NUMERICAL STUDY OF NATURAL GAS – OXYGEN ROTATING DETONATION ROCKET ENGINE OPERATION AND PERFORMANCE

S. N. Medvedev[1,2], S. M. Frolov[1,2,3], and V. S. Ivanov[1,2]

[1]N. N. Semenov Institute of Chemical Physics (ICP)
Russian Academy of Sciences
Moscow, Russia
e-mail: smfrol@chph.ras.ru
[2]Center for Pulsed Detonation Combustion
Moscow, Russia
[3]National Research Nuclear University MEPhI
(Moscow Engineering Physics Institute)
Moscow, Russia

The computational investigations of detonation liquid rocket engine (DLRE) operating on natural gas (NG)–oxygen mixture have been performed to examine the impact of the DLRE configuration and fuel supply parameters on the operation process and thrust performance. The results of DLRE fire tests were used to explore the predictive capabilities of the ICP computational technology designed for full-scale simulation of the operation process in detonation combustors. Comparison of the predicted results with measurements proved that the calculations accurately predict the number of detonation waves circulating in the tangential direction of the annular DLRE combustor and the chaotic near-limiting operation mode resembling the mode with longitudinally pulsating detonation in the DLRE with converging-diverging (CD) nozzle extension. Calculations predict with reasonable accuracy both detonation propagation velocity and detonation rotation frequency. In addition, the calculations correctly predict the trends in the variation of DLRE operation parameters in an engine of a particular design. As in the experiments, the use of nozzle extension increases thrust. As for the thrust values, the calculations were shown to systematically overestimate them by at least 7%–10% compared with the measurements.

Introduction

The use of liquefied NG as a propellant and the use of continuous-detonation combustion of the fuel mixture in a liquid rocket engine are considered as promising directions of development of modern space engines. The energy efficiency of the DLRE was first proved theoretically by Zel'dovich in 1940 [1] and experimentally by Frolov *et al.* in 2014–2015 [2–4]. The first experiments with continuous-detonation combustion of methane–oxygen mixture in an annular combustor were made in Novosibirsk [5]. Similar experiments were carried out in [6–10]. Described in [9, 10] are the experiments with thrust measurements of the DLRE operating on NG–oxygen mixture at relatively low pressure (up to 10 bar) in the annular combustor and the compositions of the fuel mixture from the fuel-lean (equivalence ratio of 0.5) to fuel-rich (2.0). The maximum value of specific impulse obtained in [9, 10] was 185 s.

In this paper, the authors continue the study launched in [9] but from the computational rather than experimental side. Thus, the objective of the investigations described below was to explore the predictive capability of the computational technology developed at ICP in terms of reproducing all DLRE operation modes detected in the experiments. The experiments used for this purpose are those partly published in [9, 10].

Problem Formulation

Figure 1 shows a longitudinal section (Fig. 1*a*) and one-quarter perspective view (Fig. 1*b*) of the DLRE of several different configurations with oxygen and NG collectors and a piece of oxygen-feeding manifold. In addition to these DLRE configurations, other configurations used in the experiments were also considered.

The DLRE is an annular combustor with the injector head on the one side and a jet nozzle with a conical central body on the other side [9]. The annular combustor (see Fig. 1*a*) is formed by two coaxial cylinders of 100-millimeter height: 90-millimeter inner diameter cylinder nested within a hollow outer cylinder of 100 mm in diameter, so that the gap between the cylindrical surfaces is 5 mm. The injector head consists of a replaceable thin disc with a sharpened edge attached to the inner

