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Numerical quadrature for the Prandtl Meyer function at high temperature with application for air in nozzles

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Abstract - *When the stagnation temperature of the combustion chamber or ambient air increases, the specific heats and their ratio do not remain constant any more, and start to vary with this temperature. The gas remains perfect, except, it will be calorically imperfect and thermally perfect. A new generalized form of the Prandtl Meyer function is developed, by adding the effect of variation of this temperature, lower than the threshold of dissociation. The new relation is presented in the form of integral of a complex analytical function, having an infinite derivative at the critical temperature. A robust numerical integration quadrature is presented in this context. The classical form of the Prandtl Meyer function of a perfect gas becomes a particular case of the developed form. The comparison is made with the perfect gas model for aim to present a limit of its application. The application is for air.*

Résumé – *Lorsque la température de stagnation de la chambre de combustion ou de l'air ambiant augmente, la chaleur spécifique et de leur rapport ne reste pas plus constant, et commence à varier avec cette température. Le gaz reste parfait, à l'exception, il sera imparfait en calories et parfait thermiquement. Une nouvelle forme générale de la fonction de Prandtl Meyer est développée, en ajoutant l'effet de variation de cette température, qui est basse au seuil de dissociation. La nouvelle relation est présentée sous la forme d'une intégrale d'une fonction analytique complexe, et ayant une dérivée infinie à la température critique. Une intégration quadratique numérique robuste est présentée dans ce contexte. La forme classique de la fonction de Prandtl Meyer d'un gaz parfait devient un cas particulier de la forme développée. La comparaison est faite avec le modèle d'un gaz parfait ayant pour but de présenter une limite de son application. L'application est l'air.*

Keywords: Supersonic flow - High temperature - Prandtl Meyer function – Gauss Legendre quadrature - Relative Error.

1. INTRODUCTION

In the Reference [1], we developed a new form of the Prandtl Meyer (PM) function at high temperature (HT) applied when the stagnation temperature (combustion chamber, ambient air) of the flow is high, as a generalisation of the PM function of the Perfect Gas (PG) model.

We know that the design of any supersonic nozzles and the calculation of a supersonic flow are based on the application of the method of characteristics which is formulated on the PM function. The supersonic flow calculation is made in each chosen point of the field, where it is necessary to calculate the value of the PM function. Then the choice of an efficiency quadrature which makes fast calculation with very high accurary is mandatory.

The aim of this work is to present a robust quadrature which can make fast calculation process answering the specificity of the function and to make comparison with the Simpson method [1]. The integration contains always the critical temperature.

With a much reduced number of points, the function can be calculated with a very high precision. The difficulty arises in the application of this quadrature is that the points of integration are non-rational number [5].

2. MATHEMATICAL FORMULATION

From reference [1], the value of ν for a Mach number $M > 1.0$ $(T < T^*)$ at high temperature is given by the following relation:

$$\nu(T) = \int_T^{T^*} F_\nu(T) \times dT \tag{1}$$

where,

$$F_\nu(T) = \frac{C_p(T)}{2H(T)} \times \sqrt{\frac{2H(T)}{a^2(T) - 1}} \tag{2}$$

The terms $M(T)$, $a(T)$ and $\gamma(T)$ are given in References [1] and [2], where:

$$M(T) = \frac{\sqrt{2H(T)}}{a(T)} \tag{3}$$

The expressions of $C_p(T)$ and $H(T)$ are presented in Refs. [1] and [2]. The PM function is connected directly with the temperature. In this relation, the temperature corresponding to the Mach number must be determined by the resolution of the {Eq. (3)}. The calculation process of T^* and T_s are presented in reference [2].

The calculation of the value of ν needs to integrate the function $F_\nu(T)$, where the analytical procedure is impossible, considering the complexity of this function. Therefore, our interest is directed towards numerical calculation. The function $F_\nu(T)$ has the following properties

- It contains only positive terms and the square root some is the interval of integration.
- It is a regular function and it hasn't a singularity. In other words, the function to be integrated is completely defined in the closed interval for any values of M_s and T_0.
- It is zero for $T = T^*$ and has an infinite derivative at this temperature. Consequently, the successive derivates of higher order present a singularity at point $T = T^*$. Then, we can write:

$$F_\nu(T^*) = 0.0, \qquad \left[\frac{d^{(n)} F_\nu}{(dT)^n}\right]_{T=T^*} = -\infty \qquad (n = 1, 2, \ldots) \tag{4}$$

The numerical integration quadratures based on the area calculation of the function (2) requires a very high discretization to have a suitable convergence, considering the result (4).

