The technique for Simulation of Transient Combustion Processes in the Rocket Engine Operating with Gaseous Fuel “Hydrogen and Oxygen”

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Abstract. The article describes the method for simulation of transient combustion processes in the rocket engine. The engine operates on gaseous propellant: oxygen and hydrogen. Combustion simulation was performed using the ANSYS CFX software. Three reaction mechanisms for the stationary mode were considered and described in detail. Reactions mechanisms have been taken from several sources and verified. The method for converting ozone properties from the Shomate equation to the NASA-polynomial format was described in detail. The way for obtaining quick CFD-results with intermediate combustion components using an EDM model was found. Modeling difficulties with combustion model Finite Rate Chemistry, associated with a large scatter of reference data were identified and described. The way to generate the Flamelet library with CFX-RIF is described. Formulated adequate reaction mechanisms verified at a steady state have also been tested for transient simulation. The Flamelet combustion model was recognized as adequate for the transient mode. Integral parameters variation relates to the values obtained during stationary simulation. A cyclic irregularity of the temperature field, caused by precession of the vortex core, was detected in the chamber with the proposed simulation technique. Investigations of unsteady processes of rocket engines including the processes of ignition were proposed as the area for application of the described simulation technique.

1. Introduction

The combustion process in a chemical rocket engine is usually regarded as a set of 4-5 steps [1, 2]. Processes of injection, gasification and combustion are preceding the mixing process depending on the fuel kind (single- or double-component, gas or liquid and solid). These intrachamber processes depend strongly on the type of fuel and engine design (i.e., the complete or partial evaporation of the components in the gas generator); there are a number of specialized techniques for calculating these processes in the open literature [3, 4, 5]; and a universal method is not claimed. But combustion in the gas phase takes place in the chamber of any chemical rocket engine, therefore the universal method for simulation of gas-phase combustion is always actual. However, the previously proposed method of calculating the intracameral combustion [1, 6] allows simulating only steady burning, excluding transient phenomena. However, in any rocket engines (especially in thrusters) nonstationary processes are important: the majority of accidents occurs when the engine starts [7]; moreover, thrusters typically operate in a pulse mode, and the chamber parameters are always unsteady.
This paper describes the method for simulation of transient combustion processes. A thruster operating using gaseous oxygen and hydrogen was taken as the object of investigation.

2. A steady-state test of combustion mechanisms

Gross-formula or a chemical reactions system can be used for modeling nonstationary processes, as in the case with the stationary mode. The use of gross-formula and stationary combustion simulation is enough for most cases. Advantages of this approach include the ability of quick obtaining of qualitative results from the first approximation, and fewer demands to the grid model and a configuration of the CFD-model. The disadvantages are excessive temperatures by the results of the calculation and incorrect modeling of unsteady operation modes [8].

The ignition process is largely determined by the unstable rapidly degradable components; therefore, using a detailed reaction system is preferred for simulation accuracy. Selecting a detailed chemical combustion mechanism in a stationary simulation is an important step: the correctness of such reactions systems (for the considered engine) must be checked intently.

Three detailed system reactions of hydrogen and oxygen were considered:
1) the reactions system from the handbook, edited by W. Gardiner [9], detailed in work [6];
2) the reactions system from article [10];
3) Flamelet-library received with the CFX RIF generator built-in ANSYS [8].

During the first step, the simulation was conducted with the first set of reactions using a combustion model “Eddy Dissipation Model” (EDM), which does not take into account the rate of chemical reactions that is conventionally acceptable simplification only for stationary processes. Calculation stably converges and gives qualitatively correct results, but the temperature was often overestimated (Figure 1), as it always happens when using combustion model EDM [8]. These results have been used later for initialization of the next simulations.

It should be noted that the stability of the calculation with the complex multi-stage reaction system caused by the feature, which consists in the reaction rate, is neglected, and calculated from the reaction products in the EDM; parameter «B» of model EDM in ANSYS CFX has default value “-1". Otherwise, combustion model EDM can only be used for the system consisting of only two reactions (if option B is equal to "0.5" as the default in the ANSYS Fluent [11]).

As has been previously noted that the usage of combustion model EDM for unsteady calculations is incorrect; therefore, at the next stage, it was replaced by combustion model Finite Rate Chemistry (FRC) that takes into account the reaction rate according to the Arrhenius equation [8]. Unfortunately, there was no results. One possible reason of volatility was the lack of pre-exponential factors of accurate values of reaction rates in the source [9]: values taken from different sources often differ by several orders of magnitude.

A more actual «oxygen-hydrogen» reaction system, consisting of 26 equations, was found in work [10]; the equations describe the direct and inverse interaction of nine components (H, H₂, O, O₂, O₃, HO₂, OH, H₂O₂, H₂O), taking into account their relative catalytic effect. This system has been adapted to the combustion process in the thruster by excluding catalytic reactions involving nitrogen and argon.

