

# Optimization of Nozzle Shape of Hydrogen-Oxygen Rocket Engine

Valeriy Matveev, Vasili Zubanov, Leonid Shabliy and Anastasia Korneeva

*Department of Aircraft Engine Theory, Samara National Research University, Samara, Russian Federation*

**Keywords:** Parametric Optimization, Rocket Engine, Combustion, Hydrogen, Oxygen, CFD-Simulation.

**Abstract:** The article presents a technique of parametric optimization of nozzle supersonic part of liquid-propellant rocket engine. Main approaches for parametric optimization were given. Two optimizers were mentioned. Thrust and specific impulse were chosen as optimization criteria. Simulation of chamber process was performed in ANSYS CFX with combustion model Eddy Dissipation. Two variants of combustion were considered: one global reaction and detailed chemical system with 8 components and 18 reactions. Comparison of results gives more smooth contours of parameters for set with detailed system against variant with one reaction for simulation of liquid-propellant rocket engine working with “hydrogen-oxygen” propellants. In result of optimization the nozzle length was shortened up to 15% virtually without thrust loss (0.18% reduction in thrust). Also the Pareto set in axis “thrust”-“nozzle length” was obtained.

## 1 INTRODUCTION

Chamber of liquid-propellant rocket engine (LPRE) is the main unit of LPRE, in which fuel components or burner gases create engine thrust during chemical reactions and efflux from nozzle.

Operating processes of LPRE chamber accompanied by energy losses. As is known, the increase of thrust, specific impulse and other operational parameters (Dobrovolskij, 2005) of modern LPRE is an actual problem of aerospace engineering. At the same time, the cost of experimental development of LPRE is significantly higher than the estimated optimization studies, which allows to create the LPRE with the best parameters at the design stage, and it reduces the creation time and the final product cost.

The technology of virtual computer simulation allows solving optimization tasks using methods based on multiple virtual simulations (Zubrilin, 2015; Baturin, 2015) appeared relatively recently.

This paper presents the technique for optimizing the shape of the expanding part of a LPRE nozzle using virtual gas-dynamic modeling in ANSYS CFX (Zubanov, 2015). The engine has a thrust of 100 kN, and it designed for the interorbital transport vehicle (Belousov, 2014).

## 2 THE MAIN APPROACHES FOR OPTIMIZATION

The traditional approach to solving any optimization problem is the general mathematical approach, where the optimized value (for example, the LPRE thrust or the specific impulse) is expressed as a function in an explicit or implicit form with several the design variables (geometric dimensions of LPRE elements, gas-dynamic flow parameters in the chamber, strength parameters, design constraints, etc.). Then, the extrema of this function and the corresponding values of the optimized parameters (Egorychev, 2016) are found using the tools of mathematical analysis. Unfortunately, the complexity of creating an adequate optimized function (verified mathematical model) exceeds the experimental development of the LPRE. After all, in order to correctly reflect in the functional form the influence of some constructive factor, for example, on the magnitude of thrust, it is necessary to carry out and mathematically generalize the corresponding experimental study.

The technology of virtual computer modeling allows solving optimization tasks using methods based on multiple virtual simulations (Kuzmenko, 2007; Shabliy, 2014) appeared relatively recently. The main feature of this approach is that the functional dependence of  $N$  optimized parameters, optimized by  $K$  criteria, is constructed in  $(N + K)$  - dimensional space solely from data on the values of the criteria

obtained from virtual models constructed for the corresponding combinations of parameters in the region of interest, completely without analyzing the physical effect of the parameters on the criteria. The latter is a very important advantage of this approach, since it allows to treat the virtual model as a "black box" without analyzing the reasons for the influence of certain parameters on the criteria. At the same time, the evaluation of the mutual influence of a parameter set on the considered criteria is performed automatically by the optimization algorithm. Algorithm of modern optimizers, such as ANSYS Design eXplorer (ANSYS, 2015) and Sigma Technology IOSO (Kuzmenko, 2007) allow simultaneous optimization by several criteria, depending on several hundred parameters (Egorov, 2007).

