Determination of a Two Variable Approximation Function with Application to the Fuel Combustion Charts

Irina-Carmen ANDREI*

*Corresponding author
INCAS – National Institute for Aerospace Research "Elie Carafoli",
B-dul Iuliu Maniu 220, Bucharest 061126, Romania,
andrei.irina@incas.ro, icandrei28178@gmail.com

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Section 1 – Launchers propulsion technologies and simulations of rocket engines

***Abstract**: Following the demands of the design and performance analysis in case of liquid fuel propelled rocket engines, as well as the trajectory optimization, the development of efficient codes, which frequently need to call the Fuel Combustion Charts, became an important matter. This paper presents an efficient solution to the issue; the author has developed an original approach to determine the non-linear approximation function of two variables: the chamber pressure and the nozzle exit pressure ratio. The numerical algorithm based on this two variable approximation function is more efficient due to its simplicity, capability to providing numerical accuracy and prospects for an increased convergence rate of the optimization codes.*

Key Words: *approximation of two-variable functions, Propellant Combustion Charts, liquid propulsion, rocket engines*

1. INTRODUCTION

Thrust evaluation or thrust prediction at different flight regimes, as well as the analysis of flight dynamics and trajectory optimization are important milestones for both the design and performance analysis of liquid propelled rocket engines.

For a realistic and accurate prediction of the rocket engines global on- and off-design performances, the **Propellant Combustion Charts** [1] are required which provide graphically the correlations between the chamber pressure p_c, exit pressure conditions p_e (i.e. burned gas expelled at ambient pressure or in vacuum) and mixture ratio r (which expresses the ratio of Oxygen to Fuel O/F), adiabatic flame temperature T_c (also referred as the Chamber Temperature), gas molecular weight M_w and specific heat ratio γ, (also referred as the adiabatic power coefficient), for different types and combinations of fuel and oxidizer, [1].

Fig. 1 ÷ Fig. 4 shows the Combustion Charts for the study case: Liquid Oxygen and Kerosene (n-Dodecane, $C_{12}H_{26}$), [1].

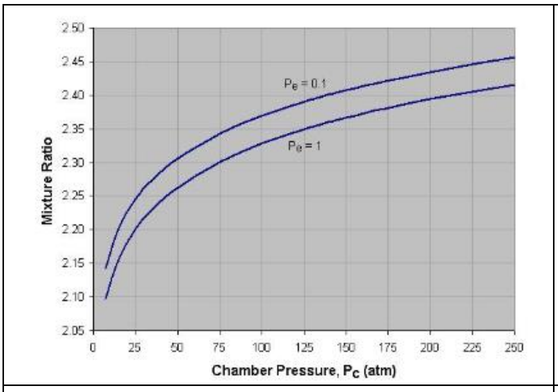

Fig. 1 - Optimum mixture ratio, LOX-K, [1]

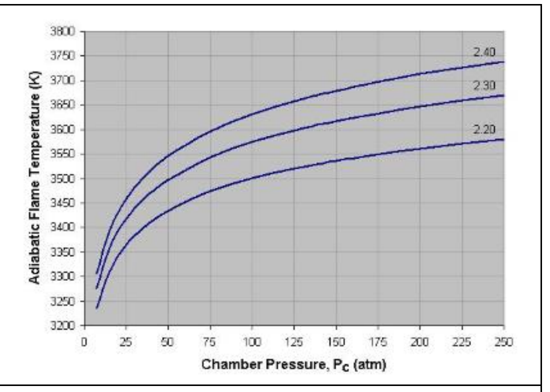

Fig. 2 - Adiabatic flame temperature, LOX-K, [1]

As one can easily notice from Fig. 1 ÷ Fig. 4, the variation with the chamber pressure of the mixture ratio, see Fig. 1, the adiabatic flame temperature, see Fig. 2, the gas molecular weight, see Fig. 3, and the specific heat ratio, see Fig. 4, is non-linear, irregardless of the exit conditions.

