Liquid rocket engine performance assessment in the context of small launcher optimisation

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Abstract: The paper presents a fast mathematical model that can be used to quickly asses the propulsive characteristics of liquid propelled rocket engines. The main propulsive parameters are computed using combustion surfaces obtained after a nonlinear data fitting analysis. This approach is much more time efficient than using standard codes which rely on frequent calls of the Fuel Combustion Charts and interpolating their data. The tool developed based on the proposed mathematical model can be used separately or it can be integrated in a multidisciplinary optimisation algorithm for a preliminary microlauncher design.

Key Words: rocket propulsion, specific impulse, nonlinear surface fitting, small launchers, multidisciplinary optimisation, mathematical model

1. INTRODUCTION

Designing a competitive and efficient small launcher, even in the preliminary conceptual phase, is a great challenge due to the fact that the complexity of the system does not significantly scale down with the decrease in payload mass [1]. A preliminary design for such a small launcher is of interest due to the increased recently demand and increase in the small satellites market, which has been booming in the last years.

A multidisciplinary approach must be used to successfully obtain a preliminary design of the microlauncher, which is often realised with the aid of a multidisciplinary design optimisation (MDO) algorithm. The MDO algorithm can vary from author to author, the block scheme for the MDO algorithm used in papers [1] and [2] can be seen in Figure 1, as an example. Here, the MDO employs an intrinsic Matlab genetic algorithm in order to search for the global optimum for the launch vehicle design problem.

The MDO tool developed core is constituted by the four main disciplines that are assessed in a cascade order: Weights & Sizing, Propulsion, Aerodynamics and Trajectory.

The objective of this paper is to present the mathematical model that can be used in the assessment of the small launchers propulsive performance, which takes place in the Propulsion block of the MDO scheme presented in Figure 1. For solution convergence, it can take up to several hundred thousand iterations [2]. Reducing the complexity of the mathematical models used is thus a very important aspect to consider.



Figure 1 - Block scheme of a MDO algorithm

2. PROPULSION ANALYSIS

Thrust curve evaluations at different altitude regimes must be accurately computed using simple mathematical models to ensure that the MDO tool can successfully asses the overall launcher performance and later optimise its configuration. For this study a total of 4 liquid propellant combinations are assessed, with oxygen as oxidizer and kerosene, methane, hydrogen and ethyl alcohol/ethanol as fuel.

The thrust of the rocket engine *T* is computed with the following formula:

$$T = q \cdot g_0 \cdot I_{sp} \tag{1}$$

The specific impulse I_{sp} is computed from papers [2], [3], [4] and [5] with:

$$I_{sp} = \eta_n \cdot \frac{C^*}{g_0} \left(\gamma_t \sqrt{\left(\frac{2}{\gamma_t - 1}\right) \cdot \left(\frac{2}{\gamma_t + 1}\right)^{\left(\frac{\gamma_t + 1}{\gamma_t - 1}\right)} \cdot \left(1 - \left(\frac{P_e}{P_c}\right)^{\left(\frac{\gamma_t - 1}{\gamma_t}\right)}\right)} + \frac{\varepsilon}{P_c} \left(P_e - P_a\right) \right)$$
(2)

Where: q, g_0 are the propellant mass flow rate and the gravitational acceleration at sea level; η_n is the nozzle efficiency, C^* is the propellants characteristic velocity, γ_t is the isentropic coefficient (also known as specific heat ratio) at the throat and ε is the nozzle expansion ratio; P_c represents the chamber pressure, P_e represents the exhaust pressure and P_a represents the atmospheric pressure.

The last term in equation 136 represents the correction with altitude of the specific impulse. At low altitudes, the atmospheric pressure is high and thus the thrust generated by the rocket engine is significantly lower than of that obtained at high altitudes, near vacuum conditions.

