

RPA: Tool for Liquid Propellant Rocket Engine Analysis C++ Implementation

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Abstract

RPA (Rocket Propulsion Analysis) is a tool for the performance prediction of the liquid-propellant rocket engines. RPA is written in C++ programming language and can be used on MS Windows™ and many Linux and UNIX systems.

This document presents the equations used for the combustion equilibrium and performance calculations. Results obtained from implementing these equations will be compared with results from equilibrium code CEA2.

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Symbols

A	area, m ²
\bar{F}	area ratio
NS	total number of species, gaseous and condensed
NG	number of gaseous species
U	number of chemical elements
a_{ij}	stoichiometric coefficient, number of the atoms of element i per mole of the species j
n_j	moles of species j
N_g	moles of gaseous species
\hat{R}	molar (universal) gas constant, $\hat{R} = 8.314472 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ (ref. 9)
\hat{H}_j^0	molar standard-state enthalpy for species j , $\text{J}\cdot\text{mol}^{-1}$
\hat{S}_j^0	molar standard-state entropy for species j , $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
\hat{G}_j^0	molar standard-state Gibbs energy for species j
p	pressure, Pa
T	temperature, K
w	velocity, m/s
ρ	density, kg/m ³
V	volume, m ³
I_s	specific impulse, m/s
c^*	characteristic exhaust velocity, m/s
C_F	thrust coefficient

Superscripts:

0	symbol for standard state
^	symbol for molar parameter
~	symbol for dimensionless parameter

Subscripts:

inj	injector face
c	end of combustion chamber, or nozzle inlet section
t	nozzle throat section
e	nozzle exit section
0	symbol for assigned, initial or stagnation condition

Analysis methods

Governing Equations for Combustion Equilibrium

The method used for obtaining equilibrium composition is based on a second law of thermodynamics, that is, if an isolated system is at equilibrium, an entropy is constant and reaches its maximum:

$$S = S_{max}; \quad dS = 0; \quad d^2 S < 0 \quad (1)$$

Applying that law to the rocket engines, it is convenient to express the condition of entropy maximization in its equivalent form through the minimization of Gibbs energy:

$$G = U - TS + pV = G_{min}; \quad dG = 0; \quad d^2 G > 0 \quad (2)$$

For the chemically reacting system the differential Gibbs energy is given by

$$dG = Vdp - SdT + \sum_{j=1}^{NS} \hat{\mu}_j dn_j \quad (3)$$

where $\hat{\mu}_j = \hat{\mu}_j^0 + \hat{R} T \ln(p_j)$ is a chemical potential of the species j .

For the isobaric-isothermal system (i.e. $dp=0$ and $dT=0$) the equilibrium conditions can be written as

$$G = \sum_{j=1}^{NS} \hat{\mu}_j n_j = G_{min}; \quad dG = \sum_{j=1}^{NS} \hat{\mu}_j dn_j = 0 \quad (4)$$

The minimization of Gibbs energy is subject to constraint based on the fundamental physical principle: the mass of the isolated system is conserved. That is given by

$$\sum_{j=1}^{NS} a_{ij} \hat{m}_i n_j - b_{i,0} = 0 \quad (i=1 \dots v) \quad (5)$$

where a_{ij} are the stoichiometric coefficients, a_{ij} are the number of the atoms of element i per mole of the species j , the index v is the number of chemical elements, \hat{m}_i are atomic mass of element i , $b_{i,0}$ are the assigned total mass of atoms of element i in the system.

Finally, the condition for equilibrium can be written as minimization function

$$\sum_{j=1}^{NS} \hat{\mu}_j n_j = G_{min} \quad (6)$$

under the constraints

$$\sum_{j=1}^{NS} a_{ij} n_j - \frac{b_{i,0}}{\hat{m}_i} = 0 \quad (i=1 \dots v) \quad (7)$$

That conditional minimization problem can be solved by the method of Lagrange multipliers.

Defining a new function L to be

$$L(n_1, \dots, n_{NS}, \lambda_1, \dots, \lambda_v) = \sum_{j=1}^{NS} \hat{\mu}_j n_j - \sum_{i=1}^v \lambda_i \left(\sum_{j=1}^{NS} a_{ij} n_j - \frac{b_{i,0}}{\hat{m}_i} \right) \quad (8)$$

where λ_i are Lagrange multipliers, the condition for equilibrium becomes

$$\hat{\mu}_j - \sum_{i=1}^v \lambda_i a_{ij} = 0 \quad (j=1 \dots NS) \quad (9a)$$

$$\sum_{j=1}^{NS} a_{ij} n_j - \frac{b_{i,0}}{\hat{m}_i} = 0 \quad (i=1 \dots v) \quad (9b)$$

where

$$\hat{\mu}_j = \begin{cases} \hat{\mu}_j^0 + \hat{R} T \ln \frac{n_j}{N_g} + \hat{R} T \ln \frac{p}{p_0} & (j=1, \dots, NG) \\ \hat{\mu}_j^0 & (j=NG+1, \dots, NS) \end{cases}, \quad \hat{\mu}_j^0 = \frac{G_j^0}{n_j} = \hat{G}_j^0, \quad (10)$$

$N_g = \sum_{j=1}^{NG} n_j$ is the total mole number of gaseous species, and p_0 is a standard-state pressure.

Reducing expressions and separating terms for gaseous and condensed phases, the final equations become

$$\hat{G}_j^0 + \hat{R} T \ln \frac{n_j}{N_g} + \hat{R} T \ln \frac{p}{p_0} - \sum_{i=1}^v \lambda_i a_{ij} = 0 \quad (j=1 \dots NG) \quad (11a)$$

$$\hat{G}_j^0 - \sum_{i=1}^v \lambda_i a_{ij} = 0 \quad (j=NG+1 \dots NS) \quad (11b)$$

$$\sum_{j=1}^{NS} a_{ij} n_j - \frac{b_{i,0}}{\hat{m}_i} = 0 \quad (i=1 \dots v) \quad (11c)$$

$$\sum_{j=1}^{NG} n_j - N_g = 0 \quad (11d)$$

The set (11) consists of $NS+v+1$ simultaneous equations and can be solved for variables $\{N_g, n_1, \dots, n_{NS}, \lambda_1, \dots, \lambda_v\}$, providing the equilibrium composition for the isobaric-isothermal problem with assigned pressure and temperature $(p, T) = \text{const.}$

For the combustion chamber and nozzle of rocket engines, the temperature of the equilibrium composition is an unknown variable that has to be determined as well.