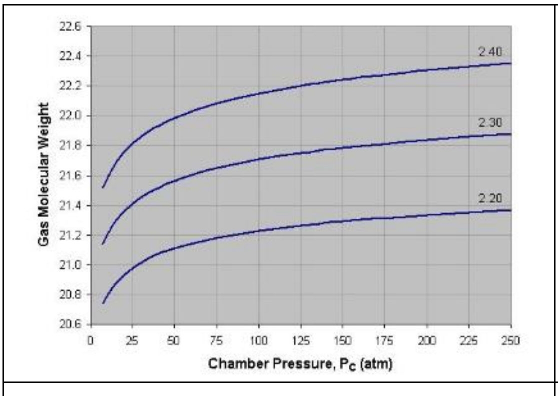

Fig. 3 - Gas Molecular Weight, LOX-K, [1]

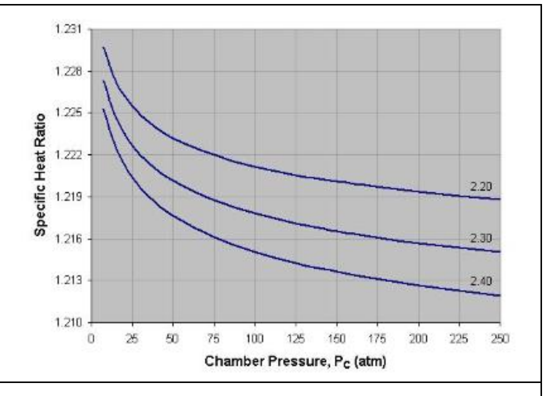

Fig. 4 - Specific Heat Ratio, LOX-K, [1]

An investigation of the liquid propelled rocket engines, which has been carried on as a part of an **INCAS** project for the European Space Agency **ESA**, focused on Liquid Oxygen **LOX** as oxidizer and Kerosene $C_{12}H_{26}$, Liquid Methane CH_4 and Ethyl Alcohol CH_3CH_2OH as potential fuel; the selection followed the consideration of lower costs, operational safety, more environmental friendly in comparison with other combinations, such as LOX - Liquid Hydrogen, LOX - UDMH, Red - Fuming Nitric Acid - Kerosene, Red - Fuming Nitric Acid - MMH, Red - Fuming Nitric Acid - UDMH, Nitrogen Tetroxide - MMH, Nitrogen Tetroxide - Aerozine 50, Hydrogen Peroxide - Kerosene.

Therefore, since the input data are the combustion chamber pressure p_c [atm] and the nozzle exit pressure p_e [atm], then the two-variable approximation is necessary. As mentioned above and as one can notice from Fig. 1 ÷ Fig. 4, the variation is non-linear, so the two-dimensional non-linear approximation is in question.

Although the bilinear approximation is more often used and it is detailed in many papers and books [7-12], the applications of 2D non-linear approximation are less used, since the algorithm associated to numerical simulation can be very complex, intricate, requiring large memory capacities.

The problems of ill-conditioning and divergence can be ameliorated by either finding initial parameter estimations that are near to the optimal values, which can be difficult sometimes, or by using analytical functions or accurate approximation methods, customized for the analyzed applications.

The focus in this paper is to determine a non-linear approximation function, of two variables, so as to be as accurate as possible numerically and less time consuming for the flight dynamics and trajectory optimization code.

2. STUDY CASE

The research presented in this paper is focused on the **LOX - Kerosene Charts**, which are shown in Figs. 1 ÷ 4; in order to highlight the proposed methodology, only the Targeted Investingation TI # 1 (i.e. the variation of the mixture ratio r versus the combustion chamber pressure p_c [atm] and the nozzle exit pressure p_e [atm]) is presented in this paper.

3. METHODOLOGY

For the particular case of the two-variable approximation of the Propellant Combustion Charts, the author proposes a methodology based on a hybrid approach, which consists in fulfilling two steps:

1. the 1st step refers to the least squares approximation of the variation of mixture ratio (and adiabatic flame temperature, gas molecular weight and specific heat ratio, respectively), with the chamber pressure; also, a comparison between the linear regression and non-linear curve fitting for the least squares approximation method was done;
2. the 2nd step refers to the determination of the variation with the exit pressure, based on interpolating the coefficients of the function calculated at the 1st step.