The nozzle area ratio or expansion ratio is computed with the formula given below:

$$\varepsilon = \frac{\left(\frac{2}{\gamma_t + 1}\right)^{\frac{1}{\gamma_t - 1}} \cdot \left(\frac{P_c}{P_e}\right)^{\frac{1}{\gamma_t}}}{\sqrt{\left(\frac{\gamma_t + 1}{\gamma_t - 1}\right) \cdot \left[1 - \left(\frac{P_e}{P_c}\right)^{\frac{\gamma_t - 1}{\gamma_t}}\right]}}$$
(3)

The propellant characteristic velocity is computed based on the following formula:

$$C^* = \eta_c \cdot \frac{\sqrt{\gamma_t \cdot R \cdot T_f}}{\gamma_t \cdot \left(\frac{2}{\gamma_t + 1}\right)^{\frac{\gamma_t + 1}{2(\gamma_t - 1)}}}$$
(4)

Where: η_c is the combustion efficiency, *R* is the exhaust gas constant and T_f is the adiabatic flame temperature.

The exhaust gas constant is considered to be ratio between the universal gas constant R_u and the gas molecular weight M_w . The adiabatic flame temperature is the temperature achieved by a combustion reaction that takes place adiabatically for the given reactants, measured in Kelvin. The exhaust gas molecular weight is the average molar weight of the combustion products, being the ratio between the mass of the exhaust gas divided by the number of moles, measured in kg/kmol.

The set of data shown in Table 1 is used for some of the parameters that appear in the presented model.

| Key parameter | Value |
|---------------|---|
| g_0 | 9.80665 $\frac{m}{s^2}$ |
| P_a | 0 atm for vacuum conditions 1 atm for sea level conditions |
| η_n | 98% |
| η_c | 96% for LOX/ethanol; 96% for LOX/kerosene; 98% for LOX/methane; 99% for LOX/hydrogen |
| R_{u} | $8314.3 \frac{J}{kmol \cdot K}$ |

Table 1 – Key model parameters

The propellant mass flow, together with the chamber and exhaust pressures are considered to be optimisation variables in the multidisciplinary optimisation context. Based on these 3 parameters and the flight regime, thrust generated by the liquid rocket engine can be computed. This is possible because the four main propulsive parameters (mixture ratio, adiabatic flame temperature, specific heat ratio at the throat and the molecular mass at combustion) can be approximated with the aid of propellant combustion charts [6]. The mixture ratio R_m does not explicitly appear in the mathematical model, but the other 3 propulsive parameters are computed with respect to it.

The combustion charts are generated after a thermochemical equilibrium analysis with the aid of STANJAN code [7]. The thermochemical data are based on the JANAF Thermochemical Tables [8]. For specific impulse computations only the chamber pressure P_c and exhaust pressure P_e are needed.

3. NONLINEAR APPROXIMATION FUNCTION

The typical approach to obtain the main four propulsive parameters is by directly calling the combustion charts and interpolating their data multiple times. Doing this several million times until the launcher configuration converges, the need for a simpler model arises.

Thus, this paper proposes to determine a two-variable nonlinear function that provides accurate results for the pressure range of interest.

Figure 2 shows the combustion charts for one of the four bipropellant combinations studied (LOX/kerosene), as presented in [6]. The data were extracted from these charts using a plot digitizer tool [9].



Figure 2 – LOX/kerosene combustion charts [6]

For the nonlinear surface generation, a two-variable power function has been chosen having the following form:

$$f(x, y) = a + b \cdot x^c + d \cdot y^e \tag{5}$$

The aim of the data fitting analysis is to find the optimum values of the 5 coefficients (a, b, c, d, e) such that the surface z = f(x, y) accurately represents the data in the propellant combustion charts.

The nonlinear regression is attempted with the Trust-region algorithm detailed in [10], [11], [12] and the Levenberg-Marquardt algorithm detailed in [13], [14] which minimize the summed square of residuals. The main disadvantage of least-squares fitting is its sensitivity to outliers. The outliers are the extreme values that can appear in the input data and usually tend to be at the range frontiers. Two robust methods for outlier influence minimisation are also used, these being the LAR and Bisquare methods, with the aid of the Matlab surface fitting tool [15].