Assuming the combustion in the chamber of the rocket engine to be isobaric-adiabatic (i.e., the pressure is constant and no heat is transferred to or from the chamber), from the first law of thermodynamics follows

$$dH = dQ + Vdp = 0 \quad (12)$$

The last equation states that the combustion is an isenthalpic process, that is it proceeds without any change in enthalpy. That can be expressed as

$$\sum_{j=1}^{NS} n_j \hat{H}_j^0 - H_0 = 0 \quad (13)$$

where \hat{H}_j^0 are the molar enthalpy of the species j , H_0 is a constant equal to enthalpy of the propellant components.

The final equations that permit the determination of equilibrium composition for thermodynamics state specified by an assigned pressure and enthalpy become

$$\hat{G}_j^0 + \hat{R} T \ln \frac{n_j}{N_g} + \hat{R} T \ln \frac{p}{p_0} - \sum_{i=1}^v \lambda_i a_{ij} = 0 \quad (j=1 \dots NG) \quad (14a)$$

$$\hat{G}_j^0 - \sum_{i=1}^v \lambda_i a_{ij} = 0 \quad (j=NG+1 \dots NS) \quad (14b)$$

$$\sum_{j=1}^{NS} a_{ij} n_j - \frac{b_{i,0}}{\hat{m}_i} = 0 \quad (i=1 \dots v) \quad (14c)$$

$$\sum_{j=1}^{NG} n_j - N_g = 0 \quad (14d)$$

$$\sum_{j=1}^{NS} n_j \hat{H}_j^0 - H_0 = 0 \quad (14e)$$

The set (14) consists of $NS+v+2$ simultaneous equations and can be solved for variables $\{N_g, n_1, \dots, n_{NS}, \lambda_1, \dots, \lambda_v, T\}$, providing the equilibrium composition for the isobaric-isenthalpic problem with assigned pressure and enthalpy $(p, H) = \text{const.}$

In order to determine the equilibrium composition for the nozzle flow, it is assumed that the entropy of the composition remains constant during expansion through the nozzle:

$$\sum_{j=1}^{NS} n_j \hat{S}_j - S_0 = 0 \quad (15a)$$

$$\hat{S}_j = \begin{cases} \hat{S}_j^0 - \hat{R} \ln \frac{n_j}{N_g} - \hat{R} \ln \frac{p}{p_0} & (j=1, \dots, NG) \\ \hat{S}_j^0 & (j=NG+1, \dots, NS) \end{cases} \quad (15b)$$

where $N_g = \sum_{j=1}^{NG} n_j$ is the total mole number of gaseous species, p_0 is a standard-state pressure, and S_0 is an entropy of the composition at the end of the combustion chamber.

Substituting last terms into the initial equations, and separating equations for gaseous and condensed phases, the final equations become

$$\hat{G}_j^0 + \hat{R} T \ln \frac{n_j}{N_g} + \hat{R} T \ln \frac{p}{p_0} - \sum_{i=1}^v \lambda_i a_{ij} = 0 \quad (j=1 \dots NG) \quad (16a)$$

$$\hat{G}_j^0 - \sum_{i=1}^v \lambda_i a_{ij} = 0 \quad (j=NG+1 \dots NS) \quad (16b)$$

$$\sum_{j=1}^{NS} a_{ij} n_j - \frac{b_{i,0}}{\hat{m}_i} = 0 \quad (i=1 \dots v) \quad (16c)$$

$$\sum_{j=1}^{NG} n_j - N_g = 0 \quad (16d)$$

$$\sum_{j=1}^{NG} n_j \left(\hat{S}_j^0 - \hat{R} \ln \frac{n_j}{N_g} - \hat{R} \ln \frac{p}{p_0} \right) + \sum_{j=NG+1}^{NS} n_j \hat{S}_j^0 - S_0 = 0 \quad (16e)$$

The set (16) consists of $NS+u+2$ simultaneous equations and can be solved for variables $\{N_g, n_1, \dots, n_{NS}, \lambda_1, \dots, \lambda_u, T\}$, providing the equilibrium composition for the isobaric-isentropic problem with assigned pressure and entropy $(p, S) = \text{const}$.

Iteration Equations for Combustion Equilibrium

The equations (11), (14) and (16) are not all linear and an iteration procedure is required. A Newton method is used to solve for corrections to initial estimates of variables.

After applying a Newton-type linearization to equations (11), (14) and (16) the linearized equations for corresponding problems are as follows:

for the problem $(p, T) = \text{const}$

$$\Delta \ln(n_j) - \Delta \ln(N_g) - \sum_{i=1}^u a_{ij} \pi_i = -\frac{\hat{G}_j^0}{\hat{R}T} - \ln n_j + \ln N_g - \ln \frac{p}{p_0} \quad (j=1 \dots NG) \quad (17a)$$

$$\sum_{i=1}^u a_{ij} \pi_i = \frac{\hat{G}_j^0}{\hat{R}T} \quad (j=NG+1 \dots NS) \quad (17b)$$

$$\sum_{j=1}^{NG} a_{ij} n_j \Delta \ln(n_j) + \sum_{j=NG+1}^{NS} a_{ij} \Delta n_j = \frac{b_{i,0}}{\hat{m}_i} - \sum_{j=1}^{NS} a_{ij} n_j \quad (i=1 \dots u) \quad (17c)$$

$$\sum_{j=1}^{NG} n_j \Delta \ln(n_j) - N_g \Delta \ln(N_g) = N_g - \sum_{j=1}^{NG} n_j \quad (17d)$$

for the problem $(p, H) = \text{const}$

$$\Delta \ln(n_j) - \Delta \ln(N_g) - \sum_{i=1}^u a_{ij} \pi_i - \frac{\hat{H}_j^0}{\hat{R}T} \Delta \ln(T) = -\frac{\hat{G}_j^0}{\hat{R}T} - \ln n_j + \ln N_g - \ln \frac{p}{p_0} \quad (j=1 \dots NG) \quad (18a)$$

$$\sum_{i=1}^u a_{ij} \pi_i + \frac{\hat{H}_j^0}{\hat{R}T} \Delta \ln(T) = \frac{\hat{G}_j^0}{\hat{R}T} \quad (j=NG+1 \dots NS) \quad (18b)$$