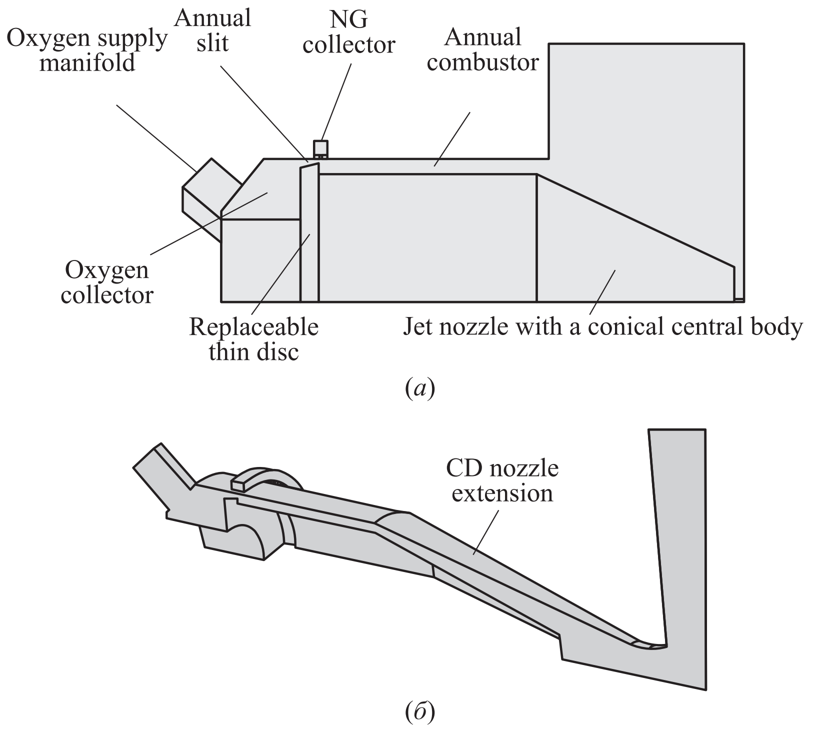


Figure 1 Longitudinal section (*a*) and a perspective view of a quarter (*b*) of DLRE of two different configurations with oxygen and NG collectors and pieces of oxygen-feeding manifold

cylinder of the combustor so that it forms an annular slit of width δ with the outer combustor wall. Gaseous oxygen is supplied to the combustor through this annular slit in the axial direction. Natural gas is fed through the equally distributed radial holes 0.8 mm in diameter drilled in the outer wall of the combustor in the cross section located at a distance of 0.5 mm downstream from the disc. The number of radial holes is 144. During firing, the DLRE is water cooled. In one of the test series, a CD conical nozzle extension was attached to the edge of the external cylinder of the combustor (see Fig. 1*b*). In this

DLRE configuration, the minimum cross-sectional area was 50% of the cross-sectional area of the annular combustor channel.

Three-dimensional numerical simulation of physical and chemical processes in the DLRE of Fig. 1 was carried out according to the procedure described in detail in [11, 12]. The flow of viscous compressible gas is described by the Reynolds-averaged unsteady Navier–Stokes equations supplemented by energy equation and continuity equations of all chemical components of a multicomponent mixture. Turbulent fluxes of mass, momentum, and energy are modeled by a standard k–ε-turbulence model for compressible flow. Because all the physical and chemical processes in the combustor under consideration take place within a very short time, the contribution of frontal (controlled by transport processes) combustion in chemical sources in the energy and species continuity equations was neglected. The contribution of volumetric reactions in these chemical sources was determined by the Lagrangian Monte-Carlo-based Particle Method (PM) in which the average rates of chemical reactions in a turbulent flow are calculated with due regard for the effect of turbulent fluctuations of temperature and species concentrations (the effect of "turbulence–chemistry interaction"). The governing equations are closed with the caloric and thermal equations of state of an ideal gas mixture with variable specific heats, as well as with initial and boundary conditions. All other thermal parameters of the gas were also considered variable. In contrast to [11], where the calculations were performed for continuous-detonation combustor with separate supply of hydrogen and air, the calculations described in [12] and herein are made for separate supply of NG and oxygen.

For simulating volumetric chemical transformations in the NG–oxygen mixture, the technique proposed in [13,14] was used. The chemical conversion of the fuel mixture was assumed to occur in two stages: the first stage corresponds to the self-ignition delay, and the second to the establishment of thermodynamic equilibrium in the combustion products. Upon the completion of the first stage, the initial fuel mixture was assumed to immediately convert into the thermodynamically equilibrium reaction products (HP-problem is solved for the entire computational cell; here, H is the enthalpy and P is the pressure).

