

APPLICATION OF DIFFERENT INTERPOLATION SCHEMES FOR REACTIVE FLOWS IN ROCKET NOZZLE ENGINES

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Abstract. *The accuracy of a numerical solution is strongly related to which interpolation scheme is used to discretize a mathematical model. Two of the most used schemes are the UDS (Upstream Differencing Scheme) and the CDS (Central Differencing Scheme). Although the CDS presents second order of accuracy, it can exhibit numerical oscillations and even numerical divergence, depending of the studied problem. On the other hand, the UDS presents much easier convergence but it exhibits numerical diffusion. In order to avoid UDS and CDS problems, other approximations schemes were developed, such as the TVD (Total Variation Diminishing) ones. TVD is not a single interpolation scheme, but actually a family of schemes, which basically differs one to another by the limiting functions. In this work, different TVD schemes are employed for frozen and local equilibrium reactive flows in rocket nozzle engines. Such flows presents a strongly variation in gases speed: it starts with nearly null velocities and achieves supersonic flow in the exit region of the nozzle. Reactive models includes from three to eight chemical species for hydrogen/oxygen reactions, which are usually employed as propellants for high performance rocket engines. In order to evaluate numerical uncertainties of results, numerical verification techniques are used. By analyzing numerical results, it was observed that TVD Min-Mod presents better performance for reactive flows in studies, especially for local equilibrium flows, since it provides numerical results with equivalent uncertainties and accuracy of CDS results, with smaller computational processing time.*

Keywords: TVD, frozen flow, local equilibrium flow, rocket nozzle engines, H_2/O_2 .

1. INTRODUCTION

Different interpolation functions for reactive compressible flows inside a rocket nozzle engine are studied in this work. Two different physical models are included in numerical tests: the frozen and the local equilibrium flows. Both models are limiter cases of the actual reactive flow into a rocket nozzle: while for the frozen flow the chemical composition remains constant throughout space and time, the local equilibrium flow implies infinite chemical and vibrational reaction rates (Anderson Jr, 2003).

Studying reactive flows in rocket nozzles, Wang (2006) noted that: simulations in structured meshes have better results than in unstructured meshes; the effects of heat exchange due to radiation are small compared to the convective effects, with little influence on thrust; a generally finite rate models show better results than the local chemical equilibrium; and consideration of thermal losses in regeneratively cooled engine improves thrust prediction. However, none estimate of numerical errors for the numerical results were provided.

The accuracy of numerical solutions is dependent on the chosen interpolation schemes. While first order schemes, such as UDS, are subjected to the false diffusion phenomenon, higher order schemes, such as CDS, are subjected to numerical spurious oscillations, usually called as "wiggles" (Versteeg and Malalasekera, 2007). In recent years, efforts have been made to build interpolation schemes which can give high order of accuracy without introducing spurious oscillations and converge to physically correct solution (Kumar and Kadalbajoo, 2008). Such schemes must attempt a special feature known as monotonicity preserving, which consists on the following facts: (i) they must not create local extrema, and (ii) the value of an existing local minimum must be non-decreasing and that of a local maximum must be non-increasing (Versteeg and Malalasekera, 2007).

Concerning about the oscillation control schemes, many studies have been carried out since the late 1970s and several important concepts, such as: the Total Variation Diminishing (TVD), proposed by Harten (1983); the Total Variation Bounded (TVB); and the Essentially Non-Oscillatory (ENO) schemes, among other ones. All these schemes have been proposed focusing the achievement of better convergence and stable calculation (Kim and Kim, 2005).

The key idea of ENO schemes is to use the smoothest stencil among several candidates in evaluating fluxes at a cell boundary which should yield higher order spatial accuracy and essential non-oscillatory profile near shocks. TVB

concept allows oscillations only if spurious oscillations do not grow unboundedly large as time evolves. Although TVB or ENO avoids unphysical clipping at extrema and enhances accuracy, it is inevitable to yield undershoot and/or overshoot which in turn influences convergence badly (Kim and Kim, 2005).