The following regression metrics were computed to quantify the accuracy of data approximation:

| Regression metric | Formula |
|--|---|
| Mean Squared Error (MSE) | $MSE = \frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$ |
| Root Mean Squared Error (RMSE) | $RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2} = \sqrt{MSE}$ |
| Mean Absolute Error (MAE) | $MAE = \frac{1}{N} \sum_{i=1}^{N} \left y_i - \hat{y}_i \right $ |
| Mean Absolute Percentage Error [%] (MAPE) | $MAPE = \frac{1}{N} \sum_{i=1}^{N} \frac{ y_i - \hat{y}_i }{y_i} \cdot 100$ |
| Max Absolute Percentage Error [%] (MaxAPE) | $MaxAPE = \max\left(\frac{ y_i - \hat{y}_i }{y_i} \cdot 100\right)$ |

Table 2 – Regression metrics

In Table 2: *N* is the number of data input points (ranging from 50 to 75 for all the combustion graphs); y_i is the actual expected output and \hat{y}_i is the model's prediction.

From all nonlinear regression methods earlier presented, the one which has yielded the lowest Mean Absolute Percentage Error has been chosen as the optimum solution. For the LOX/kerosene propellant combination, the optimum values of the 5 desired coefficients are shown in Table 3.

The validity range of the model is: $P_c \in [10 - 250]$ atm and $P_e \in [0.1 - 1]$ atm, which corresponds to $R_m \in [2.2 - 2.4]$. A couple of LOX/kerosene combustion surfaces together with the residuals are shown in Figure 3, while the corresponding regression metrics are presented in Table 4.

| Propulsive | Fun var | ction iable | Coefficient | | | | | |
|----------------------|------------|----------------|-------------|------------|---------|-----------|----------|--|
| parameter | х | у | а | b | с | d | e | |
| Mixture ratio | P_c | P_e | 0.40488 | 1.80306 | 0.04244 | -0.27005 | 0.07216 | |
| Flame temperature | P_{c} | R_m | -96657.5664 | 100008.738 | 0.00111 | -20471.89 | -5.10454 | |

Table 3 - LOX/kerosene approximation function coefficients

| Gas molecular weight | P_c | R_m | -61.87059 | 35.50626 | 0.00568 | 39.03287 | 0.22586 |
|-------------------------|-------|-------|-----------|----------|---------|----------|----------|
| Specific heat ratio | P_c | R_m | 2.83175 | -1.6644 | 0.00204 | 0.16136 | -1.06601 |



Figure 3 - LOX/kerosene mixture ratio and gas molecular weight approximations

| Table 4 – LOX/kerosene regres | sion metrics |
|-------------------------------|--------------|
| | |

| Propulsive | Approximation errors | | | | | | | | |
|----------------------|----------------------|-----------|-----------|----------|------------|--|--|--|--|
| parameter | MSE | RSME | MAE | MAPE [%] | MaxAPE [%] | | | | |
| Mixture ratio | 1.443E-06 | 1.201E-03 | 8.185E-04 | 0.036 | 0.169 | | | | |
| Flame temperature | 9.994E+01 | 9.997E+00 | 7.185E+00 | 0.205 | 1.099 | | | | |
| Gas molecular weight | 5.583E-04 | 2.363E-02 | 1.739E-02 | 0.081 | 0.444 | | | | |
| Specific heat ratio | 9.962E-08 | 3.156E-04 | 2.373E-04 | 0.019 | 0.107 | | | | |

It can be clearly seen that the proposed two-variable power function accurately predicts the propulsive data of interest for the LOX/kerosene liquid propellant combination. The residuals are low for the majority of the models validity range, being slightly above average towards the end of the chamber pressure limits. Overall, the proposed power function yields very good results, as seen in Table 4.