A major disadvantage for those quadratures is that no information on the error can be given, considering the error calculation is based on the maximum value of the derived from the function $F_v(T)$ and the derived from higher order [3] in the interval of integration.

The function $F_v(T)$ has consequently a term known by *weight function*, that is responsible for the singularity of derived and the higher orders derivatives from the function in point $T = T^*$. Our interest is thus based on the decomposition of the function, so removing the singularity and to consider remains to it function for the numerical integral calculation.

The function under the sign square root in the expression (2) has a root $T = T^*$. We can show this result starting from the relation (3), when $M = 1$ $(T = T^*)$. Then this expression is divisible by $(T^* = T)$.

This relation can be written by multiply and divide at the same time by $\sqrt{T^* = T}$. In the obtained result, we did not prefer the Euclidean division for reason taking the general case independently of the interpolation of $C_p(T)$.

Let us take the following variable change for aim to transform the interval $[T_s, T^*]$ to $[0, 1]$:

$$T = T^* - (T^* - T_s) \times x \tag{5}$$

then $dT = -(T^* - T_s)\,dx$. When $x = 0$, one has $T = T^*$, and when $x = 1$ one obtains $T = Ts$. Consequently, the value v_s can be obtained by the evaluation of the following integral in the interval $[0, 1]$. We obtain:

$$v_s = \int_0^1 w(x)\, f(x)\, dx \tag{6}$$

where, $w(x) = \sqrt{x}$ and

$$f(x) = \frac{(T^* - T_s)^{3/2} \times C_p(T)}{2H(T)\,a(T)} \times \sqrt{\frac{2H(T) - a^2(T)}{T^* - t}} \tag{7}$$

In this relation, the temperature is given by the relation (5). The obtaining value of v_s depends on M_s and T_0.

We can write from (7):

$$\lim_{T \to T^*} \frac{2H(T) - a^2(T)}{T^* - T} = \frac{0}{0} = 2a(T^*) \left.\frac{da}{dT}\right|_{T=T^*} + 2\,C_p(T) \neq 0 \tag{8}$$

Then, the function $f(x)$ has a finite value at $x = 0$.

In the relation (7), the developed integration quadrature does not need to know the value of the function $f(x)$ when $x = 0$, $(T = T^*)$.

The function $f(x)$ and the successive higher order derivatives $f'(x)$, $f''(x)$, …, $f^{(n)}(x)$ do not present any singularity in the closed interval $[0,1]$, and in particularity at $x = 0$. Then for $x = 0$, one has:

$$\left(\frac{d^{(n)} f}{(dx)^n}\right)\Bigg|_{x=0} = \text{finite value} \qquad (n = 0,1,2,3,...) \tag{9}$$

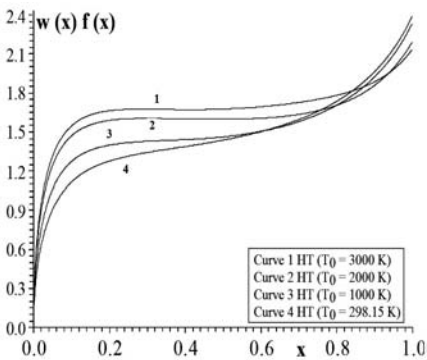

Fig. 1: Graph of the function $w(x)\,f(x)$ for $M_s = 6.00$

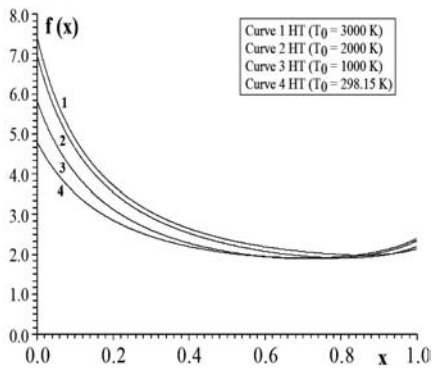

Fig. 2: Graph of the function $f(x)$ for $M_s = 6.00$

Figures 1 and 2 respectively represent the form of $w(x)\,f(x)$ and $f(x)$. The presented functions are selected for $M_s = 6.00$. For the other values of M_s, one obtains the same pace with different values.

On figure 1, one can view clearly that the function $w(x)\,f(x)$ has a infinite derivative at $x = 0$. Figure 2 shows us that the function $f(x)$ is regular in the interval $[0,1]$ some is T_0 and M_s.

Considering the form of the function $f(x)$, one can say that the higher successive derivative $\left|f^{(2n)}(x)\right|$ $(n=1,2,3,...)$ of an even nature reach the maximum value at the point $x = 0$.