The selection of the approximation method, which can be the interpolation or the least squares approximation (by either linear on non-linear curve fitting) is done by taking into consideration both criteria: the numerical accuracy provided by the chosen method and the prospective for minimizing the computational time for an in-house developed code dedicated to design and optimization of launch vehicles, Huzel [2], Sutton [3], flight dynamics optimization and control, Balesdent [4], Brevault [5], Casiano [6].

In case of small perturbation in input data (e.g. from reading), the least squares approximation smoothens the errors of the resulting function, while any interpolation method amplifies them; this feature represents an additional reason for considering the least squares approximation. The global polynomial interpolation methods are often used for the single variable approximation, e.g. Newton polynomial, Lagrange polynomial, Berbente [7], which are simpler, but sometimes fail on numerical accuracy. More accurate are the split interval polynomial interpolation methods (again, for single variable interpolation), such as the spline functions, Berbente [7].

The best accuracy is provided by the 3rd order spline function (cubic spline), and then, following the decreasing order of the accuracy, are 2nd order (parabolic spline) and 1st order (linear) spline functions.

Note that in case of a trajectory optimization code based on genetic algorithm, the spline function must be called repeatedly, at each iteration, for a general number of iterations of about 10000 or even larger.

4. LEAST SQUARES APPROXIMATION BASED ON LINEAR REGRESSION VERSUS NON-LINEAR CURVE FITIING

4.1 Least Squares Approximation by Linear Regression

The linear regression is the simplest way to determine a least squares approximation, but in certain cases, it is not convenient, due to the lack of accuracy.

The linear regression (3) determined for a general function:

$$y = f\left(x\right) \tag{1}$$

which for many practical applications is not given analytically, but is defines on nodes:

$$y_i = f\left(x_i\right)\Big|_{i=\overline{1,n}} \tag{2}$$

which crosses the mean values point$\left(\overline{x},\overline{y}\right)$, is determined by the correlation coefficient c (4) , the *x*-variation σ_x (5), and the mean values $\overline{x}$ (7) and $\overline{y}$ (8), as follows:

$$g\left(x\right) = \frac{c}{\sigma_x}\cdot\left(x-\overline{x}\right)-\overline{y} \tag{3}$$

$$c = \overline{xy}-\overline{x}\cdot\overline{y} \tag{4}$$

$$\sigma_x^2 = \overline{x^2}-\left(\overline{x}\right)^2 \tag{5}$$

$$\sigma_y^2 = \overline{y^2}-\left(\overline{y}\right)^2 \tag{6}$$

$$\overline{x} = \frac{1}{n}\cdot\sum_{i=1}^{n}x_i \tag{7}$$

$$\overline{y} = \frac{1}{n}\cdot\sum_{i=1}^{n}y_i \tag{8}$$

4.2 Least Squares Approximation by Non-Linear Curve Fitting

The non-linear curve fitting is basically a non-linear regression determined for the least squares approximation, based on non-linear functions, such as the logarithm or the exponential functions.

Next is presented the case of non-linear curve fitting, by using the exponential function (9), where k and α are both constant, which will be further determined:

$$y = k\cdot\exp\left(\alpha\cdot x\right) \tag{9}$$

Following the coordinate transformation (10) and (11), then the problem of non-linear regression in coordinates (*x*,*y*) turns into the determination of a linear regression in the new coordinates (X,Y). With respect to the new coordinates *X*(10) and *Y*(11), one obtained the linear regression as (12):

$$X = x \tag{10}$$

$$Y = \ln(y) \tag{11}$$

$$\ln(Y) = \ln(k) + (\alpha \cdot X) \tag{12}$$

Relation (12) can be expressed as (13), which is similar to the equation of the linear regression (3):

$$g(y) = (\alpha \cdot x) + \ln(k) \tag{13}$$

5. NUMERICAL RESULTS AND CONCLUSIONS

Application # 1 introduces a comparison between the linear regression (14) and non-linear regression (non-linear curve fitting) (9) used for the least squares method, [13,14]:

$$y = a \cdot x + b \tag{14}$$

Table 1 – Generic test function, defined (2) by nodes, [13,14]

i	x_i	y_i
1	1	2
2	2	1
3	4	4
4	5.5	5
5	7	9

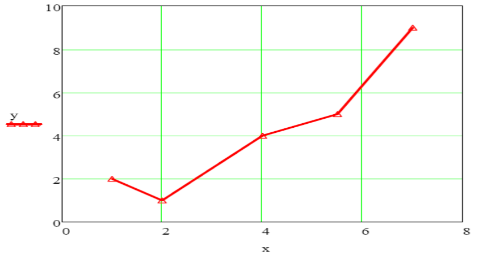

Fig. 5 – Generic Test Function, [13,14]