Although with ENO and WENO schemes there are higher-order alternatives, TVD schemes are still in widespread use; one reason for that is the simple implementation (Kemmm, 2011). TVD schemes are conservative, generally (at most times) second-order accurate, non-oscillatory in nature and capable of resolving discontinuity in the solution (Kumar and Kadalbajoo, 2008). However, Guerrero (2015) notes that the choice of the limiter function dictates the order of the scheme and its boundedness. In order to study the effects of such limiter functions on numerical solution for compressible reactive flows, two TVD schemes are compared, both proposed by Roe (1985): the SUPERBEE and the Min-Mod ones.

2. MATHEMATICAL MODEL

Especially for preliminary design studies, the combustion gases flow inside a rocket nozzle can be modeled by the quasi-one-dimensional model, which overpredicts the actual rocket performance by 1 to 6% (Sutton and Biblarz, 2010). Such model consists of the mass, momentum and energy conservation equations, as well as by the perfect gas state equation, given by

$$\frac{d}{dx}(\rho u S) = 0 \quad (1)$$

$$\frac{d}{dx}(\rho u S u) = -S \frac{dP}{dx} + F' \quad (2)$$

$$c_p \frac{d}{dx}(\rho u S T) = u S \frac{dP}{dx} + q' + S_{eq} \quad (3)$$

$$P = \rho R T \quad (4)$$

where: ρ [kg/m^3], u [m/s], P [Pa] and T [K] are the four variables of interest, representing density, velocity, pressure and temperature respectively; x [m] is the axial coordinate of the nozzle; S [m^2] cross-sectional area along the longitudinal axis of the nozzle; R [J/kgK] is the gas constant mixing within the nozzle and c_p [J/kgK] the specific heat at constant pressure; F' and q' are the effects of shear strength and gain or loss of heat; S_{eq} is a chemical source term, which is null for frozen flow and, for local equilibrium flow is evaluated by

$$S_{eq/lf} = -\sum_{i=1}^N h_i \frac{d}{dx}(\rho u S Y_i) \quad (5)$$

in which h_i is the enthalpy of chemical specie i , Y_i is the weight fraction of the chemical specie i and N is the total number of chemical species.

For both frozen and local equilibrium flows, chemical species involve the reaction between H_2 and O_2 , one of the highest performance rocket propellant pair. Such propellants are used in the Delta IV launcher, Centaur upper stage, the Space Shuttle main engine, and upper stage space engines developed in Japan, Russia, Europe, India, and China (Sutton and Biblarz, 2010). Table 1 summarizes the chemical reaction schemes implemented in the numerical code used in this work. In such Table: N is related to the number of species, which varies from 3 to 8; and L is the number of chemical reaction equations, which varies from null to 18.

Table 1. Available chemical reaction schemes in numerical code for frozen and local equilibrium flows.

Model	L	N	Species	Observations
0	0	3	H_2O, O_2, H_2	Ideal model
1	1	3	H_2O, O_2, H_2	–
2	2	4	H_2O, O_2, H_2, OH	–
3	4	6	H_2O, O_2, H_2, OH, O, H	4 reactions with 3 rd body – Barros <i>et al.</i> (1990) and Smith <i>et al.</i> (1987)
4	4	6	H_2O, O_2, H_2, OH, O, H	4 reactions – Svehla (1964)
5	8	6	H_2O, O_2, H_2, OH, O, H	8 reactions (4 with 3 rd body) – Barros <i>et al.</i> (1990)
7	8	6	H_2O, O_2, H_2, OH, O, H	8 reactions (4 with 3 rd body) – Smith <i>et al.</i> (1987)
10	6	8	$H_2O, O_2, H_2, OH, O, H, HO_2, H_2O_2$	4 reactions from model 3 and 2 from Kee <i>et al.</i> (1990) – all the reactions including 3 rd body
9	18	8	$H_2O, O_2, H_2, OH, O, H, HO_2, H_2O_2$	18 reactions (5 with 3 rd body) – Kee <i>et al.</i> (1990)

