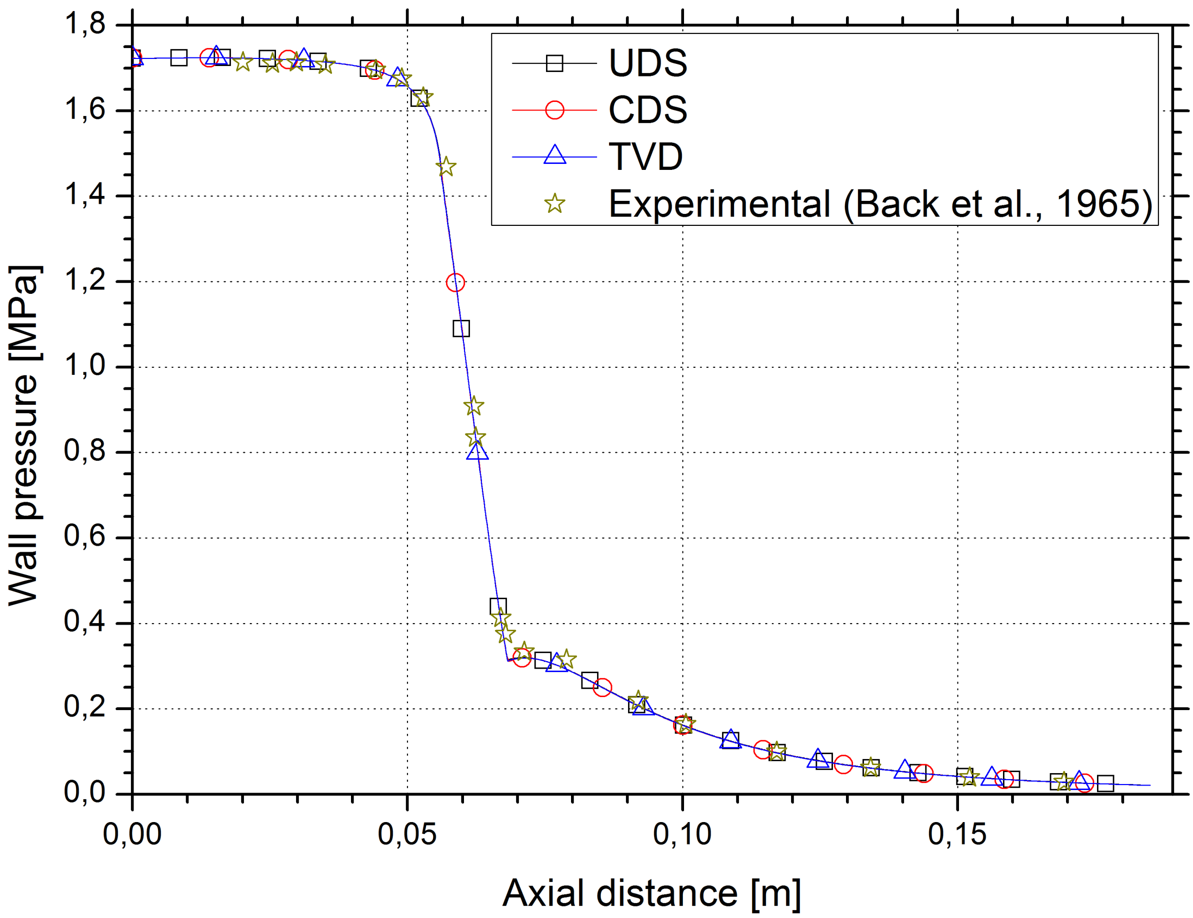

Figure 1: Wall pressure due to experimental data and numerical solutions.

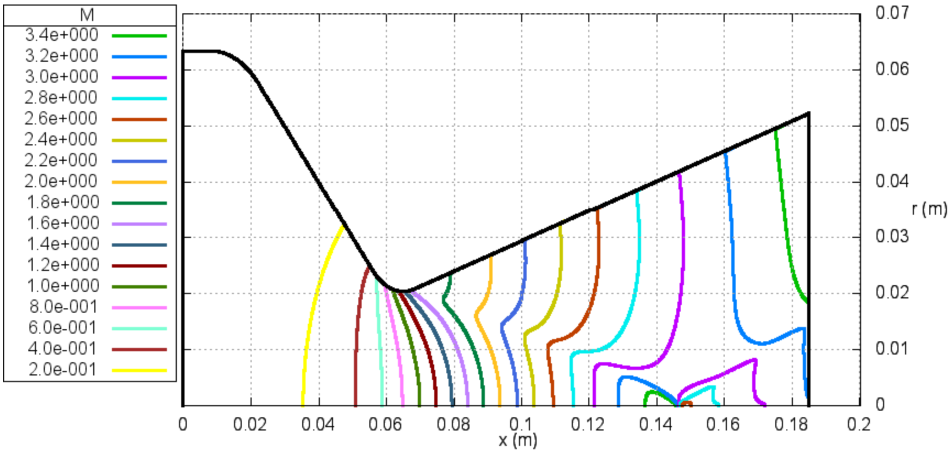

Figure 2: Isolines for Mach number in the finest mesh UDS solution.