Figure 1 shows a diagram of the process of constructing an approximating optimization surface using as a virtual model the CFD model of the flow in the chamber of a liquid rocket engine. Similarly, lower-level models, both higher, up to the full three-dimensional model of a virtual LPRE, can be applied, which includes not only CFD modeling of currents in all engine paths, considering phase transitions and chemical transformations, but also a FEM-evaluation of the structural strength of the structure. Similarly, models of both low and high levels can be applied. As models of a low level, the mathematical functions of the traditional approach can be used. As models of a high level, the full three-dimensional model of a virtual LPRE including not only workflow CFD-simulation in all engine paths, considering phase transitions and chemical transformations, but also the FEM-evaluation of structural strength can be used. Also, combined and multilevel models can be used. For example, modeling of fuel flow through pipelines is carried out in a one-dimensional setting, the quality of its spraying by nozzles is estimated by zero-dimensional criterial dependencies, and modeling of combustion in the chamber is performed in a three-dimensional nonstationary setting. Naturally, since the values obtained from the "black box" cover the investigated area with a mesh model of finite density, this approach to optimization contains a methodological error: the approximating surface in the general case cannot guarantee the search for a global extremum under sharp changes in the criterion (Figure 2). However, as practice shows, the existing technologies of optimizer programs can reduce the probability of error (Shabliy, 2014).

### 3 CFD-SIMULATION OF COMBUSTION PROCESS IN LPRE CHAMBER WITH FUEL COMPONENTS «HYDROGEN & OXYGEN»

This section presents the methodology of simulation in ANSYS CFX of combustion process in the chamber of small thrust rocket engine operating on gaseous oxygen and hydrogen (Zubakov, 2017). Chemical kinetics was modeled in two variants: using a single global reaction (molecular formula) and set of chemical reactions.

For first calculation, the single reaction in the pre-processor CFX-Pre was chosen from the library ANSYS CFX the global combustion reaction "Hydrogen Oxygen", which involves three components: H<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>O. The reacting mixture of these three gases, defined based on the selected reaction was set as a working fluid. The mass flow rate, the temperature and mass fraction components were set as the input boundary conditions of calculation area.

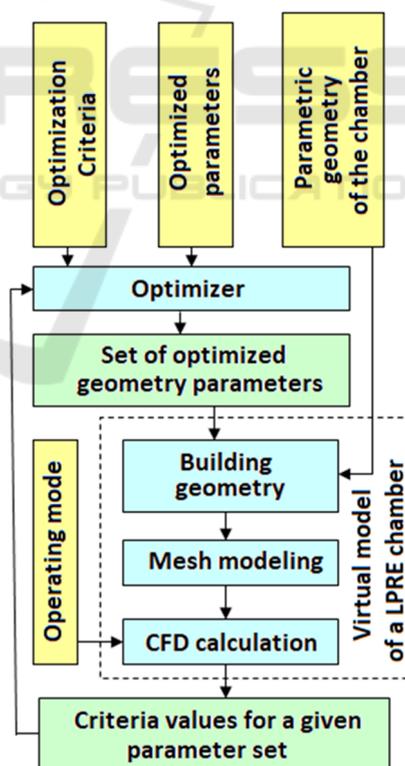


Figure 1: The optimization scheme through multiple virtual simulations (for example, CFD simulation of a LPRE chamber).

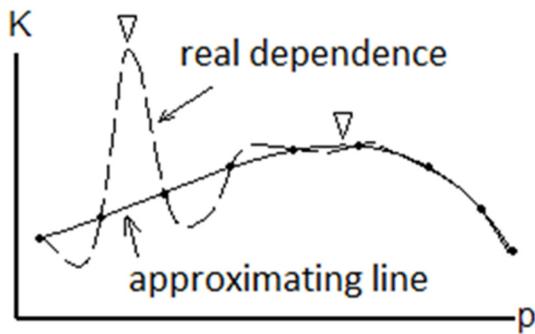


Figure 2: Error estimating the global maximum of the optimized criterion in the case of insufficient discretization of the approximation domain.