To calculate the self-ignition delay of the NG–oxygen mixture, the overall reaction mechanism containing five reactions was used, similar to the mechanism proposed in [14]:

$$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O\,; \qquad (I)$$
$$CO + H_2O \rightarrow CO_2 + H_2\,; \qquad (II)$$
$$CO_2 + H_2 \rightarrow CO + H_2O\,; \qquad (III)$$
$$H_2 + H_2 + O_2 \rightarrow H_2O + H_2O\,; \qquad (IV)$$
$$CO + CO + O_2 \rightarrow CO_2 + CO_2 \qquad (V)$$

with tabulated Arrhenius parameters, preexponential factor A, and activation energy E, in the expression for the rate of reaction (I):

$$W = -A[O_2][CH_4]\exp\left(-\frac{E}{RT}\right),$$

i. e., reaction (I) is considered as a bimolecular reaction. Arrhenius parameters for other reactions (II)–(V) are the same as in [14]. A similar approach was used in [11] and gave good results in all measured characteristics of the operation process in a hydrogen–air continuous-detonation combustor.

Table 1 shows the values of Arrhenius parameters A and E for NG–oxygen mixture in the range of initial temperature from 1100 to

Table 1 Arrhenius parameters A and E of reaction (I) in the range of initial temperature from 1100 to 1400 K

Φ	P, atm	A, cm^3/mol/s	E, kcal/mol
0.5	1	$6 \cdot 10^{14}$	48
1	1	$4 \cdot 10^{14}$	48
2	1	$3 \cdot 10^{14}$	48
4	1	$2 \cdot 10^{14}$	48
0.5	12	$1.5 \cdot 10^{14}$	46
1	12	$1 \cdot 10^{14}$	46
2	12	$8 \cdot 10^{13}$	46
4	12	$8 \cdot 10^{13}$	46
0.5	50	$4 \cdot 10^{13}$	43
1	50	$2.7 \cdot 10^{13}$	43
2	50	$1 \cdot 10^{13}$	40
4	50	$1 \cdot 10^{13}$	40

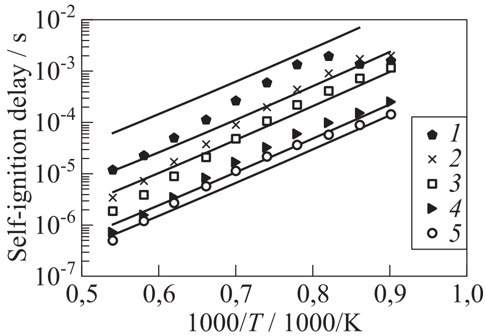


Figure 2 Example of calculated dependences of self-ignition delay on the initial temperature at different initial pressures obtained by mechanism (I)–(V) (curves) and DKM (symbols) at $\Phi = 1$: *1* — $P = 1$ atm; *2* — 5; *3* — 12; *4* — 50; and *5* — $P = 80$ atm

1400 K, initial pressure from 1 to 80 atm, and fuel-to-oxygen equivalence ratio Φ from 0.5 to 4.0. These values are derived from the best fit of self-ignition delay predicted by mechanism (I)–(V) with the self-ignition delay predicted by a thoroughly validated detailed kinetic mechanism (DKM) [15]. In the calculations with the DKM, NG had the following composition: $[CH_4] = 92.8\%$; $[C_2H_6] = 3.9\%$; $[C_3H_8] = 1.1\%$; $[C_4H_{10}] = 0.4\%$; $[C_5H_{12}] = 0.1\%$; $[N_2] = 1.6\%$; and $[CO_2] = 0.1\%$.

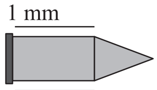
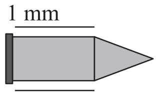
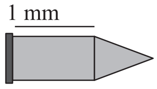
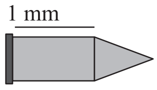
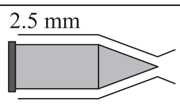
Figure 2 shows the example of calculated dependences of the self-ignition delay on the initial temperature at different initial pressures obtained by mechanism (I)–(V) (curves) and DKM (symbols) at $\Phi = 1.0$. For the calculation of equilibrium parameters of the combustion products, the approach of [16] was used.

The above-described model of a two-stage chemical transformation of the fuel mixture was validated on the one-dimensional problem of detonation initiation by a strong shock wave. The results were compared with the results of calculations based on the DKM for NG–oxygen mixture. In both cases, very similar values of self-ignition delays, equilibrium temperature and pressure, and equilibrium concentrations of the main species in the combustion products, as well as the values of the detonation velocity were obtained.