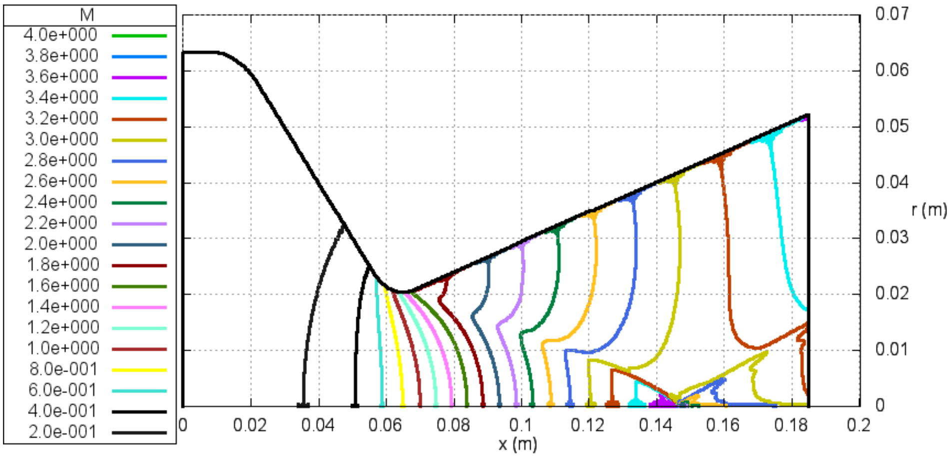

Figure 3: Isolines for Mach number in the finest mesh CDS solution.

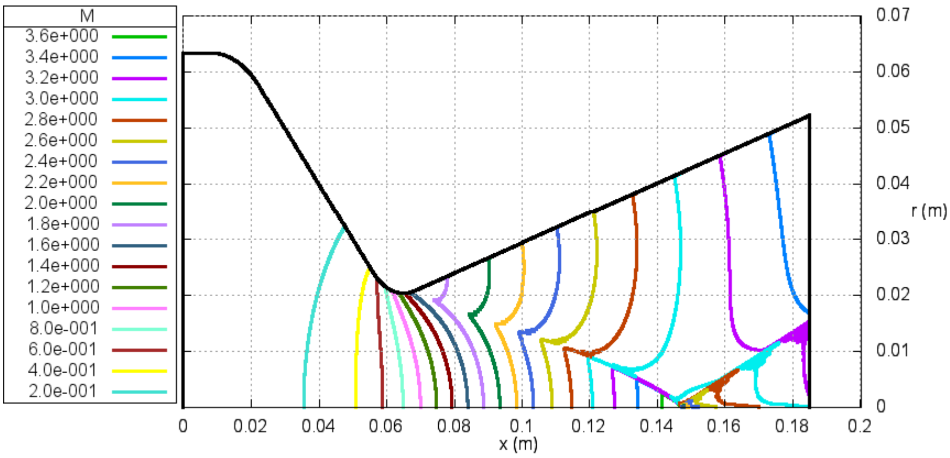

Figure 4: Isolines for Mach number in the finest mesh TVD solution.

The absolute numerical errors and orders for the discharge coefficient of the schemes can be seen in Fig. 5 and 6.

Figure 5 shows that only UDS without RRE had a stable and expected behaviour. The CDS