The applied model of combustion Eddy Dissipation was developed to describe turbulent flows of a premixed mixtures. It suggests that chemical reactions cause the reacting mixture to equilibrium, i.e. the chemical reaction rate is much higher than the rate of mixing of fuel and oxidizer (Matveev, 2014). Using one global reaction does not allow to fully describe a branched chain reaction in mixtures of hydrogen with oxygen and assess the education progress of the reaction intermediates. A detailed kinetic scheme of chemical reactions with these components includes more than 20 elementary reactions with participation of free radicals in the reacting mixture. The set of reactions of (Gardiner, 1984), described in more detail in (Zubakov, 2014) was used in this study. It consists of 18 chemical reactions (including reversible 5) with the participation of 8 components:  $H_2$ ,  $O_2$ ,  $H_2O$ ,  $H$ ,  $O$ ,  $OH$ ,  $H_2O$ ,  $H_2O_2$ .

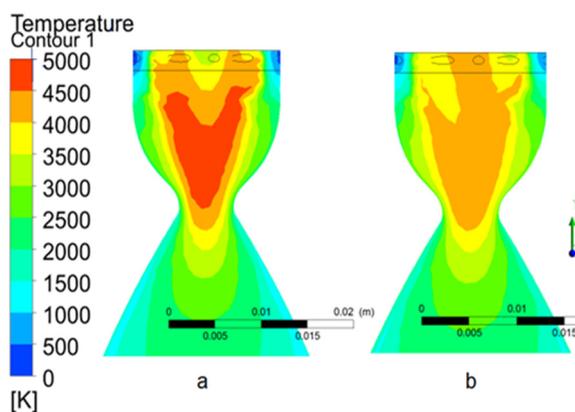


Figure 3: The temperature distribution along the length of the chamber when using: a – single global reaction; b – set of 18 reactions.

The rate of each reaction is determined by the Arrhenius equation. The components and products involved in this reaction, the stoichiometric coefficients and the reaction order were set manually for describe each reaction in CFX-Pre. The parameters of the chemical reaction speed rate (preexponential multiplier  $A$ , temperature exponent  $n$ , activation energy  $E$  and activation temperature  $T$  were taken from (Gardiner, 1984), (Solovieva-Sokolova, 2016) and (Kozlov, 2015).

After reactions specifying all substances was included in the reacting gas mixture of fluid domain. Further steps of the modeling did not differ from the previous simulation using global-reaction. When modeling complicated systems of reactions, the instability of the solution was increased that was required to increase the number of iterations, and consequently, increased the total solution time in comparison with using a single global reaction.

Verification of shown above simulation methodology was performed on the test small thrust rocket engine (25 N thruster), since there were experimental data for it. A comparison of the CFD model results with experimental data showed that the resulting specific impulse in the void corresponds to the experimental one with an accuracy of 3%.

After verification the current LPRE was simulated. The obtained results (Figures 3 and 4) show that the simulation with a single reaction overestimates the local temperature, and the flow is more uniform, axisymmetric. But the calculation with a complicated system of reactions gives has more gradual change in temperature along the length of the chamber and looks more “physical”.

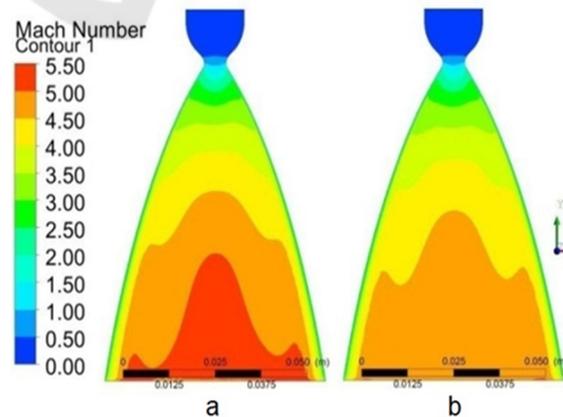


Figure 4: The Mach number distribution along the length of the chamber when using: a – single global reaction; b – set of 18 reactions.

#### 4 DESCRIPTION OF LPRE CHAMBER PARAMETRIC MODEL

The rocket engine with a thrust of 100 kN designed for the interorbital transport vehicle was chosen as the optimization object, because it should have a large nozzle to provide the high specific impulse and thrust.