Results of Calculations

Following [10], Table 2 shows the conditions of 5 sample tests with the indication of DLRE configuration, the width of the annular slit δ, oxygen and NG absolute pressures P_{O_2} and P_{CH_4} in collectors, fuel mixture mass flow rate G, specific (per unit area of injector holes for fuel mixture supply) mass flow rate G_{sp}, fuel-to-oxygen equivalence ratio Φ, as well as the results of the tests in terms of the average absolute pressure in the combustor P_c near the injector head, the number of detonation waves n, detonation velocity D, the frequency f of detonation rotation, thrust T, and specific impulse I_{sp} calculated as thrust T divided by gG where g is the acceleration of gravity.

Table 2 Results of five selected tests performed under normal atmospheric conditions

No.	Configuration	P_{O_2}, atm	P_{CH_4}, atm	G, kg/s	G_{sp}, kg/s/m^2	Φ	P_c, atm	n	D, m/s	f, kHz	T, kgf	I_{sp}, s
1	2	3	4	5	6	7	8	9	10	11	12	13
1[a]		8	21	0.70	2243	0.87	1.0	—	—	—	19	28
2		8	19	0.46	1474	1.1	4.5	4	1880	24	64	140
3		6	14	0.37	1186	1.1	3.2	3	2090	20	47	128
4[b]		6	13	0.30	962	1.12	3.2	1	2320	7	38	127
5[c]		7	15	0.36	430	1.15	6.6	1	—	5	59	162

[a] Test without ignition.
[b] Replaceable thin disc displaced 2 mm downstream.
[c] Near-limiting mode with a detonation wave pulsating longitudinally rather than circulating in the tangential direction.

In Tests 1 to 4, the DLRE of basic design with the annular slit width of $\delta = 1$ mm without CD nozzle extension was used (see schematic in column 2). In Test 4, the replaceable thin disc was displaced 2 mm downstream relative to the fuel injector holes, so that NG was injected radially 1.5 mm upstream from the annular slit. In Test 5, the annular slit was expanded to $\delta = 2.5$ mm.

In addition, Test 5 was made with CD nozzle extension. In Test 1, the fuel mixture components were purged through the DLRE without ignition to measure the baseline thrust created by the cold flow. In Tests 2 and 3, stable operation modes with four and three equidistant detonation waves simultaneously circulating in the same tangential direction were detected. In Test 4 with the DLRE of basic configuration, a steady operation mode with a single detonation wave circulating in a tangential direction was observed. It is worth noting that at the mass flow rate of fuel mixture close to that in Test 3, the thrust in Test 5 appeared to be higher than in Test 3: 51 instead of 41 kgf.

In the calculations, structured nonuniform computational grids of the DLRE were used. The minimum size of the computational cells in the reaction zone was 0.2 mm. Round radial holes in the outer wall of the combustor (for NG supply) are modeled by a set of rectangular cells with the same hydraulic resistance. The total number of cells together with the nozzle and the buffer zone attached to the engine outlet was $4.5 \cdot 10^5$–$5.5 \cdot 10^5$.

At the entrance of NG collector and oxygen manifold, fixed mass flow rates of NG and oxygen were specified. At all solid walls, no-slip conditions and a constant temperature of 293 K were adopted. At the outlet boundary of the buffer zone normal to the engine axis and located at a large distance from the nozzle exit, a constant static pressure of 1 atm was adopted, whereas at the side boundaries of the buffer zone, the symmetry conditions were specified.

At the beginning of calculation, the annular combustor was filled with air under normal conditions, and the NG and oxygen collectors were filled with NG and oxygen at a pressure equal to the corresponding experimentally measured values at the cutoff valves. Initially, all gases were assumed to be quiescent. Each calculation started from purging of the combustor with gases accompanied by turbulence generation, molecular mixing processes, and followed by the procedure of detonation initiation. To initiate detonation, a certain number of ignition sources were placed in the combustor annulus. The ignition sources were the localized finite regions with fast burnout of fuel mixture. After a transition period, a quasi-stationary operation process with one or several detonation waves circulating in the same or in different tangential directions, or a chaotic operation mode resembling a mode with longitudinally pulsating detonation wave was set in the combustor.