$$\sum_{j=1}^{NG} a_{ij} n_j \Delta \ln(n_j) + \sum_{j=NG+1}^{NS} a_{ij} \Delta n_j = \frac{b_{i,0}}{\hat{m}_i} - \sum_{j=1}^{NS} a_{ij} n_j \quad (i=1 \dots u) \quad (18c)$$

$$\sum_{j=1}^{NG} n_j \Delta \ln(n_j) - N_g \Delta \ln(N_g) = N_g - \sum_{j=1}^{NG} n_j \quad (18d)$$

$$\sum_{j=1}^{NG} n_j \frac{\hat{H}_j^0}{\hat{R}T} \Delta \ln(n_j) + \sum_{j=NG+1}^{NS} n_j \frac{\hat{H}_j^0}{\hat{R}T} \Delta \ln(n_j) + \sum_{j=1}^{NS} n_j \frac{\hat{C}_{p,j}^0}{\hat{R}} \Delta \ln(T) = \frac{H_0}{\hat{R}T} - \sum_{j=1}^{NS} n_j \frac{\hat{H}_j^0}{\hat{R}T} \quad (18e)$$

for the problem $(p, S) = \text{const}$

$$\Delta \ln(n_j) - \Delta \ln(N_g) - \sum_{i=1}^v a_{ij} \pi_i - \frac{\hat{H}_j^0}{\hat{R}T} \Delta \ln(T) = -\frac{\hat{G}_j^0}{\hat{R}T} - \ln n_j + \ln N_g - \ln \frac{p}{p_0} \quad (j=1 \dots NG) \quad (19a)$$

$$\sum_{i=1}^v a_{ij} \pi_i + \frac{\hat{H}_j^0}{\hat{R}T} \Delta \ln(T) = \frac{\hat{G}_j^0}{\hat{R}T} \quad (j=NG+1 \dots NS) \quad (19b)$$

$$\sum_{j=1}^{NG} a_{ij} n_j \Delta \ln(n_j) + \sum_{j=NG+1}^{NS} a_{ij} \Delta n_j = \frac{b_{i,0}}{\hat{m}_i} - \sum_{j=1}^{NS} a_{ij} n_j \quad (i=1 \dots v) \quad (19c)$$

$$\sum_{j=1}^{NG} n_j \Delta \ln(n_j) - N_g \Delta \ln(N_g) = N_g - \sum_{j=1}^{NG} n_j \quad (19d)$$

$$\begin{aligned} \sum_{j=1}^{NG} \left[\frac{\hat{S}_j^0}{\hat{R}} - \left(\ln n_j - \ln N_g + \ln \frac{p}{p_0} + 1 \right) \right] n_j \Delta \ln n_j + \sum_{j=NG+1}^{NS} n_j \frac{\hat{S}_j^0}{\hat{R}} \Delta \ln n_j + \sum_{j=1}^{NS} n_j \frac{\hat{C}_{p,j}^0}{\hat{R}} \Delta \ln T + \\ \sum_{j=1}^{NG} n_j \Delta \ln N_g = \frac{S_0}{\hat{R}} - \sum_{j=1}^{NG} \left[\frac{\hat{S}_j^0}{\hat{R}} - \left(\ln n_j - \ln N_g + \ln \frac{p}{p_0} \right) \right] n_j - \sum_{j=NG+1}^{NS} n_j \frac{\hat{S}_j^0}{\hat{R}} \end{aligned} \quad (19e)$$

The set (17) consists of $NS+v+1$ linear simultaneous equations and can be solved for correction variables $\{\Delta \ln(N_g), \Delta \ln(n_1), \dots, \Delta \ln(n_{NG}), \Delta n_{NG+1}, \dots, \Delta n_{NS}, \pi_1, \dots, \pi_v\}$. The sets (18) and (19) each consist of $NS+v+2$ linear simultaneous equations and can be solved for correction variables $\{\Delta \ln(N_g), \Delta \ln(n_1), \dots, \Delta \ln(n_{NG}), \Delta n_{NG+1}, \dots, \Delta n_{NS}, \pi_1, \dots, \pi_v, \Delta \ln T\}$. Here a new variable π_i defined as $\pi_i = \frac{\lambda_i}{\hat{R}T}$.

Iteration Procedure for Combustion Equilibrium

The solutions proceeds by solving the appropriate set of linear simultaneous equations and incrementally updating the number of moles for each species n_j , the total moles N_g and the temperature T (for the (p,H) and (p,S) problems) until the correction variables are within a specified tolerance. At each iteration, the updated set of linear equations is solved using a Lower-Upper (LU) matrix decomposition algorithm.

An initial estimates and controlling the divergence are made, as suggested by Gordon and McBride (ref. 3).

Thermodynamics Derivatives from Equilibrium Solution

Derivatives from Composition With Respect to Pressure

Differentiating equations (11) with respect to pressure gives

$$\sum_{i=1}^v a_{ij} \left(\frac{\delta \pi_i}{\delta \ln p} \right)_T + \left(\frac{\delta \ln N_g}{\delta \ln p} \right)_T - \left(\frac{\delta \ln n_j}{\delta \ln p} \right)_T = 1 \quad (j=1, \dots, NG) \quad (20a)$$

$$\sum_{i=1}^v a_{ij} \left(\frac{\delta \pi_i}{\delta \ln p} \right)_T = 0 \quad (j=NG+1, \dots, NS) \quad (20b)$$

$$\sum_{j=1}^{NG} a_{kj} n_j \left(\frac{\delta \ln n_j}{\delta \ln p} \right)_T + \sum_{j=NG+1}^{NS} a_{kj} \left(\frac{\delta n_j}{\delta \ln p} \right)_T = 0 \quad (k=1, \dots, v) \quad (20c)$$

$$\sum_{j=1}^{NG} n_j \left(\frac{\delta \ln n_j}{\delta \ln p} \right)_T - N_g \left(\frac{\delta \ln N_g}{\delta \ln p} \right)_T = 0 \quad (20d)$$

The set (20) consists of $NS + v + 1$ linear simultaneous equations and can be solved for unknown terms $\left(\frac{\delta \ln n_1}{\delta \ln p} \right)_T, \dots, \left(\frac{\delta \ln n_{NS}}{\delta \ln p} \right)_T, \left(\frac{\delta \ln N_g}{\delta \ln p} \right)_T, \left(\frac{\delta \pi_1}{\delta \ln p} \right)_T, \dots, \left(\frac{\delta \pi_v}{\delta \ln p} \right)_T$.

