

Technology for Transient Simulation of Vibration during Combustion Process in Rocket Thruster

V.M. Zubanov¹, D.V. Stepanov¹ and L.S. Shabliy¹

¹ Samara National Research University, 34, Moskovskoe shosse st., Samara, Russia

E-mail: waskes91@gmail.com

Abstract. The article describes the technology for simulation of transient combustion processes in the rocket thruster for determination of vibration frequency occurs during combustion. 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. The way for obtaining quick CFD-results with intermediate combustion components using an EDM model was found. The way to generate the Flamelet library with CFX-RIF was described. A technique for modeling transient combustion processes in the rocket thruster was proposed based on the Flamelet library. A cyclic irregularity of the temperature field like vortex core precession was detected in the chamber. Frequency of flame precession was obtained with the proposed simulation technique.

1. Introduction

The combustion process in the rocket engine chamber largely determines operating parameters of rocket engine. Transient combustion processes are the most interesting for rocket engine engineers because of vibration induced by burning [1]. Also rocket thrusters often operate exclusively in pulsed mode [2]. The parameters in the chamber at this case are extremely unsteady during the entire period of the engine's operation time; the methods of research (both simulation and experimental) of stationary processes are not applicable for studying of such processes. But the CFD-simulation tool can be allowed for modeling of combustion processes in a transient mode with formally any degree of time discretization [3, 4]. The purpose of this work is to create a technology of the CFD-tools using, which will allow visualizing the unsteady workflow of any rocket thruster operating on gaseous components of oxygen and hydrogen to obtain vibration frequency. This technique was developed based on the previously published method for modeling stationary combustion [5, 6], therefore only its differences from the previous one will be indicated.

2. Features of CFD-model for transient simulation

2.1. Timestep selection

The time step should be assigned based on the average velocity of the flow along the mesh elements. The time step size usually amounts to microseconds, considering the high flow rate in the chamber. For example, with an axial velocity $V_z = 5,000$ m/s, a camera length $L = 0.1$ m and with averaged number of cells along the chamber length $N = 200$, the actual order of the time step Δt (1):

$$\Delta t = \frac{L/N}{V_z} = \frac{0,1/200}{5000} = 0,1 \text{ microsecond} \quad (1)$$



It should be noted that only an approximate order of the time step can be obtained by such calculations. The exact value is selected during trial calculations by estimating the rate of development of transient processes in the calculated zone, when the solution is stable (more small steps over time make the decision more stable).

The total simulation time is chosen to "cover" the simulation time of the process of interest with a small range. Usually it includes 200 ... 300 time steps.

2.2. Meshing

The mesh model creation for transient calculation mode does not fundamentally differ from the mesh model creation for stationary simulation [6], however, there are some features. For example, if the ignition process is modeled by setting a high-temperature boundary wall on the discharge surface of a candle, then the boundary must be represented in the grid model (Figure 1).

The size of the grid cells must be that the flow, moving with its speed, "moved" by the distance between neighboring cells in one time step Δt (with the same cell sizes, it is equal to the size of the cells themselves). Thus, the grid must have a smooth change in the cells dimensions. The *Expansion Ratio* parameter, which reflects the "growth rate" of the cells, should not exceed 10 ... 50 value. And it is necessary to correlate the rate of change in the cells dimensions with the flow velocity change in the calculated zone.

2.3. Boundary conditions

The boundary conditions can be set as constant (in this case their description does not differ from [6]) or varying with time by a given dependencies. Constant boundary conditions can be used, for example, to study the combustion process of a steady flow. However, the real process of ignition of many thrusters occurs with significantly variable fuel components flow parameters that can be specified in the form of explicit (*CEL-expression*) or tabular (*User-Function*) dependencies.

The ignition initiation can be simulated by specifying the energy transfer (*Heat transfer*) or by the high temperature (*Temperature*) in the prechamber ignition zone. This zone can be conditionally modeled by a point (*Source Point*) or an extended area of the design area (*Subdomain*) which simulated a spark discharge zone, or by heating the boundary wall (*Wall*), which is the surface of the spark plug (figure 1).

3. Setting the properties of the working fluid

Hydrogen is strictly promising rocket fuel due to its high energy and ecology [7] the properties of the working fluid must be specified as *Ideal Variable Composition Mixture* through the properties of simple components: the initial reagents and reaction products including final and intermediate ones. The component composition of the simulated mixture is determined by a specific set of reactions that are considered in the calculation and which may include several dozen reactions.