Given below is a brief description of the calculations all corresponding to the selected tests in Table 2.

The calculation of cold-flow purging (without ignition) of the DLRE in the conditions of Test 1 predicted a thrust of 21 kgf, while the experimentally measured thrust was 19 kgf. It turned out that the calculation overestimates the cold-flow thrust by approximately 11%. Note that in the calculation, the thrust was determined as the integral of pressure force and viscous friction over all DLRE rigid surfaces with regard for the curved oxygen manifold of finite length.

The upper row of Fig. 3 shows the predicted quasi-stationary fields of static pressure at the outer wall (a) and in the combustor cross section 4 mm downstream from the combustor bottom (b), as well as a static temperature at the outer wall (c) under conditions of Test 2 in Table 2. As seen, the calculation predicts the operation process with four equidistant detonation waves circulating in the same direction at a velocity of 2210 ± 30 m/s. The predicted frequency of detonation rotation is 28 kHz. According to Table 2, the operation process detected in Test 2 also exhibits four detonation waves; however, the measured detonation velocity is 14% lower (f = 24 kHz). The predicted value of thrust developed by the DLRE is 68.6 kgf, whereas the measured thrust was about 64 kgf, i. e., calculation overestimates the thrust by approximately 7%.

The middle row of Fig. 3 shows the predicted quasi-stationary fields of static pressure and static temperature under conditions of Test 3 in Table 1. The calculation predicts the operation process with three equidistant detonation waves circulating in the same direction at a velocity of 2270 ± 20 m/s. The predicted frequency of detonation rotation is 21.8 kHz. According to Table 2, the operation process detected in Test 3 also exhibits three detonation waves; however, the measured detonation velocity is 8% lower (f = 20 kHz). The predicted value of thrust developed by the DLRE is 64.2 kgf, whereas the measured

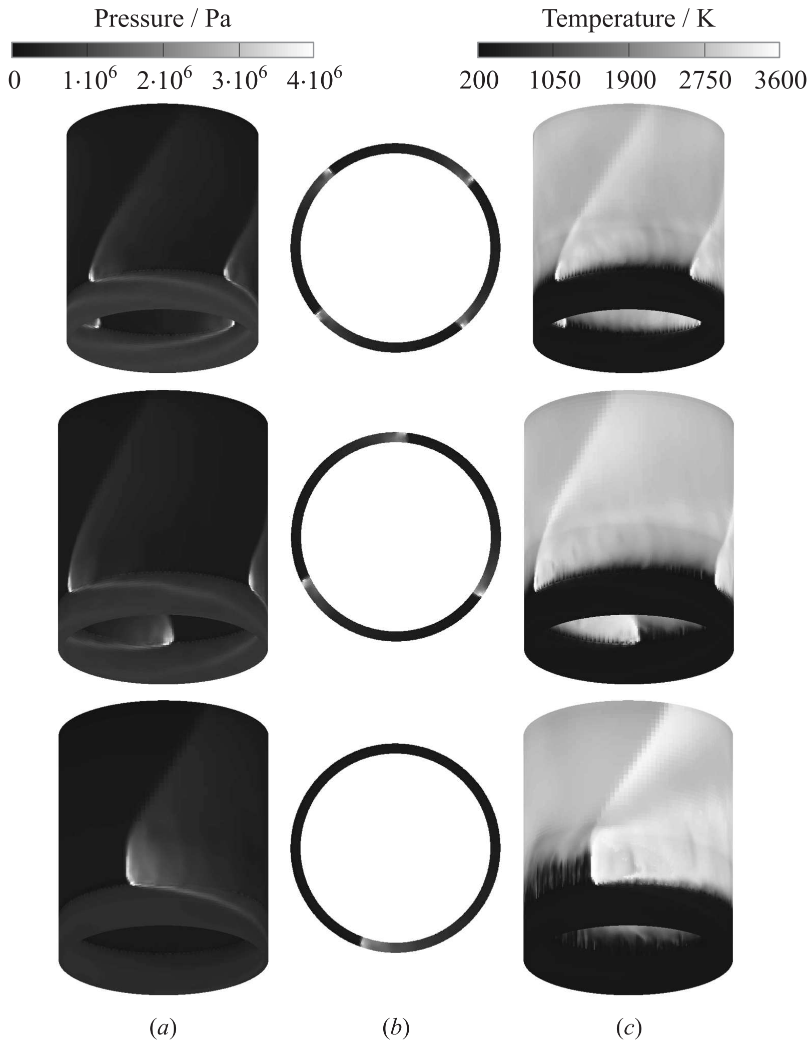


Figure 3 Predicted quasi-stationary fields of static pressure (a and b) and static temperature (c) under the conditions of experimental Tests 2 (upper row), 3 (middle row), and 4 (bottom row)