Derivatives from Composition With Respect to Temperature

Differentiating equations (11) with respect to temperature gives

$$\sum_{j=1}^{NG} a_{ij} n_j \left(\frac{\delta \ln n_j}{\delta \ln T} \right)_p + \sum_{j=NG+1}^{NS} a_{ij} \left(\frac{\delta n_j}{\delta \ln T} \right)_p = 0 \quad (i=1, \dots, v) \quad (21a)$$

$$\sum_{i=1}^v a_{ij} \left(\frac{\delta \pi_i}{\delta \ln T} \right)_p = - \frac{\hat{H}_j^0}{\hat{R} T} \quad (j=NG+1, \dots, NS) \quad (21b)$$

$$\sum_{j=1}^{NG} a_{ij} n_j \left(\frac{\delta \ln n_j}{\delta \ln T} \right)_p + \sum_{j=NG+1}^{NS} a_{ij} \left(\frac{\delta n_j}{\delta \ln T} \right)_p = 0 \quad (i=1, \dots, v) \quad (21c)$$

$$\sum_{j=1}^{NG} n_j \left(\frac{\delta \ln n_j}{\delta \ln T} \right)_p - N_g \left(\frac{\delta \ln N_g}{\delta \ln T} \right)_p = 0 \quad (21d)$$

The set (21) consists of $NS + v + 1$ linear simultaneous equations and can be solved for unknown terms $\left(\frac{\delta \ln n_1}{\delta \ln T} \right)_p, \dots, \left(\frac{\delta \ln n_{NS}}{\delta \ln T} \right)_p, \left(\frac{\delta \ln N_g}{\delta \ln T} \right)_p, \left(\frac{\delta \pi_1}{\delta \ln T} \right)_p, \dots, \left(\frac{\delta \pi_v}{\delta \ln T} \right)_p$.

Derivatives from perfect gas state equation

Differentiating equation of state $pV = N_g \hat{R} T$ with respect to temperature gives

$$\left(\frac{\delta \ln V}{\delta \ln T} \right)_p = \left(\frac{\delta \ln N_g}{\delta \ln T} \right)_p + 1 \quad (22)$$

Differentiating equation of state with respect to temperature gives

$$\left(\frac{\delta \ln V}{\delta \ln p} \right)_T = \left(\frac{\delta \ln N_g}{\delta \ln p} \right)_T - 1 \quad (23)$$

Heat Capacity and Specific Heat

Heat capacity of the thermodynamic system at constant pressure is defined as

$$C_p = \left(\frac{\delta H}{\delta T} \right)_p = \left(\frac{\delta \left[\sum_{j=1}^{NS} n_j \hat{H}_j^0 \right]}{\delta T} \right)_p \quad (24)$$

and after differentiation gives

$$C_p = \sum_{j=1}^{NG} n_j \frac{\hat{H}_j^0}{T} \left(\frac{\delta \ln n_j}{\delta \ln T} \right)_p + \sum_{j=NG+1}^{NS} \frac{\hat{H}_j^0}{T} \left(\frac{\delta n_j}{\delta \ln T} \right)_p + \sum_{j=1}^{NS} n_j \hat{C}_{p,j}^0 \quad (25)$$

Molar heat capacity and specific heat are

$$\hat{C}_p = \frac{C_p}{\sum_{j=1}^{NS} n_j} \quad (26)$$

and

$$c_p = \frac{C_p}{m} = \frac{C_p}{\hat{m} \sum_{j=1}^{NS} n_j} = \frac{\hat{C}_p}{\hat{m}} \quad (27)$$

correspondingly.

Relation between heat capacities can be expressed as

$$C_p - C_v = -T \frac{\left(\frac{\delta V}{\delta T} \right)_p^2}{\left(\frac{\delta V}{\delta p} \right)_T} = -T \frac{\frac{V^2}{T^2} \left(\frac{\delta \ln V}{\delta \ln T} \right)_p^2}{\frac{V}{p} \left(\frac{\delta \ln V}{\delta \ln p} \right)_T} = -\frac{pV}{T} \frac{\left(\frac{\delta \ln V}{\delta \ln T} \right)_p^2}{\left(\frac{\delta \ln V}{\delta \ln p} \right)_T} = -N_g \hat{R} \frac{\left(\frac{\delta \ln V}{\delta \ln T} \right)_p^2}{\left(\frac{\delta \ln V}{\delta \ln p} \right)_T} \quad (28)$$

After substitution (22) and (23) into equation (28), the heat capacity of the thermodynamic system at constant volume can be found from the previous equation:

$$C_v = C_p + N_g \hat{R} \frac{\left(\frac{\delta \ln V}{\delta \ln T} \right)_p^2}{\left(\frac{\delta \ln V}{\delta \ln p} \right)_T} \quad (29)$$

Molar heat capacity and specific heat are

$$\hat{C}_v = \frac{C_v}{\sum_{j=1}^{NS} n_j} \quad (30)$$

and

$$c_v = \frac{C_v}{m} = \frac{C_v}{\hat{m} \sum_{j=1}^{NS} n_j} = \frac{\hat{C}_v}{\hat{m}} \quad (31)$$

correspondingly.

Specific heat ratio is defined as

$$\gamma = \frac{C_p}{C_v} = \frac{\hat{C}_p}{\hat{C}_v} = \frac{c_p}{c_v} \quad (32)$$

whereas isentropic exponent is

$$k = - \frac{\gamma}{\left(\frac{\delta \ln V}{\delta \ln p} \right)_T} \quad (33)$$

Velocity of sound

The velocity of sound is defined as

$$a^2 = \left(\frac{\delta p}{\delta \rho} \right)_s \quad (34)$$

Expressing $\delta \rho = \delta \frac{m}{V} = -\frac{m}{V^2} \delta V$, the last equation can be rewritten as

$$a^2 = -\frac{V^2}{m} \left(\frac{\delta p}{\delta V} \right)_s \quad (35)$$

From the Euler's chain rule

$$\left(\frac{\delta p}{\delta V} \right)_s = -\frac{\left(\frac{\delta S}{\delta V} \right)_p}{\left(\frac{\delta S}{\delta p} \right)_V} = -\frac{\left(\frac{\delta S}{\delta V} \right)_p T \left(\frac{\delta T}{\delta T} \right)_p}{\left(\frac{\delta S}{\delta p} \right)_V T \left(\frac{\delta T}{\delta T} \right)_V} = -\frac{T \left(\frac{\delta S}{\delta T} \right)_p \left(\frac{\delta T}{\delta V} \right)_p}{T \left(\frac{\delta S}{\delta T} \right)_V \left(\frac{\delta T}{\delta p} \right)_V} \quad (36)$$