A more actual «oxygen-hydrogen» reaction system, consisting of 26 equations, was found in work [8]; the equations describe the direct and inverse interaction of nine components (H, H₂, O, O₂, O₃, HO₂, OH, H₂O₂, H₂O), considering 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. Ozone properties were taken from the open Chemistry WebBook (<http://webbook.nist.gov/chemistry>) of the National Institute of Standards and Technology (USA) [9], where they are given by the coefficients of the Shomate equation and reformatted in coefficients of NASA-polynomial by method described in details in [10].

4. Initial solution for transient calculation

Setting the initial conditions for transient calculations should be done more carefully: for transient calculation, as a rule, the initial conditions are given as the results of a preliminary stationary calculation, in contrast to the stationary calculation, while the initial conditions of the stationary

calculation can be arbitrary values. It is very important that the reaction mixture components set of the preliminary stationary calculation should be equal to the components set of transient calculation.

The initial values can be obtained using the *Eddy Dissipation Model (EDM)* of combustion. EDM does not consider the rate of chemical transformation of components in an explicit form [11]. The calculations with this model agree well and give an acceptable accuracy for specifying the initial distribution field of the parameters. Nevertheless, the EDM model, as a rule [6], overestimates the flow temperature (Figure 2).

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 [12]).

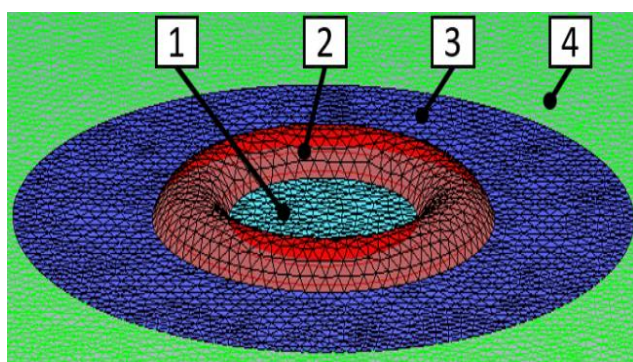


Figure 1. The discharge surface of a surface discharge plug in the prechamber mesh model: 1 - central electrode, 2 - flow zone (subdomain) around appearance of the spark, 3 - side electrode, 4 - prechamber wall

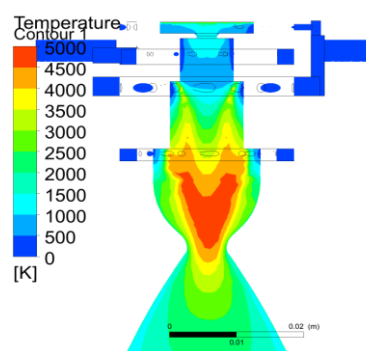


Figure 2. Static temperature distribution along the thruster chamber using EDM combustion model with chemical scheme of 24 reactions [13]

5. Combustion model and chemical reaction scheme

The choice of the combustion model and the system of chemical equations is a rather complicated task as in the case of stationary calculation [6]. An assessment of the different combustion models applicability for the transient processes modeling in thrusters in combination with different sets of reactions was the main objective of this study. To solve it, the combustion model *Finite Rate Chemistry (FRC)* [11] and *Flamelet* model of micro-flame combustion were considered. FRC model considers the rate of chemical reactions, calculated by the Arrhenius equation. The EDM combustion model was immediately excluded from consideration, since its application is justified only for combustion processes in which the rate of chemical reactions strongly prevails over the rate of their mixing (Damköhler number $Da \gg 1$); the latter cannot be guaranteed for combustion in a rapidly moving flow in the thruster chamber.

Combustion in the transient processes simulation can be described both by a single gross reaction and by a set of chemical reactions of varying detail degrees (as in the case of stationary processes [6]). A smaller number of reactions makes possible to obtain a faster and more stable solution by ignoring the intermediate chemical processes; the combustion temperature is usually overestimated, since the losses from underburning of the intermediate components are not considered. The most branched reaction scheme with the most detailed component description is necessary for modeling the transient combustion processes, including ignition; since the ignition process is largely determined by the interaction of unstable rapidly decomposing components present in the reacting mixture at low concentrations.

The following combinations of the "combustion model" - "set of reactions" were considered:

- FRC model with a reaction system [6], composed of 24 equations taken from [13], involving 8 components;
- FRC model with a reaction system [8], composed of 26 equations, involving 9 components (with addition of ozone O₃);
- Flamelet-model, which uses Flamelet-library of 8 components to describe the combustion scheme.