3. NUMERICAL MODEL

The presented mathematical model for reaction gas products is discretized using the Finite Volume Method (Versteeg and Malalasekera, 2007). A co-located grid arrangement, appropriated for all speed flows is used (Marchi and Maliska, 1994). Pressure and velocity are coupled by SIMPLEC algorithm (Van Doormaal and Raithby, 1984), in order to convert the mass equation in a pressure (or better, in a pressure-correction) one. So, the mass conservation equation, Eq. (1), is used for determination of a pressure-correction (P'). Velocity (u) is obtained from Eq. (2), and the energy equation, Eq. (3), is taken for temperature (T) determination. Density (ρ) is gotten from the state equation, Eq. (4). It must be noted that axial velocity (u) is evaluated from very reduced values (near null values) until supersonic ones, and not only for supersonic values, as commonly found in literature.

The implemented numerical model also includes different approximation schemes: (1) the Upwind Differencing Scheme (UDS); (2) the Central Differencing Scheme (CDS); and two TVD schemes - Superbee and Min-Mod, both proposed by Roe (1985). These two TVD schemes vary only according to the limiter function ψ_e , which is defined as

$$\psi(r) = \max[0; \min(2r; 1); \min(r; 2)] \quad (6)$$

for Superbee; and is

$$\psi(r) = \begin{cases} \min(r; 1), & \text{if } r > 0 \\ 0, & \text{if } r \leq 0 \end{cases} \quad (7)$$

for Min-Mod. The value of r is obtained by the following expressions:

$$r_e = \frac{\phi_P - \phi_W}{\phi_E - \phi_P} \text{ and } r_w = \frac{\phi_W - \phi_{WW}}{\phi_P - \phi_W} \quad (8)$$

where ϕ represents the variable of interest and subscripts are related to the control volumes.

The development of TVD schemes is related to the computational research during the past three or four decades, which has focused on developing non-linear, non-oscillatory approximation schemes (Bidadi and Rani, 2014). Compared to other high-order methods, such as ENO and WENO, to two or three space-dimensional problems, TVD presents simpler implementation, compact stencil and robustness (Kemmm, 2011). Unfortunately, in literature only a few works are related to the TVD limiters comparison, especially for reactive flows.

Sweby (1984) introduced a requirement for second-order accuracy of TVD limiters, which is known as symmetry property. According to this property, all limiters that stay inside the blue area of Fig. 1 on the r - ψ diagram represent second-order accurate schemes. Such region is lower limited by the Min-Mod function, while the Superbee scheme follows the upper limit. Because of this both functions were chosen to be studied in the current work.

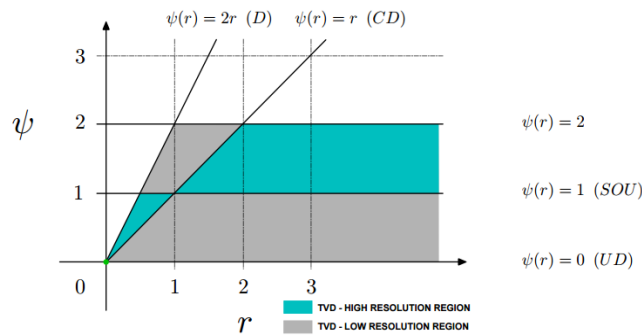


Figure 1. r - ψ diagram (Guerrero, 2015)

For both frozen and local equilibrium flows, the simulations were made for at least three different grids, to allow the determination of apparent convergence order (Marchi, 2001; Marchi and Silva, 2005). Some pieces of information about numerical errors and error estimators can be found in Tannehill *et al.* (1997), Marchi (2001), and Ferziger and Perić (2001). Asymptotic error order depends on the chosen discretization model, while apparent order, for constant refinement ratio, is evaluated by

$$p_U(h_1) = \frac{\log(\psi_U)}{\log(q)} \quad (9)$$

in which h is the grid spacing or distance between two successive grid points, the subscript 1 refers to the fine grid, q is the grid refinement ratio ($q = h_2 / h_1$), and ψ_U is the numerical solution convergence ratio for analytical one, defined by

$$\psi_U = \frac{(\phi_2 - \phi_3)}{(\phi_1 - \phi_2)} \quad (10)$$

where ϕ_1 , ϕ_2 and ϕ_3 correspond, respectively, to the numerical solution for the fine, intermediate and coarse grids. Besides, the numerical uncertainties can be evaluated by estimators, such as the GCI, proposed by Roache (1997), whose expression is given by

$$GCI(\phi_1, p) = FS \frac{|\phi_1 - \phi_2|}{(q^{p_L} - 1)}, \quad (11)$$

where p_L is related to the asymptotic order and FS is the safety factor, which is suggested to be equal 3.