Since $T \left(\frac{\delta S}{\delta T} \right)_p = C_p$, $T \left(\frac{\delta S}{\delta T} \right)_V = C_v$ and (from the Euler's chain rule again)

$$\left(\frac{\delta T}{\delta p} \right)_V \left(\frac{\delta V}{\delta T} \right)_p = -\left(\frac{\delta V}{\delta p} \right)_T, \text{ the equation (36) can be reduced to}$$

$$\left(\frac{\delta p}{\delta V} \right)_s = \frac{\gamma}{\left(\frac{\delta V}{\delta p} \right)_T} = \frac{p}{V} \frac{\gamma}{\left(\frac{\delta \ln V}{\delta \ln p} \right)_T} \quad (37)$$

Substituting (37) into equation (35), velocity of sound is expressed as

$$a^2 = -p v \frac{\gamma}{\left(\frac{\delta \ln V}{\delta \ln p} \right)_T}$$

Recalling the equation of perfect gas state, the velocity of sound can now be written as

$$a^2 = -\frac{\gamma}{\left(\frac{\delta \ln V}{\delta \ln p} \right)_T} \frac{\hat{R} T}{\sum_{j=1}^{NG} n_j \hat{m}_j} \quad (38)$$

Density

$$\rho = \frac{p}{1000 N_g \hat{R} T} \sum_{j=1}^{NS} n_j \hat{m}_j$$

Thermodynamic Derivatives for Frozen Flow

It can be shown, that for the “frozen” flow where composition remains fixed, the mentioned derivatives can be reduced to

$$C_{p,f} = \sum_{j=1}^{NS} n_j \hat{C}_{p,j}^0, \quad (39)$$

$$C_{v,f} = C_{p,f} + \sum_{j=1}^{NS} n_j \hat{R}, \quad (40)$$

$$k_f = \gamma_f = \frac{C_{p,f}}{C_{v,f}} = \frac{\hat{C}_{p,f}}{\hat{C}_{v,f}} = \frac{c_{p,f}}{c_{v,f}} \quad (41)$$

$$a_f^2 = k_f \frac{\hat{R}}{\hat{m}} T \quad (42)$$

Thermodynamic Data

The program supports the thermodynamic database in ASCII format (ref. 6) and can utilize original NASA database of McBride (ref. 4) as well as its enlargements (e.g. provided by Burcat and Ruscic, ref. 7). Both databases are included with the current program distribution.

For each reaction species the thermodynamic functions heat capacity, enthalpy and entropy as functions of temperature are given in the polynomial form using 9 constants as follows:

$$\frac{\hat{C}_p^0}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 \quad (43)$$

$$\frac{\hat{H}^0}{RT} = -a_1 T^{-2} + a_2 \ln(T) T^{-1} + a_3 + \frac{a_4}{2} T + \frac{a_5}{3} T^2 + \frac{a_6}{4} T^3 + \frac{a_7}{5} T^4 + a_8 T^{-1} \quad (44)$$

$$\frac{\hat{S}^0}{R} = -\frac{a_1}{2} T^{-2} - a_2 T^{-1} + a_3 \ln(T) + a_4 T + \frac{a_5}{2} T^2 + \frac{a_6}{3} T^3 + \frac{a_7}{4} T^4 + a_9 \quad (45)$$

Theoretical Rocket Engine Performance

The following assumptions are made for the calculation of the theoretic rocket performance: adiabatic, isenthalpic combustion; adiabatic, isentropic (frictionless and no dissipative losses) quasi-one-dimensional nozzle flow; ideal gas law; no dissipative losses.

Combustion Chamber Conditions

The analysis is started by obtaining the combustion chamber equilibrium composition assuming the isobaric-isenthalpic combustion, followed by calculation of the thermodynamics derivatives from the equilibrium solution. The results include the number of moles for each species, combustion

temperature, heat capacity, enthalpy and entropy of the reacting mixture, as well as specific heat ratio, isentropic exponent and velocity of sound.

Once the combustion equilibrium composition obtained, the throat conditions can be found.

Throat Conditions for Infinite-area combustion chamber

When the chamber section is large compared to the nozzle throat section, the velocity in the combustion chamber is comparatively small. This leads to the tiny pressure and temperature drop, and the conditions at the nozzle inlet can be considered as identical to that at the injector face. The last statement can be expressed as

$$p_{inj} = p_c = p_{0c} = \text{const} \quad (46a)$$

$$h_{inj} = h_c = \text{const} \quad (46b)$$

$$s_{inj} = s_c = \text{const} \quad (46c)$$

$$w_{inj} = w_c = 0 \quad (46d)$$

where p_{0c} is a stagnation pressure.

Knowing the conditions at nozzle inlet and assuming isentropic expansion in the nozzle, the equilibrium routine for the problem $(p, S)_t = \text{const}$ can be utilized to determine the composition at throat section.

Because the pressure p_t is unknown, an iterative procedure is conducted with initial estimate

$$p_t^{(0)} = p_c \left(\frac{2}{k_c + 1} \right)^{\frac{k_c}{k_c - 1}} \quad (47)$$

At each iteration, the solution of the problem $(p_t^{(i)}, S_t) = \text{const}$ is used to determine the flow velocity and Mach number at throat section:

$$w_t^{(i)} = \sqrt{2(h_c - h_t^{(i)}) + w_c^2} \quad (48)$$

$$M_t^{(i)} = \frac{w_t^{(i)}}{a_t^{(i)}} \quad (49)$$

where the chamber velocity w_c is comparatively small and term w_c^2 can be neglected.