The properties of all components, except ozone (O₃), were taken from the «Gas Phase Combustion» ANSYS CFX library, where heat capacity, enthalpy and entropy are given depending on the temperature via NASA-polynomials:

(1)
where \( C_p \) – specific heat capacity \([\text{J/(kg·K)}]\), \( H \) – enthalpy \([\text{J/kg}]\), \( S \) - entropy \([\text{J/(kg·K)}]\), \( R \) - gas constant of the current gas \([\text{J/(kg·K)}]\), \( T \) - static temperature \([\text{K}]\), \( a_1 \ldots a_7 \) – NASA-polynomial coefficients.

Ozone properties were taken from the open online database of the National Institute of Standards and Technology (USA) [12, 13], where they are given by the \( A \ldots G \) coefficients of the Shomate equation:

\[
\frac{H}{1000} = M = A t + B t^2 + C t^3 + D t^4 - \frac{E}{t} + F,
\]

\[
S = M = A \ln(t) + B t + C t^2 + D t^3 - \frac{E}{2 t^2} + F,
\]

where \( M = 47.9982 \times 10^{-3} \text{ kg/mol} \) – the molar mass of ozone, \( t = T / 1000 \) – the temperature in thousands of Kelvin degrees.

As can be seen from equations (1) ... (6), the explicit algebraic conversion coefficients of the Shomate equation into NASA-format for a subsequent use in ANSYS CFX is impossible. Therefore, it was evaluated in the following manner: 5 coefficients of NASA-polynomial \( C_p a_1 \ldots a_5 \) were obtained by solving a system of five equations closed on the basis of data of the ozone characteristics obtained by the Shomate equation (Table 1 and 2). Coefficients \( a_6 \) and \( a_7 \) were obtained by solving equations (2) and (3), correspondingly. The performed verification showed that the obtained NASA-polynomial give the ozone properties values that are different from the original data (Shomate equation) by not more than 0.2% in the whole range of values (Figure 2).

### Table 1. Initial coefficients of Shomate equation for ozone properties

| Temperature range | A         | B            | C          | D         | E          | F          | G          |
|-------------------|-----------|--------------|------------|-----------|------------|------------|------------|
| \( T_{\text{min}} \) K | \( T_{\text{max}} \) K | \( A \)   | \( B \)    | \( C \)   | \( D \)    | \( E \)    | \( F \)    |
| 300              | 1200      | 21.66157     | 79.86001   | -66.02603 | 19.58363   | -0.079251  | 132.9407   | 243.6406   |
| 1200             | 6000      | 57.81409     | 0.730941   | -0.039253 | 0.00261    | -3.560367  | 115.7717   | 294.5607   |

### Table 2. Calculated coefficients of NASA-polynomials for ozone properties

| Temperature range | \( a_1 \) | \( a_2 \) K\(^{-1}\) | \( a_3 \) K\(^{-2}\) | \( a_4 \) K\(^{-3}\) | \( a_5 \) K\(^{-4}\) | \( a_7 \) |
|-------------------|-----------|-----------------|-----------------|-----------------|-----------------|-----------|
| \( T_{\text{min}} \) K | \( T_{\text{max}} \) K | \( a_1 \) | \( a_2 \) K\(^{-1}\) | \( a_3 \) K\(^{-2}\) | \( a_4 \) K\(^{-3}\) | \( a_5 \) K\(^{-4}\) | \( a_7 \) |
| 300              | 1200      | 372.96         | 1.999565       | -1.949401 \times 10\(^{-3}\) | 8.498051 \times 10\(^{-7}\) | -1.2676 \times 10\(^{-10}\) | -167190   | -2612.66   |
| 1200             | 6000      | 1021.5         | 0.186437       | -6.350789 \times 10\(^{-5}\) | 1.025164 \times 10\(^{-8}\) | -6.1116 \times 10\(^{-13}\) | -1305734  | 672041.1   |
During this work, the authors were unable to achieve stable "combustion" in the LPRE chamber using the FRC model. The reason probably lies in the parameters of the individual rates of chemical reactions which were obtained for the other conditions; the reaction rate was used from the synthesis of gas and air at low pressures, not only hydrogen in oxygen at high pressures.

At the third stage of combustion, simulation mechanisms in the flame front (Flamelet-model) were investigated. Combustion reactions data were obtained with the CFX RIF flamelet libraries generator built-in ANSYS CFX.

Figure 3 shows a static temperature distribution along the rocket engine chamber using reactions of the Flamelet-library. Comparison of the results with the first system (Figure 1) showed that using flamelet combustion model eliminates overestimation of the maximum temperature in the chamber: 3500 K with flamelet vs 5000 K with EDM. Also, combustion with flamelet occurs at the fuel-oxidant front and not so fast, evidenced by the presence of the unreacted fuel components in the critical section; it gives more physical distribution of all parameters.