A virtual CFD model of the gas-dynamic flow in the nozzle was created earlier (Figures 3 and 4). The thrust, the specific impulse, and the static pressure distribution on the inner surface were determined for the given working conditions of the projected nozzle. The working conditions of the projected nozzle were the workflow parameters at the inlet, the pressure at the inlet and outlet. It is noteworthy that the simulation accuracy was acceptable for a multivariate optimization study: the calculated thrust by CFD-modeling of the base nozzle version, constructed according to the technique (Egorychev, 2016), was 99.14 kN, and the specific impulse was 4323 m/s. By the technique (Dobrovolskij, 2005; Egorychev, 2016) the thrust was 100 kN, and the specific impulse was 4357 m/s with the combustion chamber coefficient 0.98.

The expanding part of the nozzle composed of a circular arcs and a Bezier-splines constructed by three knots (Figure 5). The expanding part of the nozzle was parameterized by six parameters with the following ranges of variation (the basic value and relative changes are indicated in parentheses):

- the length of the expanding nozzle part was  $L_a = 935 \dots 1155$  ( $1100^{+5\%}_{-5\%}$ ) mm;
- the arc radius after the critical section was  $R_{c3} = 2 \dots 20$  ( $14^{+40\%}_{-85\%}$ ) mm;
- the expansion angle of the nozzle in the critical section was  $\beta_m = 30 \dots 70^\circ$  ( $50^{+40\%}_{-40\%}$ );
- the expansion angle of the nozzle in the output section was  $\beta_a = 5 \dots 19^\circ$  ( $15^{+30\%}_{-70\%}$ );
- the distance of the spline control points from its ends for the critical (cr) section was  $spline\_cr = 1 \dots 99\%$  (basic - 5%);
- the distance of the spline control points from its ends for the output (out) section was  $spline\_out = 1 \dots 99\%$  (basic - 5%).

For optimization, ANSYS Design Exploration tools were used, namely: the sensitivity of the parameters (*Local Sensitivity*), the construction of the response surface in the second order polynomials (*Response Surface*), and the optimization algorithm for screening geometry variants (*Screening Optimization*) (ANSYS, 2015; Shabliy, 2014).

#### 5 OPTIMIZATION RESULTS

A preliminary assessment of the sensitivity of the parameters showed that parameters  $\beta_a$  and  $\beta_m$ ,  $spline\_cr$  and  $spline\_out$  have the determining influence on the thrust and momentum, while parameter  $L_a$  affects to a lesser extent, and the influence of parameter  $R_{c3}$  is insignificant (Figures 6 and 7).

In the first case, optimization was carried out according to the criteria of maximum thrust and specific impulse, and it was possible to increase the thrust by 0.6%, and the specific impulse by 0.2%, and with the nozzle length  $L_a$  reduced to 1093 mm (base value of  $L_a$  was 1100 mm). Since the mass of the engine depends strongly on the length of the nozzle, it was decided to supplement the optimization task by the criterion of minimizing  $L_a$ . As a result, the nozzle was shortened by 15% (up to 936 mm) with a slight (by 0.18%) reduction in thrust. Changes of the nozzle shape, corresponding to the first (I) and the second (II) tasks, are shown in Figure 8. The Pareto set corresponding to the second task is shown in Figure 9.

Thus, the technique for optimizing the shape of the expanding part of a LPRE nozzle by calculation was created to obtain maximum thrust with the minimum nozzle length.

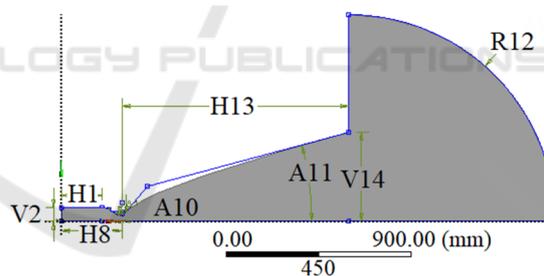


Figure 5: Parametrized nozzle model.