Similar to the LOX/kerosene, the other 3 propellant combinations have been analysed and the results are presented in Table 5, Table 6 and Table 7. The validity range of the model is still: $P_c \in [10 - 250]$ atm and $P_e \in [0.1 - 1]$ atm, which corresponds to $R_m \in [2.7 - 2.9]$ for LOX/methane, $R_m \in [5 - 6]$ for LOX/hydrogen and $R_m \in [1.25 - 1.33]$ for LOX/ethanol.

| Propulsive | Function variable | | Coefficient | | | | | | |
|----------------------|----------------------|-------|---------------|--------------|---------|-------------|----------|--|--|
| parameter | х | у | а | b | с | d | e | | |
| Mixture ratio | P_c | P_e | -0.88149 | 3.17521 | 0.03058 | 0.03777 | -0.34131 | | |
| Flame temperature | P_c | R_m | -283663.22149 | 200294.10397 | 0.00045 | 84639.97654 | 0.01976 | | |

Table 5 - LOX/methane approximation function coefficients

| Gas molecular weight | P_c | R_m | -332.49854 | 372.70801 | 0.00045 | -36.22978 | -0.51958 |
|-------------------------|-------|-------|------------|-----------|---------|-----------|----------|
| Specific heat ratio | P_c | R_m | 2.1738 | -2.66329 | 0.00105 | 1.78059 | -0.0395 |

| Propulsive | Function variable | | Coefficient | | | | | |
|-------------------------|----------------------|-------|--------------|-------------|----------|-------------|----------|--|
| parameter | х | у | а | b | с | d | e | |
| Mixture ratio | P_c | P_e | 6.13493 | -91.65097 | -1.26518 | 0 | 0 | |
| Flame temperature | P_c | R_m | -30566.91615 | 12651.74602 | 0.00705 | 18970.35078 | 0.05811 | |
| Gas molecular weight | P_c | R_m | -11.04871 | -1.59875 | -0.11377 | 13.13317 | 0.37008 | |
| Specific heat ratio | P_c | R_m | 6.18754 | -4.99755 | 0.00058 | 0.52031 | -1.78262 | |

Table 6 - LOX/hydrogen approximation function coefficients

Table 7 – LOX/ethanol approximation function coefficients

| Propulsive | Function variable | | Coefficient | | | | | |
|-------------------------|----------------------|-------|--------------|-------------|---------|------------|----------|--|
| parameter | х | у | а | b | с | d | e | |
| Mixture ratio | P_c | P_e | -45.27899 | 46.40622 | 0.00084 | 0.00198 | -0.81443 | |
| Flame temperature | P_c | R_m | -33290.54725 | 26893.55167 | 0.00297 | 8940.82886 | 0.12003 | |
| Gas molecular weight | P_c | R_m | -101.38495 | 66.57454 | 0.00253 | 55.2925 | 0.15025 | |
| Specific heat ratio | P_c | R_m | 3.6356 | -5.26427 | 0.00047 | 2.83722 | -0.0138 | |

For a better overall understanding of the regression metrics of the proposed functions the global MAPE and MaxAPE of all 4 propulsive parameters are shown in Table 8. It can be seen that the global mean absolute percentage errors (of all 4 propulsive parameters) are very small, the maximum being of almost 0.5%, while the global maximum absolute percentage error occurs for the LOX/hydrogen combination and is around 4.4%.

Table 8 - Global average errors - proposed two-variable power function

| Propellant combination | Global average errors (of all 4 propulsive parameters) | | | | |
|------------------------|---|------------|--|--|--|
| | MAPE [%] | MaxAPE [%] | | | |
| LOX/kerosene | 0.085 | 0.455 | | | |
| LOX/methane | 0.074 | 0.607 | | | |
| LOX/hydrogen | 0.451 | 4.391 | | | |
| LOX/ethanol | 0.072 | 0.431 | | | |

4. RESULTS

A total of 11 liquid propelled rocket engines have been analysed, ranging from 30kN to 7.7MN. All four bipropellant liquid combinations earlier presented have been analysed to validate the proposed mathematical model.