3. Methods for transient simulation of combustion
Simulation of combustion in the rocket engine was conducted in two variants of calculation: calculation with the second reactions system using the FRC combustion model and calculation with the Flamelet model.
Usage of the FRC model with transient statement confirmed that it is incorrect to use FRC system reactions: combustion was «non-self-sustaining », which led to the flame attenuation within the first simulation steps (Figure 4).

In case of the non-stationary Flamelet model, the simulation of the combustion proceeds steadily and parameters are slightly changed with respect to the values obtained at the stationary modeling. This reaction mechanism gives a qualitative and adequate picture of the combustion in unsteady simulations: the flame front oscillates a little bit about their average stationary position.

A periodically rotating circle of flame unevenness was unexpectedly found in the cylindrical section of the subcritical tapered nozzle on the conical section of the LPRE chamber during analysis of obtained data when testing the non-stationary methods. It is similar to a vortex core precession (Figure 5).

![Figure 4. Static temperature distribution along the LPRE chamber using a set of reactions for two timestamps: 0.01 µs and 0.08 µs.](image)

![Figure 5. Static temperature distribution in the cylindrical section of the LPRE chamber.](image)

### 4. Conclusion

Several modeling methods of the hydrogen-oxygen transient combustion in the chamber thruster were investigated using detailed chemical kinetics and the mechanisms of the different combustion models in ANSYS CFX were analyzed. From the considered combustion mechanisms only the Flamelet combustion model allowed obtaining the qualitatively adequate results. Using the FRC combustion model is unreasonably difficult due to the large variation of rate constants input data of the Arrhenius equation for a set of elementary chemical reactions. The EDM combustion model can be used for quick obtainment of reference solutions for initialization, despite the overestimated temperatures. The Flamelet combustion model was recognized as a qualitatively adequate model; it can be used in the future to study instabilities of combustion processes and transient processes, including ignition. However, it should be subjected to a detailed verification for this purpose [14].

### 5. Acknowledgments

This work was supported by the Ministry of Education and Science of the Russian Federation in the framework of the implementation of the Program “Research and development on priority directions of the scientific-technological complex of Russia for 2014–2020".
References
[1] Egorychev V.S., Shabliy L.S., Zubanov V.M. 2016 *Modeling intracameral workflow of small thrust rocket engine operating on gaseous oxygen and hydrogen in ANSYS CFX*. (Samara: Samara National Research University Publ.) p 140
[2] Kozlov V. E., Chechet I. V., Matveev S. G., Titova N. S., Starik A. M. 2015 Modeling study of combustion and pollutant formation in HCCI engine operating on hydrogen rich fuel blends. *International Journal of Hydrogen Energy*
[3] Matveev S. S., Zubrilin I. A., Orlov M. Y., Matveev S. G. 2015 Numerical investigation of the influence of flow parameters nonuniformity at the diffuser inlet on characteristics of the GTE annular combustion chamber. Paper presented at the Proceedings of the ASME Turbo Expo
[4] Biryuk V., Kayukov S., Zvyagintsev V., Lysenko U. 2014 Ways of speed increase for internal combustion engine fuel injectors. *Research Journal of Applied Sciences* 9(11) 721-724
[5] Dobrovol'skij M.V. 2005 Zhidkostnye raketnye dvigateli. *Liquid propellant rocket engines. Basics of designing*. (Moscow: MGTU Publ.) p 488
[6] Vasiliy Zubanov, Vitaliy Egorychev, Leonid Shabliy 2015 Design of Rocket Engine for Spacecraft Using CFD-Modeling. *Procedia Engineering* 104 29–35
[7] Ivanov V.K., Kashkarov A.M., Romasenko E.N., Tolstikov L.A. 2006 LRE turbopump unit of NPO Energomash. *Conversion in engineering*. 1 15-21
[8] ANSYS CFX-Solver Modeling Guide, 2011, ANSYS Inc.
[9] Gardiner W.C. 1984 Combustion Chemistry. (Springer-Verlag New York) p 351
[10] Gerasimov G.Ya., Shatalov O.P. 2013 Kinetic mechanism of combustion of hydrogen-oxygen mixtures. *Journal of Engineering Physics and Thermophysics* 86 5
[11] ANSYS FLUENT User's Guide, 2011, ANSYS Inc.
[12] NIST Chemistry WebBook http://webbook.nist.gov/chemistry/ National Institute of Standards and Technology
[13] Chase M.W., Jr., 1998 NIST-JANAF Thermochemical Tables, Fourth Edition, *J. Phys. Chem.* 9 1-1951
[14] Zubanov V. M., Shabliy L. S., & Krivcov A. V. 2015 Rational technique for multistage centrifugal pump CFD-modeling. Paper presented at the Proceedings of the ASME Turbo Expo, Vol. 2B