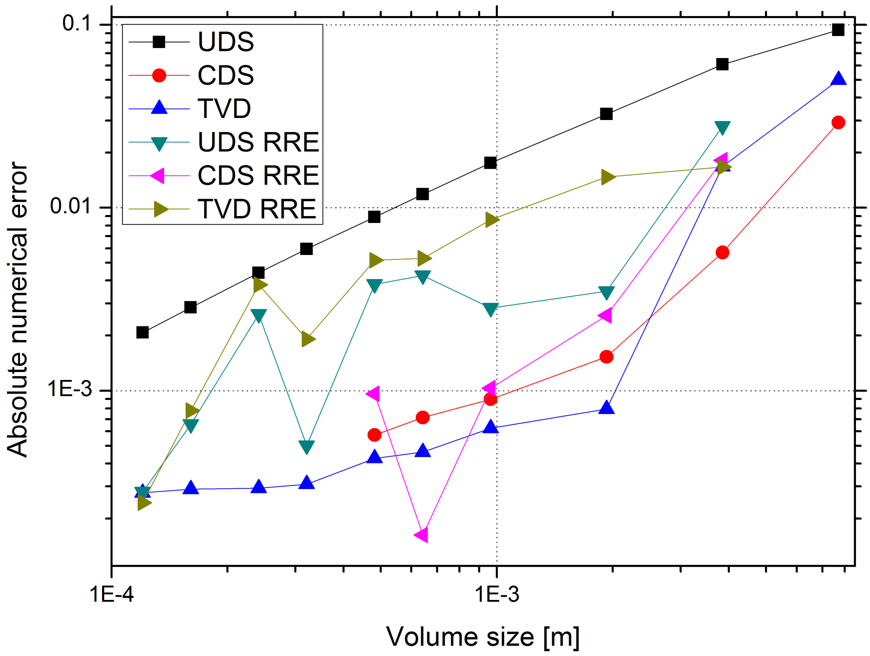

Figure 5: Absolute numerical errors with and without RRE for discharge coefficient.

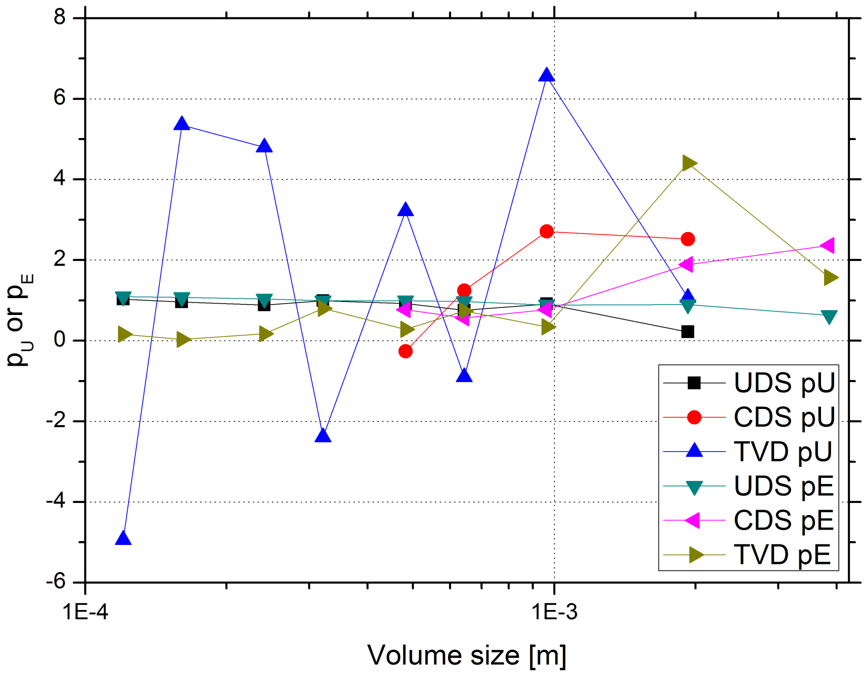

Figure 6: Apparent and effective orders for discharge coefficient.

without RRE error is close to expected stability and behaviour, while TVD errors oscillate in both cases. Now, comparing the asymptotic order, one for UDS and TVD and two to CDS, we observe that only apparent and effective UDS orders are close to the asymptotic value. In other words, with these meshes only the UDS could be verified. It is necessary more meshes to verify the TVD solution and we are unable to verify the CDS solution, since it had diverged for the thinnest meshes.

4 CONCLUSIONS

We have presented a valid model to compute two-dimensional axisymmetric inviscid under-expanded supersonic flows in nozzles. In verification process only the UDS solution could be evaluated, more meshes are necessary to verify the TVD solution. The TVD procedure could not avoid completely the oscillations, it was only before the shock wave and its reflection. Due to great oscillation problems the CDS solution had diverged since mesh 7.

With the aid of a post-processing tool, RRE in our case, the numerical error of a less accurate approximation can be reduced to the same magnitude of a more accurate scheme with shorter time. In practical applications, where the numerical error do not need to be such small, this magnitude error is reasonable. Furthermore, it does not present numerical oscillations.

Despite reducing the error in some cases, the RRE could not reach its optimal performance. This is specially valid for CDS and TVD, which did not reach their expected behaviour, as shown in Fig. 5. In the case of UDS the error presented the expected behaviour. However, RRE did not reached its optimal performance and we suppose that another error source is present, besides the discretization error. This performance issue has already been observed in a one-dimensional with normal shock wave study by Silva and Araki (2014). Therefore, it is necessary improve the RRE performance with shocks to allow a fast error reduction.

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