4. NUMERICAL RESULTS AND DISCUSSION

The geometry of the rocket propulsion thruster chosen for the numerical studies presented in the current work is the same used by Marchi *et al.* (2000; 2004) and Araki and Marchi (2006), which consists on a cylindrical section, called combustion chamber (with radius r_{in} and length L_C) assembled to a nozzle device, whose longitudinal section is defined by a cosine curve (with neck nozzle radius r_g and length L_n). The radius r , for $x > L_C$, is evaluated by the following equation:

$$r = r_g + \frac{(r_{in} - r_g)}{2} \left\{ 1 + \cos \left[2\pi \frac{(x - L_C)}{L_n} \right] \right\}, \quad (12)$$

where x corresponds to the position where the radius is evaluated.

For all studies presented in this work, the values used for geometrical parameters are: $r_g = 0.1$ m; $r_{in} = 0.3$ m; $L_C = 0.1$ m; $L_n = 0.4$ m. Inside the combustion chamber, the stagnation temperature (T_0) is taken as 3420.33 K, while the stagnation pressure value (P_0) is 20 MPa and liquid oxygen and liquid hydrogen are injected at the stoichiometric composition ($OF = 7.936682739$). For isentropic analytical solution, the gas constant (R) is taken as 526.97 J/kg·K and the ratio between specific heats (γ) is 1.1956.

The aim of numerical solutions is given by the evaluation of some parameters of interest, cited in the following:

1. Nozzle discharge coefficient (C_d): defined as the ratio between numerical mass flux ($\dot{m}_{num}$) and the theoretical one ($\dot{m}_{th}$), obtained from isentropic analytical solution:

$$C_d = \frac{\dot{m}_{num}}{\dot{m}_{th}}. \quad (13)$$

2. Non-dimensional momentum thrust (F^*): defined by the ratio between numerical and theoretical thrusts (F_{num} and F_{th} , in this order), given by

$$F^* = \frac{F_{num}}{F_{th}}, \quad (14)$$

where F corresponds to the thrust values and can be obtained by the following relation between mass flux ($\dot{m}$) and exit velocity (u_{ex}):

$$F = \dot{m} \cdot u_{ex}. \quad (15)$$

3. Pressure (P_{ex}), temperature (T_{ex}), density (ρ_{ex}), velocity (u_{ex}) and Mach number (M_{ex}) for gas products, at the nozzle exit.

All simulations were performed in a Dell Optiplex 7010 Computer, with Intel® Core™ i5 3.20 GHz and 4 GB RAM. For numerical studies, the coarsest grid used presented 50 control volumes and the finest one, 12800 for frozen flow and 1600 for local equilibrium flow; the chosen refinement ratio was $q = 2$. Numerical results presented in the current work refers to the model 2, listed in Tab. 1, which presents four species (H_2 , O_2 , H_2O and OH) and two reaction equations. All simulations were performed until the achievement of the round-off error, in order to allow the numerical verification, by the use of Eqs. (9) to (11).

Computational processing time (CPU time) requirements are presented in Tab. 2 and 3. It can be noted that CPU time is dependent on the chosen approximation scheme, with UDS as the fastest scheme for most of tests. It must be observed, however, that UDS presents only first order accuracy, while CDS and TVD are second order schemes. Among CDS and TVD, it can be seen that for the frozen flow, most of tests present smaller CPU time for CDS when compared to both TVD schemes. Such behavior, however, is not seen for the local equilibrium flow: for such physical model, TVD Min-Mod is faster than CDS for all tests. Comparing only the CPU time of TVD schemes, however, is inconclusive by the fact that, in some cases, TVD Min-Mod is faster than TVD Superbee, while for other ones, this behavior is totally the opposite one. The higher CPU time requirement observed for the local equilibrium flow compared to the frozen flow, for all approximation schemes is related to the fact that, for the former the chemical composition of the mixture of gases must be evaluated in each iteration, while for the frozen flow model, it is evaluated with a much smaller frequency.