Iteration is repeated until the difference $|M_t^{(i)} - 1|$ is within a specified convergence tolerance. For the next iteration $(i+1)$ the improved throat pressure is calculated as

$$p_t^{(i+1)} = p_t^{(i)} \frac{k(M_t^{(i)})^2 + 1}{k + 1} \quad (50)$$

Throat Conditions for Finite-area combustion chamber

As stated in ref. 10, when the chamber has a cross section that is larger than about four times the throat area ($\bar{F}_c = A_c/A_t > 4$), the chamber velocity can be neglected. To the contrary, in combustion chambers with relatively small cross section, the expansion of the gases is accompanied by significant acceleration and pressure drop. The acceleration process in the chamber is assumed to be adiabatic, but not isentropic, and the pressure drop leads to the lower pressure at nozzle inlet p_c . This causes a

small loss in specific impulse.

Because both nozzle inlet pressure p_c and nozzle throat pressure p_t are unknown, two-level iterative procedure is conducted with initial estimates

$$p_c^{(0)} = \frac{1}{\pi(\lambda_c) \left[1 + \frac{k_{inj} M_c^2}{(\beta_T p)_{inj}} \right]} \quad (51a)$$

where λ_c is a characteristic Mach number at nozzle inlet obtained for subsonic flow from equation

$$\frac{1}{\bar{F}_c} = \left(\frac{k+1}{2} \right)^{\frac{1}{k-1}} \lambda_c \left(1 - \frac{k-1}{k+1} \lambda_c^2 \right)^{\frac{1}{k-1}} \quad \text{with assumption } k = k_{inj} ; \quad M_c \text{ is a Mach number that}$$

corresponds to the calculated characteristic Mach number;

$$\beta_T = - \frac{\left(\frac{\delta \ln V}{\delta \ln p} \right)_T}{p} \quad \text{and} \quad \pi(\lambda_c) = \left(1 - \frac{k-1}{k+1} \lambda_c^2 \right)^{\frac{k}{k-1}} \quad \text{also with assumption } k = k_{inj} ;$$

$$\rho_c^{(0)} = \rho_{inj} \quad (51b)$$

For the assigned chamber contraction area ratio $\bar{F}_c = A_c / A_t$, the iteration proceeds as follows:

1. Assuming that velocity at injector face can be neglected, the velocity at the nozzle inlet is obtained from the momentum equation for steady one-dimensional flow:

$$w_c^{(i)} = \sqrt{\frac{p_{inj} - p_c^{(i)}}{\rho_c^{(i)}}} \quad (52)$$

2. If acceleration process in the chamber is adiabatic, the total enthalpy per unit mass is constant. Recalling that velocity at injector face can be neglected, the specific enthalpy at nozzle inlet can be expressed as

$$h_c^{(i)} = h_{inj} - \frac{(w_c^{(i)})^2}{2} \quad (53)$$

3. Solution of the problem $(p, H)_c = \text{const}$ for the nozzle inlet section provides the entropy at nozzle inlet $S_c^{(i)}$.

4. Known conditions at nozzle inlet and assumption about an isentropic expansion in the nozzle allow to obtain the throat conditions (including throat pressure $p_t^{(i)}$ and density $\rho_t^{(i)}$), utilizing the procedure similar to that for the infinite-area combustion chamber (equations 47 to 50).

5. From the continuity equation for steady quasi-one-dimensional flow, find the velocity at the nozzle inlet for the specified chamber contraction ratio:

$$\tilde{w}_c = \left(\frac{\rho_t w_t}{\rho_c} \right)^{(i)} \frac{1}{\bar{F}_c} \quad (54)$$

6. From the momentum equation, find the pressure at injector face that corresponds to the calculated pressure and velocity at the nozzle inlet:

$$\tilde{p}_{inj} = p_c^{(i)} + \rho_c^{(i)} \tilde{w}_c^2 \quad (55)$$

Iteration is repeated until the relative deviation $\frac{|p_{inj} - \check{p}_{inj}|}{p_{inj}}$ is within a specified convergence tolerance. The improved nozzle inlet pressure for the next iteration ($i+1$) is calculated as

$$p_c^{(i+1)} = p_c^{(i)} \frac{p_{inj}}{\check{p}_{inj}} \quad (56)$$

The stagnation pressure at nozzle inlet section can be computed from

$$p_{0c} = p_c \left[1 + (k_c - 1) \frac{w_c^2 \rho_c}{2 k_c p_c} \right]^{\frac{k_c}{k_c - 1}} \quad (57)$$

Nozzle Exit Conditions

Equilibrium Conditions

Equilibrium conditions at section specified by assigned pressure p_e

Knowing the conditions at nozzle throat and assuming isentropic expansion in the nozzle, the equilibrium routine for the problem $(p, S)_e = \text{const}$ can be directly utilized to determine the composition at nozzle exit section.

The corresponding nozzle area ratio can be obtained from

$$\bar{F}_e = \frac{\rho_t a_t}{\rho_e w_e} \quad (58)$$

Equilibrium conditions at section specified by assigned nozzle area ratio $\bar{F}_e = A_e / A_t$

Knowing the conditions at nozzle throat and assuming isentropic expansion in the nozzle, the equilibrium routine for the problem $(p, S)_e = \text{const}$ can be utilized to determine the composition at nozzle exit section.

Because the pressure p_e is unknown, an iterative procedure is conducted with initial estimate

$$p_e^{(0)} = p_c \left(1 - \frac{k-1}{k+1} \lambda_e^2 \right)^{\frac{k}{k-1}} \text{ with assumption } k = k_t \quad (59)$$

where λ_e is a characteristic Mach number at nozzle exit obtained for supersonic flow from equation

$$\frac{1}{\bar{F}_e} = \left(\frac{k+1}{2} \right)^{\frac{1}{k-1}} \lambda_e \left(1 - \frac{k-1}{k+1} \lambda_e^2 \right)^{\frac{1}{k-1}} \text{ also with assumption } k = k_t .$$

At each iteration, the solution of the problem $(p^{(i)}, S)_e = \text{const}$ is used to determine the nozzle area ratio that corresponds to the assumed nozzle exit pressure:

$$w_e^{(i)} = \sqrt{2(h_c - h_t^{(i)}) + w_c^2} \quad (60)$$

$$\bar{F}_e^{(i)} = \frac{\rho_t a_t}{\rho_e^{(i)} w_e^{(i)}} \quad (61)$$

Iteration is repeated until the relative deviation $\frac{|\bar{F}_e - \bar{F}_e^{(i)}|}{\bar{F}_e}$ is within a specified convergence tolerance. The improved nozzle exit pressure for the next iteration ($i+1$) is calculated as

$$p_e^{(i+1)} = p_e^{(i)} \left(\frac{\bar{F}_e^{(i)}}{\bar{F}_e} \right)^2 \quad (62)$$

Frozen Conditions

For the frozen conditions it is assumed that chemical equilibrium is established within the nozzle section r between nozzle throat and nozzle exit. Once the reaction products passed through that section, the composition is considered to be invariant (frozen), and does not change.