The suitable numerical integration quadrature is that of Gauss Legendre (GL) when the function to be integrated has a weight function $w(x)$ form $\sqrt{x}$. The general form of the quadrature is given by [3]:

$$\nu_s = \int_0^1 \sqrt{x} \times f(x) \times dx = \sum_{j=1}^{j=N} b_j \times f(\eta_j) \tag{10}$$

The weight function does not intervened in the calculation of the right sum of the relation (10). The integration points n_j and the coefficients b_j for $N = 12$ are

presented in **Table 1**. They are given starting from the positive roots of the odd Legendre polynomial of order 25 by the following relations [3, 8, 9]:

$$\eta_j = \xi_j^2, \qquad b_j = 2\,\sigma_j \times \xi_j^2 \qquad j = 1, 2, \ldots, N \tag{11}$$

More details and extensive collection of tables of abscissas and weights for Gaussian quadrature formulas is contained in Ref. [8].

To determine the quadratures of order N, it is necessary initially to determine the roots and the corresponding coefficients of the Legendre polynomial of order $2\ N + 1$, and used the {Eq. (11)} *only for the positive roots to determine the considered quadrature.*

In the general case, one interested to determine the value of the Mach number in the supersonic flow points. The obtaining of the PM function value is only a way for calculation.

If $\nu_s > 0$ is given, it is necessary to determine the correspondent value of $T_s < T^*$ as solution of (6). This problem is called by inverse problem. Physically there is one solution. By substitution the obtained value of T_s in (3), one cans deduct the value of M_s.

Table 1: X-coordinates and associated coefficients of the Gauss Legendre with weight function for $N = 12$

j	n_j	b_j
1	0.0150957326903243	0.0036906784746633
2	0.0594710569757861	0.0142083221076484
3	0.1304454344836689	0.0299654709534825
4	0.2237315839551131	0.0485585350762163
5	0.3336944609748679	0.0670965784946015
6	0.4536916527396207	0.0825975254591715
7	0.5764746285191373	0.0923981606785536
8	0.6946266154271490	0.0945224752917305
9	0.8010106761709498	0.0879584949065280
10	0.8892010419046903	0.0728062821925218
11	0.9538724158796266	0.0502785894275588
12	09911336801673817	0.0225855546319901

The solution of the inverse problem of (6) is made by the use of the bisection algorithm [3], with $T_s < T^*$ (each value of T_0 has his correspondent value of T^* [2]). One can choose the beginning interval containing T_s by $T_1 = 0$ K and $T_2 = T^*$ or T_0. The value of T_s can be given with a precision ε if the interval of subdivision number K is satisfy by the following condition [10]:

$$K = 1.4426 \times \mathrm{Log}\left(\frac{T_0}{\varepsilon}\right) + 1 \tag{12}$$

If $\varepsilon = 10^{-6}$ is taken, the number K can't exceed 32.

3. APPLICATION

To obtain the supersonic Minimum Length Nozzle (MLN) giving a uniform and parallel flow at the exit section ($M = M_E$ and $\theta = \theta_E = 0$), it is necessary to diving the wall of an angle θ^* at the throat by [4]:

$$\theta^* = \nu_E / 2 \tag{13}$$

This situation is presented in figure 3. The relation (13) is valid for the two dimensional MLN. For the axisymmetric geometry MLN [11], the relation between θ^* and ν_E must be determined numerically. Where the relation (13) is not valid for this case.

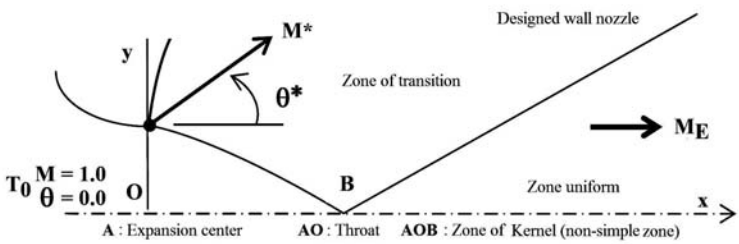

Fig. 3: Expansion center for MLN configuation

For the Plug Nozzle, the deviation of the nozzle at the throat is given by [5] $\theta^* = \nu_E$. The term ν_E is equal to the value of the PM function corresponding to the exit Mach number of the nozzle.

The Mach number M^* just after the expansion can be consequently given. It corresponds to the PM function when $\nu(M^*) = \theta^*$.