Table 2. Computational processing time requirements for the frozen flow model (in seconds)

Grid / Scheme	UDS	CDS	TVD Min-Mod	TVD Superbee
50	2.06×10^0	2.25×10^0	4.18×10^0	4.13×10^0
100	6.40×10^0	7.04×10^0	1.55×10^1	1.24×10^1
200	1.98×10^1	2.17×10^1	5.98×10^1	1.19×10^2
400	4.87×10^1	5.34×10^1	2.36×10^2	3.50×10^2
800	1.91×10^2	2.11×10^2	4.66×10^2	9.49×10^2
1600	5.78×10^2	1.06×10^3	1.87×10^3	2.81×10^3
3200	1.49×10^3	4.13×10^3	1.37×10^4	9.35×10^3
6400	3.06×10^3	1.68×10^4	7.32×10^4	2.81×10^4
12800	2.79×10^4	8.29×10^4	1.86×10^4	9.41×10^3

Table 3. Computational processing time requirements for local equilibrium flow (in seconds)

Grid / Scheme	UDS	CDS	TVD Min-Mod	TVD Superbee
50	3.78×10^1	2.40×10^1	7.83×10^0	8.14×10^0
100	7.18×10^1	7.29×10^1	2.93×10^1	2.93×10^1
200	1.96×10^2	1.99×10^2	1.13×10^2	1.71×10^2
400	5.61×10^2	5.67×10^2	4.60×10^2	5.71×10^2
800	2.52×10^3	2.53×10^3	2.02×10^3	3.80×10^3
1600	6.80×10^3	1.32×10^4	1.10×10^4	2.00×10^4

Analysis of the apparent order (p_U) of all variables of interest were also made. Figures 2 and 3 provides the behavior of p_U for the pressure at nozzle exit for both frozen and local equilibrium flows. Such behavior was also observed for the other variables of interest and, because of this, none of all other variables are present in the current work. It can be noted in Fig. 2 that all approximation schemes present the expected behavior in relation to p_U : UDS results tend to the unitary value when the grid is refined, as well as both TVD schemes and CDS show a tendency of p_U to 2. For the local equilibrium flow, however, such behavior was not observed: UDS, CDS and TVD Min-Mod present a tendency of p_U to a unitary value; TVD Superbee, by its turn, presents an inconclusive tendency – numerical results for more refined grids should be analyzed to provide an accurate result of p_U . Such tendency of p_U to a unitary value can be attributed to the chemical source term of Eq. (3), S_{eq} , evaluated by Eq. (5), whose discretization needs more attention by the fact that this term inserts numerical instabilities for the energy equation; because of this, all discretization procedures tends to the UDS interpolation scheme, which implicates in a lower accuracy for all schemes.

Figure 4 presents the temperature profile for all numerical studies. It also includes CEA results - CEA is referred to a numerical code named "Chemical Equilibrium with Applications" (Glenn Research Center, 2005). According to Fig. 4, temperature profiles for both frozen and local equilibrium flows, the four numerical schemes (UDS, CDS, TVD Min-Mod and TVD Superbee) seem to converge to the same numerical results. They differ a little from CEA results since for CEA nine chemical species were taken into account - the same four ones for other results plus H , O , H_2O_2 , HO_2 and O_3 . As can be seen, CEA temperature for local equilibrium flow are quite higher than for other results; otherwise, when the frozen flow model is compared, CEA results are quite smaller than the ones for other models.