That is, the nozzle exit composition is defined as $\{N_g, n_1, \dots, n_{NS}\}_e = \{N_g, n_1, \dots, n_{NS}\}_r = \text{const}$.

The remainder procedure is as follows.

Frozen conditions at section specified by assigned pressure p_e

In that case the unknown variable T_e can be determined from equation

$$\left(\sum_{j=1}^{NS} n_j \hat{S}_j \right)_e - S_r = 0 \quad (63a)$$

$$\text{where } \hat{S}_j = \begin{cases} \hat{S}_j^0 - \hat{R} \ln \frac{n_j}{N_g} - \hat{R} \ln \frac{p}{p_0} & (j=1, \dots, NG) \\ \hat{S}_j^0 & (j=NG+1, \dots, NS) \end{cases} \quad (63b)$$

Frozen conditions at section specified by assigned nozzle area ratio $\bar{F}_e = A_e / A_t$

In that case the unknown variables $\{T_e, p_e\}$ can be found from the following equations:

$$\left(\sum_{j=1}^{NS} n_j \hat{S}_j \right)_e - S_r = 0 \quad (64a)$$

$$\text{where } \hat{S}_j = \begin{cases} \hat{S}_j^0 - \hat{R} \ln \frac{n_j}{N_g} - \hat{R} \ln \frac{p}{p_0} & (j=1, \dots, NG) \\ \hat{S}_j^0 & (j=NG+1, \dots, NS) \end{cases}$$

$$\frac{p}{\rho_g} \sum_{j=1}^{NG} n_j \hat{m}_j = N_g \hat{R} T \quad (64b)$$

$$\bar{F}_r = \frac{(\rho w)_t}{(\rho w)_r} \quad (64c)$$

$$\left(h + \frac{w^2}{2} \right)_e = \left(h + \frac{w^2}{2} \right)_r \quad (64d)$$

The set of simultaneous equations (64a) to (64d) can be solved for variables $\{p, T, \rho, w\}_e$.

Theoretical Rocket Engine Performance

The following equations for the theoretical rocket engine performance obtained from ref. 10 and 11.

Characteristic exhaust velocity:

$$c^* = \frac{p_{0c}}{a_t \rho_t} \quad (65)$$

Specific impulse in a vacuum:

$$I_s^{vac} = w_e + \frac{p_e}{w_e \rho_e} \quad (66)$$

Specific impulse at ambient pressure p_H :

$$I_s^H = w_e + \frac{p_e - p_H}{w_e \rho_e} \quad (67)$$

Optimum specific impulse ($p_e = p_H$):

$$I_s^{opt} = w_e \quad (68)$$

Thrust coefficient in vacuum:

$$C_F^{vac} = \frac{I_s^{vac}}{c^*} \quad (69)$$

Optimum thrust coefficient:

$$C_F^{opt} = \frac{I_s^{opt}}{c^*} \quad (70)$$

Note that the equation (67) can be used for nozzle conditions without flow separation caused by over-expansion. In order to correctly predict the nozzle performance under highly over-expanded conditions, a more accurate model that considers flow separation and shock waves is required.

Computer Program RPA

Graphical User Interface

Input Parameters

The minimal set of input parameters include

- combustion chamber pressure (expressed in Pascal, atm, bar or psia)
- propellant combination
- mixture ratio "O/F" or oxidizer excess coefficient (α) or mass fractions of each component;
- list of components at standard conditions or at assigned temperature (K);
- assigned enthalpy (kJ/kg or J/mol, optional).

When the minimal set of parameters is defined, the program calculates combustion equilibrium and

determines the properties of the reaction products.

Additional set of input parameters include nozzle analysis options:

- nozzle exit conditions
 - assigned nozzle exit pressure (Pascal, atm, bar or psia) or nozzle exit area ratio;
 - nozzle inlet conditions (optional)
 - assigned chamber contraction area ratio or mass flux ($\text{kg}/\text{m}^2 \cdot \text{s}$);
 - frozen flow (optional)
 - freezing at the assigned pressure (Pascal, atm, bar or psia) or at the assigned nozzle area ratio.
- The complete set of input parameters can be stored in and loaded from the file system.

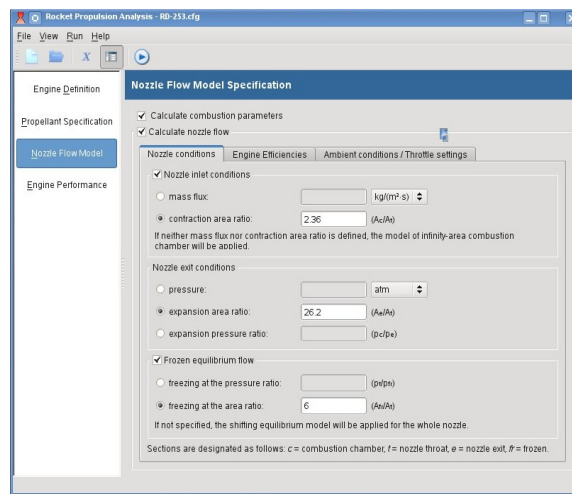


Illustration 1. Input parameters GUI

Output Data

For the minimal set of input parameters, results of thermodynamic calculations include combustion parameters and composition.

For the set of input parameters that includes nozzle analysis options, conditions at nozzle throat and nozzle exit, as well as theoretical rocket engine performance, will be determined.

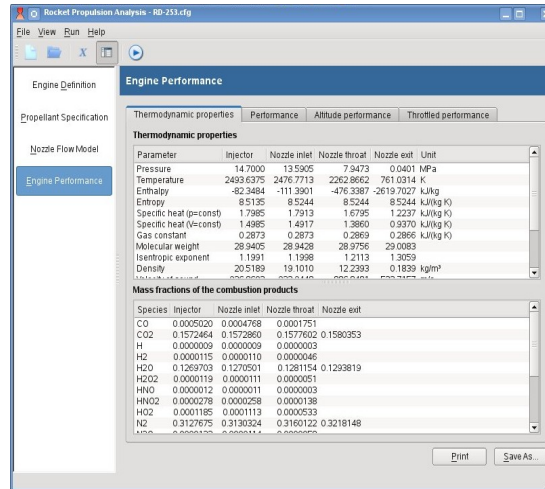


Illustration 2. Output data GUI

Verification

The tool was compared with a code CEA2 (Chemical Equilibrium and Applications 2) developed by Gordon and McBride (ref. 4) at NASA Glenn/Lewis Research Center.