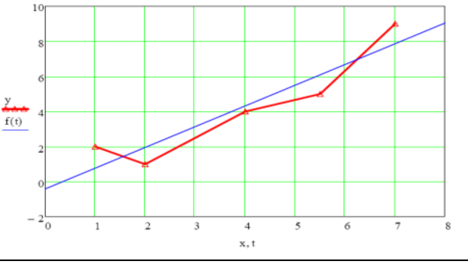

Fig. 6 – Least squares approximation, linear regression, [13,14]

The coefficients calculated for the linear regression (14) and for the non-linear regression (9) are summarized in Table 2.

Table 2 – Coefficients of linear and non-linear regressions

Linear regression	Non-linear regression
$y = a \cdot x + b$	$y = k \cdot \exp(\alpha \cdot x)$
$a = 1.1818$	$k = 0.9667$
$b = -0.4091$	$\alpha = 0.3105$

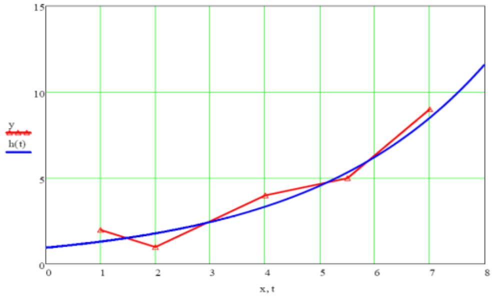

Fig. 7 – Least squares approximation, non-linear regression, [13,14]

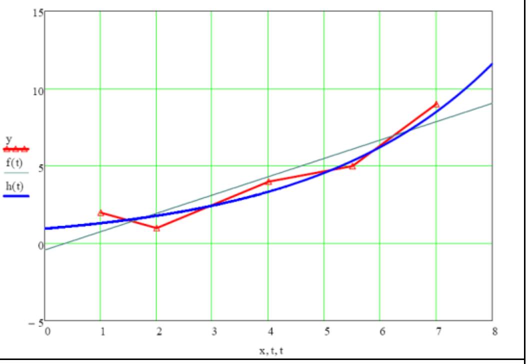

Fig. 8 – Least squares approximation, linear versus non-linear regression, [13,14]

<u>Application # 2</u> refers to the study case, presenting the step by step determination of the two-variable non-linear approximation of mixture ratio r with the chamber pressure p_c and nozzle exit pressure p_e; the methodology for developing the hybrid function comes forward.

Fig. 1 expresses the variation of the mixture ratio with the chamber pressure, for the given nozzle exit pressure, in case of Liquid Oxygen and Kerosene **LOX-K**, [1], summarized in Table 3:

Table 3 – Mixture ratio, chamber pressure, nozzle exit pressure, defined (2) by nodes, for LOX-K

Index	Chamber pressure p_c [atm]	Mixture ratio [---] at given nozzle exit pressure p_e = 1 [atm]	Mixture ratio [---] at given nozzle exit pressure p_e =0.1 [atm]
i	x_i	$y1_i$	$y2_i$
1	6	2.100	2.140
2	25	2.200	2.240
3	50	2.265	2.315
4	75	2.300	2.340
5	100	2.335	2.370
6	125	2.350	2.395
7	150	2.370	2.410
8	175	2.380	2.430
9	200	2.395	2.440
10	225	2.410	2.445
11	250	2.420	2.455

The approach of the proposed methodology is to determine distinct one-variable approximations of the mixture ratio versus the chamber pressure for each value of the nozzle exit pressure.

As one can notice in Fig. 10, the linear regression used for the least squares approximation of the mixture ratio with respect to the chamber pressure, for both cases of the nozzle exit pressure (in blue contours, the nozzle exit pressure = 1 [atm], while in red contours, the nozzle exit pressure = 0.1 [atm]), is not satisfactory, since it provides only a rough approximation.