The first two systems are a traditional representation of chemical interactions in the form of chemical equations, and the third is a tabulated information on the combustion products concentration at different fuel / oxidizer ratios in the flame front. The Flamelet library must be created before the calculation with the CFX RIF combustion library generator [11]. The Built In algorithm of the Flamelet library creation was used based on the combustion model of hydrogen fuel in air (Fuel Module - H₂) with Kinetic Scheme – without NO_x. The replacement of air with pure oxygen was accomplished by changing the component composition of the oxidant.

Attempts to use the FRC model did not allow one to obtain a solution with any of the investigated reaction schemes. The calculation with the reaction system [6] had no converged solution. The calculation with the system [8] converged, but the simulated combustion was not self-sustaining: the flame quickly faded during the first few time steps [10].

Calculation using the Flamelet-model stably converges and gives an adequate picture (Figure 3): For transient modeling, the flame front slightly fluctuates relative to its "average" position, determined for stationary simulation, the parameters of the flow (velocity, components concentration) practically do not differ from the values obtained for stationary simulation, except for a serious drop in temperature to values only slightly exceeding the maximum temperature of hydrogen combustion in pure oxygen (3100-3200 K). Comparison of the results of stationary modeling (Figure 2) and transient (Figure 3) simulation shows that combustion with the Flamelet model occurs at the mixing boundaries of the fuel and oxidizer not so rapidly that is associated with a finite rate of chemical reactions not considered earlier in the EDM model. This is confirmed by a certain amount existence of unreacted initial fuel components and intermediate combustion products in the critical section.

Thus, Flamelet-combustion model allows obtaining a stable and adequate solution, it can be recommended for use as a basic combustion model in the calculation of transient burning processes in thrusters.

6. Results analysis of transient simulation

Figure 4 shows the change in the parameter static temperature in time. 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 thruster chamber during analysis of obtained data when testing the transient methods. It is like a vortex core precession. Figure 4 is given as an illustration of the fact that the use of transient simulation gives much more opportunities for investigating inter-chamber workflows. For example, based on the results obtained, the frequency and amplitude of the vortex precession can be calculated. From figure 4 is evident that during simulation time (0, 6 ms from 0,4 ms to 1,0 ms) flame moving was ~240 degrees on clockwise direction. So flame moving frequency can be calculated as (2):

$$f = \frac{\sim 240/360}{0.0006} \approx 1,1 \text{ kHz} \quad (2)$$

The simulation time can be increased for more accurate calculation. The application of the described technique should be accompanied by its validation under the conditions of a specific application, as in [14] and experimental verification as in [15].

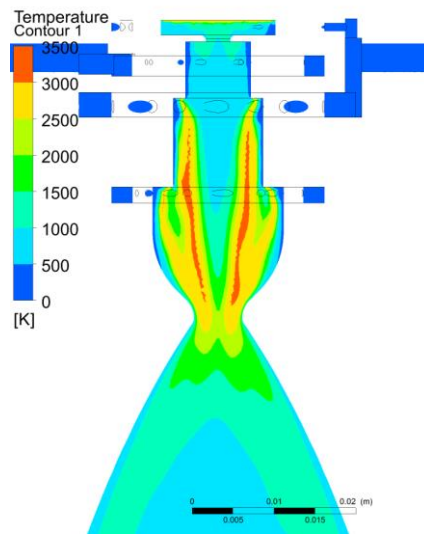


Figure 3. Static temperature distribution along the thruster chamber using *Flamelet*-combustion model

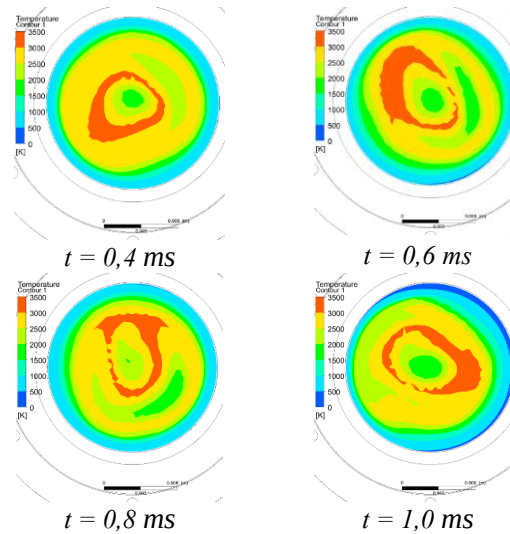


Figure 4. Static temperature distribution in the cylindrical section of the thruster chamber

7. Conclusion

Technology for transient simulation of combustion processes of rocket thruster on gashouses oxygen and hydrogen were created. 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 like precession of vortex core (PVC). PVC frequency has been determined.

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