To verify the RPA model and implementation, six test cases were selected (see Table 1).

Table 1. Test cases

	Test case 1	Test case 2	Test case 3	Test case 4	Test case 5	Test case 6
Oxidizer/Temperature, K	LOX / 90.17	LOX / 90.17	LOX / 90.17	LOX / 90.17	LOX / 90.17	LOX / 90.17
Fuel/Temperature, K	LH / 20.27	LH / 20.27	CH4 (L) / 111.643	CH4 (L) / 111.643	RP-1 / 298.15	RP-1 / 298.15
O/F ratio	5.5	5.5	3.2	3.2	2.6	2.6
Chamber pressure, MPa	10	10	10	10	10	10
Chamber contraction area ratio	—	2	—	2	—	2
Nozzle exit area ratio	70	70	70	70	70	70

For all test cases, RPA and CEA2 were executed with identical input parameters.

Tables 2 to 10 provide the results of thermodynamic calculations.

Perfect agreement was obtained between RPA and CEA2 codes.

Very good agreement with small deviations was obtained between RPA and TDC codes.

Table 2. Results of thermodynamics calculations for Test case 1

	RPA	CEA2
Chamber temperature, K	3432.01	3432.01
Characteristic velocity, m/s	2345.30	2345.30
Thrust coefficient	1.87 (opt) 1.94 (vac)	1.8728 (opt) –
Specific impulse, vac, m/s	4549.28	4549.20
Specific impulse, opt, m/s	4392.36	4392.30
Nozzle exit Mach number	4.69	4.69

Table 3. Results of thermodynamics calculations for Test case 2

	RPA	CEA2
Chamber temperature, K	3432.01	3432.01
Nozzle inlet pressure, MPa	8.98100	8.98130
Characteristic velocity, m/s	2344.62	2344.60
Thrust coefficient (opt)	1.870	1.873
Specific impulse, vac, m/s	4548.97	4548.90
Specific impulse, opt, m/s	4391.94	4391.90
Nozzle exit Mach number	4.69	4.69

Table 4. Mole fractions in combustion chamber for Test cases 1 and 2

Species	RPA	CEA2
H	0.02775	0.02775
H2	0.30152	0.30152
H2O	0.64016	0.64016
H2O2	0.00001	0.00001
HO2	0.00001	0.00001
O	0.00140	0.00140
O2	0.00115	0.00115
OH	0.02799	0.02800

Table 5. Results of thermodynamics calculations for Test case 3

	RPA	CEA2
Chamber temperature, K	3566.07	3566.07
Characteristic velocity, m/s	1862.41	1861.20
Thrust coefficient	1.91 (opt) 1.99 (vac)	1.9083 (opt) –
Specific impulse, vac, m/s	3701.07	3700.90
Specific impulse, opt, m/s	3551.82	3551.70
Nozzle exit Mach number	4.44	4.44

Table 6. Results of thermodynamics calculations for Test case 4

	<i>RPA</i>	<i>CEA2</i>
Chamber temperature, K	3566.07	3566.07
Nozzle inlet pressure, MPa	8.99100	8.99140
Characteristic velocity, m/s	1860.31	1860.30
Thrust coefficient (opt)	1.910	1.909
Specific impulse, vac, m/s	3700.35	3700.40
Specific impulse, opt, m/s	3550.90	3551.00
Nozzle exit Mach number	4.43	4.43

Table 7. Mole fractions in combustion chamber for Test cases 3 and 4

<i>Species</i>	<i>RPA</i>	<i>CEA2</i>
CO	0.19733	0.19733
CO ₂	0.11704	0.11704
COOH	0.00002	0.00002
H	0.02155	0.02155
H ₂	0.09898	0.09898
H ₂ O	0.49169	0.49169
H ₂ O ₂	0.00002	0.00002
HCO	0.00002	0.00002
HO ₂	0.00009	0.00009
O	0.00641	0.00641
O ₂	0.01221	0.01221
OH	0.05463	0.05463

Table 8. Results of thermodynamics calculations for Test case 5

	<i>RPA</i>	<i>CEA2</i>
Chamber temperature, K	3723.63	3723.63
Characteristic velocity, m/s	1800.60	1800.60
Thrust coefficient	1.92 (opt) 2.00 (vac)	1.9152 (opt) —
Specific impulse, vac, m/s	3596.50	3596.60
Specific impulse, opt, m/s	3448.37	3448.50
Nozzle exit Mach number	4.39	4.39

Table 9. Results of thermodynamics calculations for Test case 6

	<i>RPA</i>	<i>CEA2</i>
Chamber temperature, K	3723.63	3723.63
Nozzle inlet pressure, MPa	8.99	8.99
Characteristic velocity, m/s	1799.63	1799.6
Thrust coefficient (opt)	1.920	1.916

	<i>RPA</i>	<i>CEA2</i>
Specific impulse, vac, m/s	3595.96	3595.9
Specific impulse, opt, m/s	3447.67	3447.6
Nozzle exit Mach number	4,39	4,38

Table 10. Mole fractions in combustion chamber for Test cases 5 and 6

<i>Species</i>	<i>RPA</i>	<i>CEA2</i>
CO	0.31521	0.31521
CO ₂	0.15383	0.15383
COOH	0.00003	0.00003
H	0.02686	0.02686
H ₂	0.07954	0.07954
H ₂ O	0.33329	0.33329
H ₂ O ₂	0.00002	0.00002
HCO	0.00004	0.00004
HO ₂	0.00011	0.00011
O	0.01119	0.01119
O ₂	0.01785	0.01785
OH	0.06202	0.06202

Conclusion

A tool suitable for the use in preliminary or conceptual design for the prediction of the liquid-propellant rocket engines performance has been established. The implementation in C++ programming language was shown to obtain perfect agreement with industrial-quality Chemical Equilibrium and Application (CEA2) code.

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