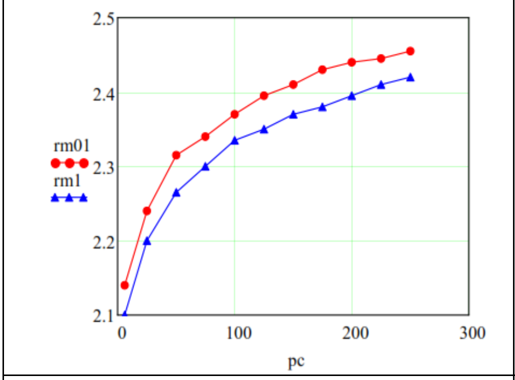

Fig. 9 – Input data for LOX-K: Mixture ratio, chamber pressure, nozzle exit pressure =1 [atm] - *blue contour*, and = 0.1 [atm] – *red contour*

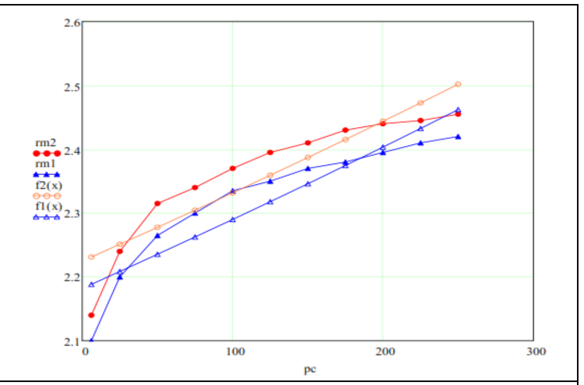

Fig. 10 – Least squares approximation, linear regression, LOX-K

Therefore, a non-linear regression (15) is proposed for the single variable approximation, and the results are concluded in Table 4:

$$y = f\left(p_c\right) = a \cdot \ln\left(p_c\right) + b \tag{15}$$

$$f\left(p_c\right)\Big|_{p_e=const} = a \cdot \ln\left(p_c\right) + b \tag{16}$$

Table 4 – Non-linear single variable approximation

Nozzle exit pressure p_e [atm]	Chamber pressure p_c [atm] range	Approximation functions $f\left(p_c\right)\Big\vert_{p_e=const}$, (16)	Coefficients	
			a	b
$p_e = 1$	$p_c \in [0, 250]$	$f\left(p_c\right)\Big\vert_{p_e=const} = a \cdot \ln\left(p_c\right) + b$	0.089332	1.926167
$p_e = 0.1$			0.089332	1.966167

The first step of the proposed methodology is completed by the determination of the non-linear single variable approximations (16) which are verified and shown graphically in Fig. 11; in blue contour is the non-linear approximation determined for the nozzle exit pressure = 1 [atm], and in red contour is the one corresponding to the nozzle exit pressure = 0.1 [atm].

The nozzle exit pressure is considered as given constant, while the chamber pressure is an input variable.

The second step consists in determining the non-linear two-variable approximation function (17) or equivalent (28) and its verification. In this case, both nozzle exit pressure and chamber pressure are input variables:

$$f\left(p_c, p_e\right) = a\left(p_e\right) \cdot \ln\left(p_c\right) + b\left(p_e\right) \tag{17}$$

The two-variable non linear approximation function is expressed by relation (17) or its equivalent (28).

The coefficients $a\left(p_e\right)$ depending on the nozzle exit pressure p_e are defined by expressions (18) ÷ (20):

$$a = \left(\frac{p_e - 0.1}{1 - 0.1} \right) \cdot a_1 - \left(\frac{p_e - 1}{1 - 0.1} \right) \cdot a_2 \tag{18}$$

$$a = \left(\frac{p_e - 0.1}{0.9} \right) \cdot a_1 - \left(\frac{p_e - 1}{0.9} \right) \cdot a_2 \tag{19}$$

$$a = \left(\frac{10}{9} \right) \cdot \left[(p_e - 0.1) \cdot a_1 - (p_e - 1) \cdot a_2 \right] \tag{20}$$