In the first case, one calculate the value of T^* as solution of (6) by substitution of θ^* in the place of ν_S. It is noticed that T^* is different to $T*$ (temperature at the throat correspond to $M=1$). By substitution T^* in the relation (3), one obtains the value of M^* just after the expansion, which correspond to the value of the Mach number in the first point of the last right running characteristics of the zone of Kernel.

We know that in the zone of Kernel, there are infinite number characteristics which result from point A and reflect on the symmetry axis. In the calculation, if one want high precision, one choose high finite number of characteristics, which result of high time processing.

To minimize the time of calculation, it is necessary to choose a robust quadrature to evaluate the integral (6), where ν_S is replaced by incremented value of θ in the point A. Thus, this point is a discontinued point in parameters, where $0 \le \theta \le \theta*$ and $1 \le M \le M*$.

4. RESULTS AND COMMENTS

Table 2 presents the effect of the developed Gauss Legendre quadrature order on the convergence of the problem. The selected example is for $T_0 = 3500$ K and $M_s = 6.00$. This example request for a raided order quadrature compared to the other values (T_0, M_s) for same desired precision.

The given quadratures results are always lower that the exact solution, ie. the convergence of the solution will take place in a monotonous way. We can deduce that only 12 points of the presented quadrature, the calculation gives as an accurary of 10^{-6}.

Then, some is (T_0, M_s), one can use the quadrature of order $N = 12$ to the maximum to have the better precision with $\varepsilon = 10^{-6}$. For the same example, the trapezoid and Simpson's quadratures with constant step request for a minimum number of points presented in **Table 3**.

Table 2: Effect of the Gauss Legendre quadrature order on convergence

N	ν	N	ν
1	84.64126548	7	97.5603689
2	95.15389223	8	97.5609629
3	96.95735518	9	97.56108289
4	97.47123155	10	97.56110527
5	97.54221288	11	97.56110958
6	97.55736411	12	97.56111080

Table 3: Effectiveness of quadratures for a given precision

	Trapezoid Ref. [10]	**Simpson** Ref. [3]	**Simpson** Ref. [1]	**GL quadrature**
$\varepsilon = 10^{-1}$	30	18	10	4
$\varepsilon = 10^{-2}$	129	70	12	5
$\varepsilon = 10^{-3}$	1869	1002	38	7
$\varepsilon = 10^{-4}$	8686	4648	158	9
$\varepsilon = 10^{-5}$	40495	21644	716	10
$\varepsilon = 10^{-6}$	195551	104174	3436	12

For the trapezoid and Simpson's quadratures, one has to control of fixation of the digits decimal for wanted precision. Since the error relations of these quadratures does not give any information's on the minimum number of points which it is necessary to obtain the desired precision, considering the properties (4).

One can have the same precision ε by using the trapezoid and Simpson's quadratures with a lower number of points that indicated in **Table 3**, if the condensation of nodes [6] is used towards the point $T = T^*$ of the interval of integration $[T_s, T^*]$.

In this case, the values given by the Simpson's quadrature are presented in **Table 3**. For example, if $\varepsilon = 10^{-6}$, we needs only 3436 points.

Of course, the evaluation of the PM function using the stretching function request some additional mathematical operations compared to that evaluated without condensation.

The values presented in the **Table 4** demonstrates that, in our flow field calculation ($T_0 < 3500$ K, $M_s < 6.00$), the maximum order of the GL quadrature can't exceeds 12 to have an accurary better than 10^{-6}.

If one take into account, the variation of $C_p(T)$, the stagnation temperature influences the size of this function. The numerical values for some values of M and T_0 are presented in **Table 5**.

The calculated PM function values for $T_0 = 298.15$ K can represent the values of the PM function, but calculated by using the HT model. For the case of $\gamma = 1.402$, the value are calculated by using the PG relations [7].

Numerical calculation shows that there is difference in spite of low temperature. For example, when $T_0 = 298.15$ K and $M = 3.00$, we obtain an error $\varepsilon = 0.006$ %.

Between the PG and HT models, when T_0 is high, the errors is not negligible which is equal to $\varepsilon = 9.70$ % if $M = 3.00$ and $T_0 = 2000$ K [1].