The two-variable power function with the earlier obtained coefficients has been implemented for the propulsive parameters of interest computation. Specific impulse and thrust values for sea and vacuum conditions obtained from the tool developed have been compared with the reference values and the errors computed. A list of all studied configurations is presented in Table 9.

| Test configuration | Engine | Fuel | Chamber pressure [atm] | Exhaust pressure [atm] | Mass flow [kg/s] | Expansion ratio | References |
|-----------------------|---------------------|----------|------------------------------|------------------------------|------------------------|--------------------|---------------------------|
| 1 | Rocketdyne F-1 | Kerosene | 65.66 | 0.441 | 2577.8 | 16 | [16], [17] |
| 2 | Merlin 1C-F9 | Kerosene | 65.26 | 0.173 | 161.5 | 14.5 | [18], [19], [20] |
| 3 | Merlin 1D | Kerosene | 95.92 | 0.421 | 236.6 | 21.4 | [20] |
| 4 | Rocketdyne J-2 | Hydrogen | 51.92 | 0.473 | 240.7 | 27.5 | [21] |
| 5 | Rocketdyne RS-25 | Hydrogen | 203.72 | 0.218 | 472.9 | 69 | [22], [23], [24] |
| ба | JAXA 30 kN class | Methane | 11.84 | 2.017 | - | 1.6 | [25], [26] |
| 6b | JAXA 30 kN class | Methane | 9.87 | 0.015 | 9.1 | 49 | [25], [26] |
| 7 | JAXA 100kN class | Methane | 51.32 | 0.020 | 28.2 | 150 | [25], [26] |
| 8 | DLR SE-12 | Methane | 252.95 | 0.591 | 1215.4 | 36.4 | [27] |
| 9 | DLR L75 | Ethanol | 57.74 | 0.025 | 24.3 | 147 | [28] |
| 10 | Glushko RD-101 | Ethanol | 21.31 | 1.174 | 172.9 | 3.42 | [29], [30], [31] |
| 11 | Glushko RD-103 | Ethanol | 24.08 | 1.029 | 196.4 | 4.1 | [29], [30], [31], [32] |

Table 9 - Engine test configurations

Some of the input data, such as chamber pressure and expansion ratio are obtained from the presented references, and in most cases the other data (exhaust pressure and mass flow) are mathematically derived based on reference data.

| | Reference values | | | | Obtained values | | | |
|------------------|----------------------|--------------------------------|---------------|---------------|----------------------|----------------------|---------------|---------|
| Engine | $I_{sp}[\mathbf{s}]$ | $I_{sp}\left[\mathbf{s} ight]$ | <i>T</i> [kN] | <i>T</i> [kN] | $I_{sp}[\mathbf{s}]$ | $I_{sp}[\mathbf{s}]$ | <i>T</i> [kN] | T [kN] |
| | s.l. | vac. | s.l. | vac. | s.l. | vac. | s.l. | vac. |
| Rocketdyne F-1 | 263 | 304 | 6770 | 7770 | 263.66 | 305.40 | 6665.14 | 7720.35 |
| Merlin 1C-F9 | 263 | 302 | 409.24 | 469.29 | 265.56 | 303.63 | 420.59 | 480.88 |
| Merlin 1D | 282 | 320 | 654.33 | 742.41 | 273.49 | 311.87 | 634.57 | 723.62 |
| Rocketdyne J-2 | - | 424 | - | 1023.09 | - | 420.74 | - | 993.23 |
| Rocketdyne RS-25 | 366 | 452.3 | 1705.83 | 2090.66 | 362.25 | 439.25 | 1679.94 | 2037.04 |
| JAXA 30 kN class | 234 | 335 | - | 30 | 225.59 | 332.73 | - | 29.79 |
| JAXA 100kN class | - | 356 | - | 98 | - | 353.34 | - | 97.78 |
| DLR SE-12 | 322.5 | 348.3 | 3844 | 4152 | 315.85 | 342.11 | 3764.72 | 4077.76 |
| DLR L75 | - | 315 | - | 75 | - | 313.75 | - | 74.64 |
| Glushko RD-101 | 214 | 240 | 363 | 402 | 221.04 | 246.02 | 374.79 | 417.14 |
| Glushko RD-103 | 220 | 251 | 432 | 500 | 224.95 | 251.49 | 433.27 | 484.37 |