There have been introduced the notations a_1 (21) and b_1 (22) corresponding to the values *a* and *b* for the case that the nozzle exit pressure is 1 [atm], while a_2 (23) and b_2 (24) match the case that the nozzle exit pressure is 0.1 [atm]:

$$a_1 = a\big|_{p_e=1} \tag{21}$$

$$b_1 = b\big|_{p_e=1} \tag{22}$$

$$a_2 = a\big|_{p_e=0.1} \tag{23}$$

$$b_2 = b\big|_{p_e=0.1} \tag{24}$$

The coefficients $b(p_e)$ also depending on the nozzle exit pressure p_e are defined by expressions (25) ÷ (27):

$$b = \left(\frac{p_e - 0.1}{1 - 0.1} \right) \cdot b_1 - \left(\frac{p_e - 1}{1 - 0.1} \right) \cdot b_2 \tag{25}$$

$$b = \left(\frac{p_e - 0.1}{0.9} \right) \cdot b_1 - \left(\frac{p_e - 1}{0.9} \right) \cdot b_2 \tag{26}$$

$$b = \left(\frac{10}{9} \right) \cdot \left[(p_e - 0.1) \cdot b_1 - (p_e - 1) \cdot b_2 \right] \tag{27}$$

Table 5 – Non-linear two variable approximation

Input variables		Approximation functions	Coefficients	
Nozzle exit pressure p_e [atm] range	Chamber pressure p_c [atm] range	$f(p_c, p_e)$, (17), (28)	$a(p_e)$	$b(p_e)$
$p_e \in [0.1, 1]$	$p_c \in [0, 250]$	$f(p_c, p_e) = a(p_e) \cdot \ln(p_c) + b(p_e)$	0.089332	1.943945

Eventually, the expression of the two-variable non linear approximation function can be deduced as (28):

$$f(p_c, p_e) = \left(\frac{10}{9} \right) \cdot \left\{ \left[(p_e - 0.1) \cdot a_1 - (p_e - 1) \cdot a_2 \right] \cdot \ln(p_c) + \left[(p_e - 0.1) \cdot b_1 - (p_e - 1) \cdot b_2 \right] \right\} \tag{28}$$

Additionally Fig. 11 shows in purple contour an intermediate approximation which was calculated from relation (28), for the nozzle exit pressure considered equal to 0.5 [atm].

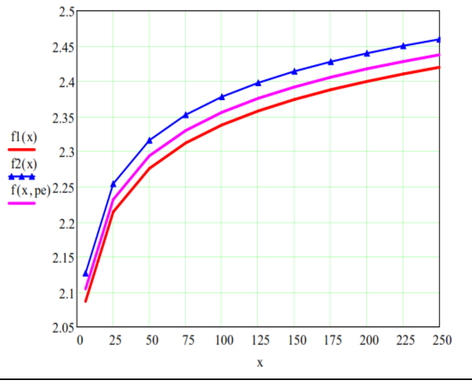

Fig. 11 – One variable least squares approximation, non-linear regression, LOX-K

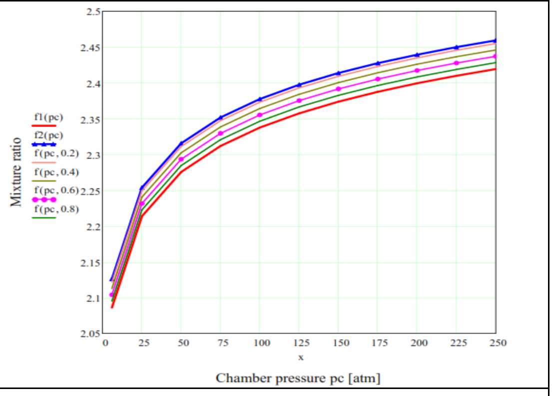

Fig. 12 – Generated Two Variable Non-Linear Approximating functions. Input variables: Chamber Pressure and Nozzle Exit Pressure, LOX-K

The two-variable non-linear approximation (17), (28) was used to generate the intermediate functions for other different values of the nozzle exit pressure, e.g. 0.2, 0.4, 0.6 and 0.8 [atm], which were depicted in Fig. 12.

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