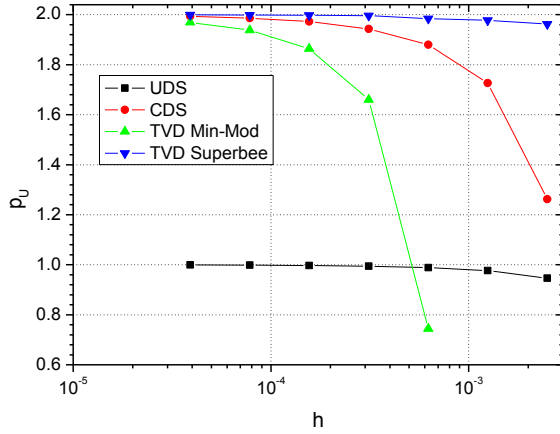


Figure 2. Apparent order (p_U) for P_{ex} – frozen flow model.

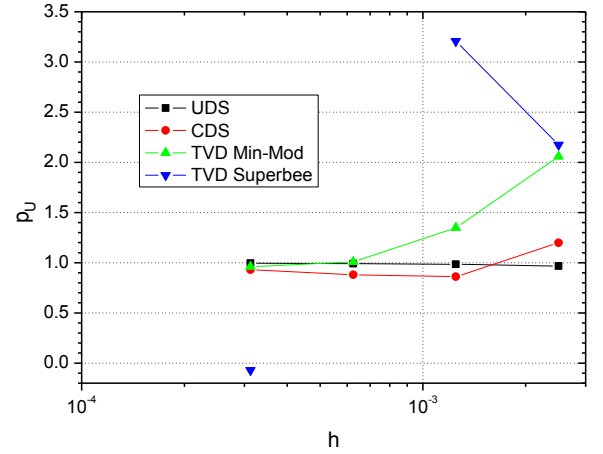


Figure 3. Apparent order (p_U) for P_{ex} – local equilibrium flow model.

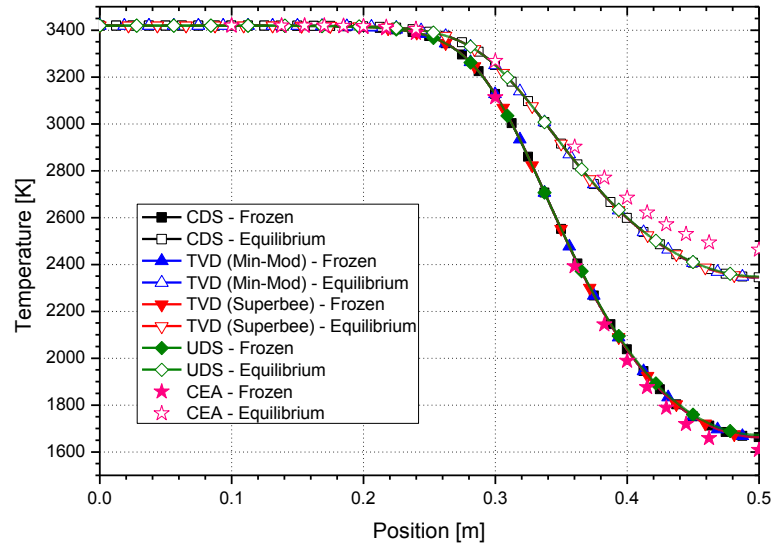


Figure 4. Temperature profile for all numerical studies.

Numerical results for different variables of interest (C_d , F^* , T_{ex} and M_{ex}) and their numerical uncertainties, given by GCI estimator, are presented in Tab. 4. Four different approximation schemes (UDS, CDS, TVD Min-Mod and TVD Superbee) were evaluated for both frozen and local equilibrium flows. CEA results are also included to provide a better comparison chart for all variables of interest. It must be noted, however, that CEA results include nine chemical species while the other ones include only four.

Analyzing the results presented in Tab. 4, it can be noted that:

1) All variables of interest are affected by the physical model (frozen or local equilibrium flow); however, while global variables of interest such C_d and F^* differ of about 1 or 2%, for local variables of interest, such M_{ex} and T_{ex} , the differences are typically superior to 5%, achieving more than 20%.

2) Numerical results for CDS, TVD Min-Mod and TVD Superbee are, in almost all cases, coincident (with numerical uncertainties ranges) or present similar results. Based on this result, it can be expected that, for situations in which CDS does not present correct results, such as shock wave studies, a TVD scheme should present better results, with higher accuracy orders.