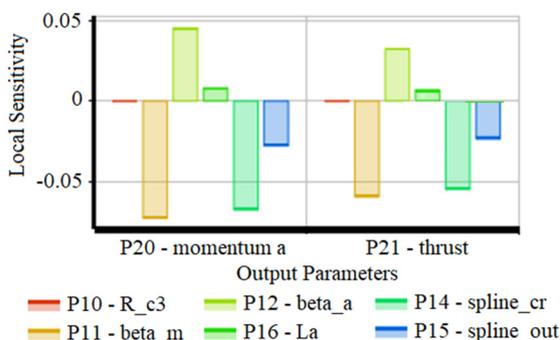


Figure 6: The sensitivity diagram for the geometric parameters and optimizing criteria.

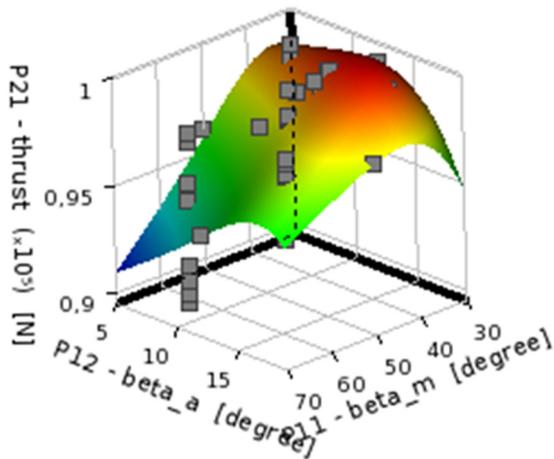


Figure 7: The response surface in assessing the effect of  $\beta_a$  and  $\beta_m$  on the thrust.

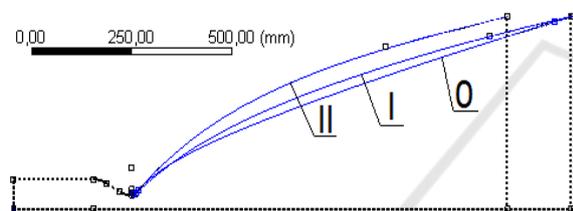


Figure 8: Changes the nozzle shape in comparison with the basic version ("0").

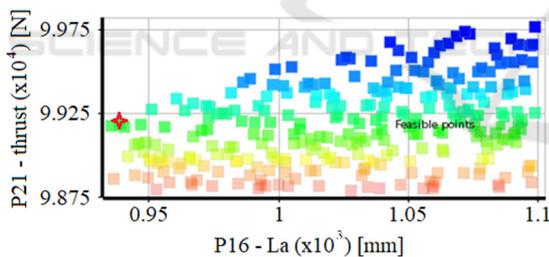


Figure 9: The Pareto set "Length La - Thrust".

## 6 CONCLUSIONS

Based on the adequate CFD-model with the set of reactions, the geometry optimization of the expanding nozzle part of the rocket engine with the thrust of 100 kN for an interorbital transport vehicle was carried out. The good solution was found of the set of pareto: the nozzle was shortened by 15% with a slight by 0.18% reduction in thrust.

CFD-modeling of the combustion process on components "hydrogen-oxygen" shows that the gross reaction results differ from the results obtained with system of chemical reactions. In General, the EDM

model gives overestimated results on temperature in comparison with results of thermodynamic calculation of the chamber. But it can be used to obtain reference solutions.

The technique for optimizing the shape of the expanding part of a LPRE nozzle by calculation was created to obtain maximum thrust with the minimum nozzle length.

The technique can be used to optimize the nozzle of a rocket engine for the second, third and interorbital transport vehicle stages of launch vehicles. But first of all it is required to obtain an adequate CFD-model with combustion of a rocket engine.

## ACKNOWLEDGEMENTS

The work was completed with the financial support of the Ministry of Education and Science of Russia in the framework of the implementation of the Program "Research and development on priority directions of scientific-technological complex of Russia for 2014–2020" and within the basic part framework of the state assignment and with Grant Council of the President of the Russian Federation in the framework of the SP-3790.2015.1 scholarship.

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