Table 10 - Proposed model results vs. reference values

The specific impulse and thrust values for sea level (s.l.) and vacuum (vac.) conditions are obtained for the input data from Table 9. The comparison between the reference values and the ones obtained with the proposed model are shown in Table 10.

Table 11 and Figure 4 present the errors between the results obtained with the Matlab tool developed based on the proposed mathematical model and the reference data. It can be seen that the model predicts real-life engine data with a high order of accuracy, the maximum absolute percentage error being of 3.2%, while the global mean absolute percentage error is at 1.65%.

| Engine | | MADE [0/] | | | | |
|------------------|---------------|---------------|--------|--------|----------|--|
| Engine | I_{sp} s.l. | I_{sp} vac. | T s.l. | T vac. | MAPE [%] | |
| Rocketdyne F-1 | 0.25 | 0.46 | 1.55 | 0.64 | 0.73 | |
| Merlin 1C-F9 | 0.97 | 0.54 | 2.77 | 2.47 | 1.69 | |
| Merlin 1D | 3.02 | 2.54 | 3.02 | 2.53 | 2.78 | |
| Rocketdyne J-2 | - | 0.77 | - | 2.92 | 1.84 | |
| Rocketdyne RS-25 | 1.03 | 2.89 | 1.52 | 2.56 | 2.00 | |
| JAXA 30 kN class | 3.59 | 0.68 | - | 0.69 | 1.65 | |
| JAXA 100kN class | - | 0.75 | - | 0.22 | 0.48 | |
| DLR SE-12 | 2.06 | 1.78 | 2.06 | 1.79 | 1.92 | |
| DLR L75 | - | 0.40 | - | 0.47 | 0.43 | |
| Glushko RD-101 | 3.29 | 2.51 | 3.25 | 3.77 | 3.20 | |
| Glushko RD-103 | 2.25 | 0.19 | 0.29 | 3.13 | 1.47 | |
| Global | 1.65 | | | | | |

Table 11 - Proposed model absolute errors



Figure 4 - Proposed model accuracy vs. combustion chamber pressure

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5. CONCLUSIONS

The proposed model can be used to quickly assess the propulsive performance for most small launcher liquid engines. The main propulsive parameters are computed using combustion surfaces obtained after a nonlinear data fitting analysis. The optimum values of the 5 coefficients used in the nonlinear two-variable power function are given in Table 3, Table 5, Table 6 and Table 7.

In the preliminary phases of a launcher design, when the propulsive assessment of a high number of configurations must be realised, models that provide fast approximations are preferred. In this paper, the specific impulse of the engine is modelled based on the combustion chamber and the exhaust pressures, together with the atmospheric conditions at the desired flight regime (sea level or vacuum). For thrust computations, the propellant mass flow is also needed as input data.

The results provide a very good approximation, as seen in the comparison with the engines reference values, the proposed model global error being under 2%. The tool developed based on this mathematical model can be used separately or it can be integrated in a more complex, multidisciplinary optimisation. Because of the low computational time needed, especially due to the nonlinear approximation functions used, the proposed mathematical model is suitable to be used in a full loop MDO algorithm.

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