3) Comparing the numerical uncertainties with experimental uncertainties provided in other studies involving rocket nozzle engines, it can be said that the 1600 control volumes grid is refined enough to provide accurate results, since numerical verification procedures were also observed.

Table 4. Variables of interest and their numerical uncertainties evaluated by GCI; results for 1600 control volumes grid.

Scheme	Variable	Frozen flow	Local equilibrium flow
UDS	C_d [-]	$1.0207 \pm 9.1 \times 10^{-3}$	$1.0014 \pm 8.4 \times 10^{-3}$
	F^* [-]	$1.0006 \pm 1.1 \times 10^{-3}$	$1.01093 \pm 5.6 \times 10^{-4}$
	T_{ex} [K]	1673 ± 29	2349 ± 13
	M_{ex} [-]	$3.188 \pm 5.0 \times 10^{-2}$	$2.929 \pm 3.2 \times 10^{-2}$
CDS	C_d [-]	$1.0176636 \pm 1.4 \times 10^{-6}$	$0.99867 \pm 2.1 \times 10^{-4}$
	F^* [-]	$1.0001922 \pm 3.7 \times 10^{-6}$	$1.010752 \pm 2.8 \times 10^{-5}$
	T_{ex} [K]	$1662.941 \pm 2.0 \times 10^{-2}$	$2344.40 \pm 4.1 \times 10^{-1}$
	M_{ex} [-]	$3.205359 \pm 3.4 \times 10^{-5}$	$2.93905 \pm 8.6 \times 10^{-4}$
TVD Min-Mod	C_d [-]	$1.0176616 \pm 6.8 \times 10^{-6}$	$0.99867 \pm 2.0 \times 10^{-4}$
	F^* [-]	$1.0001890 \pm 5.6 \times 10^{-6}$	$1.010749 \pm 1.1 \times 10^{-5}$
	T_{ex} [K]	$1662.2884 \pm 5.1 \times 10^{-3}$	$2344.40 \pm 4.2 \times 10^{-1}$
	M_{ex} [-]	$3.2053507 \pm 8.1 \times 10^{-6}$	$2.93904 \pm 9.0 \times 10^{-4}$
TVD Superbee	C_d [-]	$1.0176636 \pm 1.4 \times 10^{-6}$	$0.99867 \pm 2.1 \times 10^{-4}$
	F^* [-]	$1.000203 \pm 3.5 \times 10^{-5}$	$1.01076 \pm 1.1 \times 10^{-4}$
	T_{ex} [K]	$1662.88 \pm 1.4 \times 10^{-1}$	$2344.37 \pm 2.3 \times 10^{-1}$
	M_{ex} [-]	$3.20543 \pm 2.5 \times 10^{-4}$	$2.93909 \pm 4.4 \times 10^{-1}$
CEA (Glenn Research Center, 2005)	C_d [-]	1.000580	0.977372
	F^* [-]	0.998992	1.011553
	T_{ex} [K]	1607.91	2462.41
	M_{ex} [-]	3.231	2.986

5. CONCLUSION

Different interpolation schemes were used, in the current work, for reactive flow models in a rocket nozzle engines. The performance of two classical schemes (UDS and CDS) are compared to two TVD ones (TVD Min-Mod and TVD Superbee), for frozen and local equilibrium flows. While for frozen flow all schemes presented the expected accuracy orders for p_U , for local equilibrium flow such tendency was not verified. This behavior can be attributed to the chemical source term of energy equation, since the discretization of such term tends to the UDS scheme.

The values of the variables of interest are dependent on the chosen physical model. However, such dependency is higher for local variables, such as M_{ex} and T_{ex} , for which differences achieve more than 10%, than for global variables, for which the differences are about 1 or 2%.

Especially for local equilibrium flow, TVD Min-Mod requires smaller computational processing time (CPU time) than CDS. This fact, associated to the fact that both models provide numerical results with the same order of numerical uncertainties and equivalent order of accuracy, shows that TVD Min-Mod is a good option for the discretization of compressible reactive flow models.

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