thrust was about 47 kgf, i. e., calculation overestimates the thrust by approximately 36%.

The bottom row of Fig. 3 shows the predicted quasi-stationary fields of static pressure and static temperature under conditions of Test 4 in Table 2. The calculation predicts the operation process with one detonation wave circulating tangentially at a velocity of 2330 ± 20 m/s. The predicted frequency of detonation rotation is 7.4 kHz. According to Table 2, the operation process detected in Test 4 also exhibits one detonation wave and the measured detonation velocity is the same as in the calculation. The predicted value of thrust developed by the DLRE is 44.8 kgf, whereas the measured thrust was about 38 kgf, i. e., calculation overestimates the thrust by approximately 18%.

In the calculation corresponding to the experimental conditions of Test 5 with installed CD nozzle extension, a chaotic operation process resembling the process with one detonation wave pulsating in the longitudinal direction rather than circulating in tangential direction was obtained. In the calculation, detonation waves propagating in different tangential directions periodically appeared and disappeared in the flow. Detonation reinitiation most often occurred in the outer nozzle due to reflections of decaying shock waves and the resultant detonation waves propagated upstream towards the combustor bottom through the annulus filled with fresh fuel mixture. The mean predicted frequency of detonations in this calculation was 5.1 kHz. According to Table 2, the operation process detected in Test 5 also exhibited one detonation wave pulsating longitudinally with the same measured detonation velocity ($f = 5$ kHz). The predicted value of thrust developed by the DLRE was 64.8 kgf, whereas the measured thrust was about 59 kgf, i. e., calculation overestimates the thrust by approximately 10%.

Thus, comparison of the predicted results with measurements showed that the calculations accurately predict the number of detonation waves circulating in the tangential direction of the annular DLRE combustor of a certain design (four, three, or one detonation wave(s)). Moreover, the calculation predicts a near-limiting chaotic operation mode resembling a mode with detonation pulsations in the longitudinal direction in the DLRE with CD nozzle extension. Also, the calculations predict with reasonable accuracy the detonation velocity and rotation frequency. In addition, the calculations correctly predict the experimental trends in the overall performance of the DLRE of a given design: as in the experiments, the number of detonation waves, the detonation velocity and the engine thrust decrease with decreasing the mass flow rate of fuel mixture. Similar to the experiment, the use of the CD nozzle extension increases thrust. As for the thrust values, they are systematically overestimated by at least 7%–10% as compared with measurements, and a higher value of thrust is obtained even for the cold-flow purging of DLRE.

Concluding Remarks

The results of DLRE fire tests [9] were used to explore the predictive capabilities of the ICP computational technology designed for full-scale simulation of the operation process in continuous-detonation combustors. Comparison of the predicted results with measurements proved that the calculations accurately predict the number of detonation waves circulating in the tangential direction of the annular DLRE combustor (four, three, or one detonation wave(s)) and the chaotic near-limiting operation mode resembling the mode with longitudinally pulsating detonation in the DLRE with CD nozzle extension. Calculations predict with reasonable accuracy both detonation propagation velocity and detonation rotation frequency. In addition, the calculations correctly predict the trends in the variation of DLRE operation parameters with decreasing the mass flow rate of fuel mixture in an engine of a particular design: as in the experiment, the number of detonation waves, detonation velocity, and thrust decrease. As in the experiments, the use of nozzle extension increases the thrust. As for the thrust values, the calculations were shown to systematically overestimate them by at least 7%–10% compared with measurements. Moreover, a higher value of DLRE thrust is obtained even for the cold-flow purging of the engine. The reasons for this overestimation are currently being investigated.

Acknowledgments

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