Table 4: Minimum order of the GL quadrature giving $\varepsilon = 10^{-6}$

	Mach number					
	1.5	2.0	3.0	4.0	5.0	6.0
$T_0 = 1000$ K	4	5	8	9	10	11
$T_0 = 2000$ K	4	6	8	9	10	10
$T_0 = 3000$ K	4	6	9	10	11	12

Table 5: Numerical result of the HT Prandtl Meyer function

	$\gamma = 1.402$ [7]	Stagnation temperature T_0 (K)			
		298.15	1000	2000	3000
M = 1.5	11.890	11.890	12.400	12.715	12.822
M = 2.0	26.337	26.337	27.577	28.646	29.017
M = 3.0	49.651	49.648	51.744	54.989	56.173
M = 4.0	65.622	65.617	67.890	72.624	75.021
M = 5.0	76.714	76.707	78.983	84.262	87.617
M = 6.0	84.715	84.707	86.983	92.392	96.197

The **Table 6** presents some numerical values of Mach number when the correspondent value of the PM function is given. The aim of presentation of this **Table**

is to determine the Mach number M^* just after the expansion for the design of the supersonic nozzle for internal flow, or to determine the distribution of the Mach number on the surface of the supersonic pointed airfoil, for external flow.

For the case of PG model and HT model when T_0 = 298.15 K, one present the results by 6 digit decimals, to view clearly the deference between the two models for low temperature, because the error is letter compared to the case for high temperature, where one present only 3 digit decimals.

Table 6: Mach number correspond to the given PM function value

ν (deg)	γ = 1.402 [7]	Stagnation temperature T_0 (K)			
		298.15	1000	2000	3000
1	1.081863	1.081827	1.079	1.079	1.078
5	1.256671	1.256645	1.249	1.246	1.245
10	1.435382	1.435368	1.421	1.414	1.411
20	1.775970	1.775977	1.745	1.726	1.719
30	2.135811	2.135849	2.085	2.044	2.0331
40	2.541142	2.541227	2.465	2.389	2.366
50	3.018175	3.018335	2.912	2.780	2.741
60	3.603234	3.603517	3.461	3.243	3.173
70	4.354323	4.354814	4.164	3.821	3.692
80	5.374227	5.375098	5.111	4.587	4.348
90	6.867304	6.868933	6.469	5.670	5.243
100	9.309331	9.312729	8.627	7.319	6.580

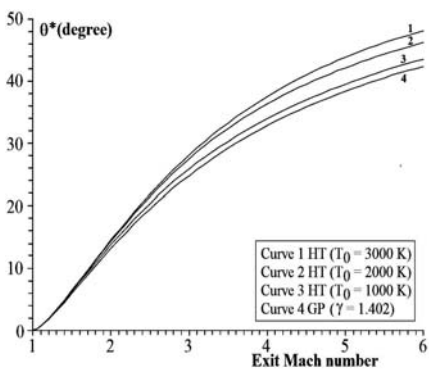

Fig. 4: Variation of θ^* versus M_E

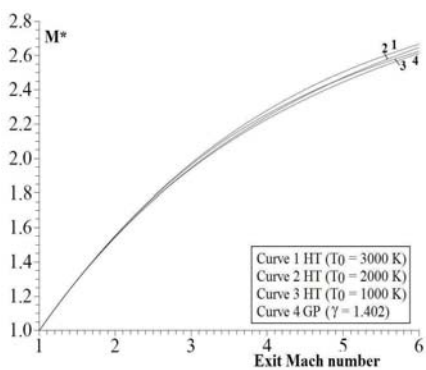

Fig. 5: Variation of M^* versus M_E

Figure 4 presents the variation of the expansion initial angle M^* at high temperature of the 2D MLN. Thus the more the value of T_0 increases, more there is opening of the wall at the throat.

The curves are almost confounded until approximately $M_S = 2.00$, then start to differentiate. Between curves 4 and 3, one can notice a small difference between the values of a PG and HT models.

On figure 5, one presented the HT variation of the Mach number M^* at point A of the throat versus M_E of the nozzle. Then, this figure shows that there is an discontinued expansion cantered at the point A which increases the Mach number of $M = 1$ to $M = M^*$.

One know that the PG model does not depend on T_0, and that the value of M^* depends on T_0 for HT model, which influences the nozzle design. Our interest of this variation is that M^* take account of the variation of T_0 and that this variation increases if T_0 increases [4].

Consequently, all the design parameters of the nozzle (length, mass of the structure, thrust coefficient, thermodynamic parameters,.) of these two types of nozzles depends primary on the stagnation temperature T_0, especially if it starts to exceed 1000 K [4, 5].

5. CONCLUSION

Gauss Legendre formulae for regular function but has singularity in first derivative has been extended to evaluate the Prandtl Meyer function at High temperature, which occur in the supersonic external and internal flow field application, lower than the dissociation threshold of the molecules.

This quadrature makes very fast calculation compared to the other existed quadrature. The profit in time processing calculation can arrive, for high precision, to 350% compared to the Simpson's quadrature with stretching function for example.

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