Comparison of efficiency characteristics of jet engines with detonation and slow combustion based on low and high fidelity computational tools

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Abstract

The main objective of the work is to compare the efficiency of thrust characteristics of direct-flow air jet engines (turbojet) with "slow" (deflagration) combustion at constant pressure and different types of air-jet engines with combustion in moving (pulsating or rotating) and stationary detonation waves. The relevance of this problem is due to the widespread allegations of a possible increase in the thrust characteristics of an air jet engine with combustion in detonation waves (primarily in pulsating - PDE and rotating - RDE) by tens of percent compared to the existing ramjet with slow combustion in the subsonic flow. These statements, however, do not rely on a direct comparison of the thrust characteristics of the respective engines, but on a comparison of their thermal efficiency and the formulas applicable only to stationary flows in inertial coordinates, linking specific thrust and pulses with thermal efficiency. For PDE, these formulas are incorrect because of the significant nonstationarity of the flow, and in RDE because of the transition to a rotating at high angular velocity noninertial coordinate system. For the correct determination of thrust characteristics of PDE, RDE and other jet engines with detonation and deflagration-detonation combustion it is assumed in the work to develop mainly based on reduced dimensions models and thermodynamic apparatus, and high-fidelity, based on CFD and chemical kinetic, computational tools. Two sub-problems and their solutions are highlighted and analyzed in the current work: comparisons of various type engines characteristics based on simple thermodynamic model and accuracy, which can be achieved with uses of detailed kinetics mechanisms for traditional ignition delay tests for model binary fuel mixture.

1. Introduction

The comparison of ideal thermal efficiency, specific thrust and specific impulses of air-breathing jet engines of different types with deflagration and detonation combustion is performed. The relevance of such comparison is due to the well-known statement about the possible increase in thrust characteristics of ABJE with combustion in detonation waves (DW) by tens of percent compared to the ramjet with deflagration combustion (DC) at constant pressure in a subsonic flow. Such statements do not rely on direct calculation of the thrust, but on a comparison of their thermal efficiency and on formulas that giving the dependence of specific thrusts and impulses with above ideal efficiency. For pulse detonation engines (PDE), these formulas are incorrect because of flow non-stationarity, which is consistent with the statement [1]: "... because of the flow non-stationarity, the calculated efficiencies can't be used directly to assess the traction characteristics of the PDE. These characteristics can only be determined by taking into account the complex gas dynamics of real PDE ... Conversion for a non-stationary system of thermal energy into traction requires a detailed analysis of the gas dynamic process in the engine ".

2.Ideal characteristics of the ABJE with detonation and deflagration combustion

In the course of the development [2-5], a thermodynamic and gas dynamic analysis of different types of ABJE with detonation and deflagration combustion was carried out. In the further investigation of the ABJE, combustion is always preceded by compression in the air intake of air coming from the atmosphere with a velocity V_0 and expansion in the nozzle of the combustion products. In the engine models under consideration, the pre-compression

of air in the air intake and the expansion of the combustion products in the nozzle to the pressure of the incident flow are isentropic and stationary.

For fixed adiabatic ratios of air, burning mixture and combustion products, when assuming the absence of losses in deceleration of air in the intake, in its mixing with the gas fuel and in the outflow of the combustion products from the nozzle(as in [5]), the ideal characteristics of the considered ABJE depend on two dimensionless parameters: Mach number of the incident flow M_0 and $q^\circ = q/(c_pT_0)$ – the dimensionless burning mixture heating value (c_p – is the heat capacity when constant pressure, T_0 – incident flow temperature). The thermal efficiency (η_{th}), the specific thrusts and specific impulses of all the considered engines are compared for $q^\circ = 6$ and for M_0 from 0.3 to 8. As demonstrated below, for all q° and M_0 , according to the ideal thrust, the PDE is slightly higher than the ABJE with combustion in constant volume (in the Humphrey cycle), and the RAMJET (in the Brighton cycle), is much higher only when $M_0 < 1.5$. With an increase in M_0 , the difference of ideal PDE thrust over ideal thrusts of other ABJE rapidly decreasing.

Part of the calculation results is shown in Figures 1. From ideal thermal efficiency, as in [3], the value of V_e/V_0 is found, where V_e is the velocity at the nozzle exit. Figure 1 shows the ratio V_e/V_0 , since the specific thrust and impulse are proportional to $(V_e/V_0- 1)$. Considered types of ABJE include engines with DC with constant pressure, as in RAMJET (in the Brighton cycle), and with constant volume (in the Humphrey cycle), pulsed detonation engines (PDE) with combustion in the detonation wave of Chapman-Jouguet (DW_{CJ}) , engines with combustion in the both: stationary DW_{CJ} with pre-deceleration of supersonic flow $(SDE_{\psi>1})$ and in oblique detonation wave (SDE_{OSW}) . An ABJE with detonation combustion, for which only thermodynamic analysis was performed in [3], is PDE.



Figure 1: Efficiency and V_e/V_0 for different engines (at $q^\circ = 6$) as a function of M₀

As can be seen from the figure 1, the efficiency of the PDE cycle is indeed higher than that of Humphrey and Brighton, as well as cycles with a direct and oblique detonation wave. The ratio of speed V_e/V_0 , consequently, the specific thrust and impulse found by the efficiency behave in the same way. However, in the case of PDE and the Humphrey cycle, as mentioned earlier, it is necessary to take into account the non-stationarity of processes in the combustion chamber. We will deal with this in the next part of this article.

3.Non-stationary model of the flow in pde

Supposing that PDE has *N* cylindrical, synchronously operating groups of detonation chambers with instantly opening and closing valves (input power walls). When the valves are open, a perfectly mixed fuel mixture enters the detonation chamber. The one period operation of detonation chamber (DC) of PDE can be divided into several stages. Opening of the valve, filling of the DC with the combustible mixture, instantaneous closing of the valve and initiation of the detonation wave at the inlet end of the DC. The arrival of the detonation wave at the right end of the DC is the cross section of the entrance to the ideally adjustable jet nozzle. Since the velocity of the detonation wave is much higher than the speed of filling the DC, this happens in a short finite time. 3. DW is reflected from the partially open right section of the detonation chamber (narrowing of the nozzle) as a shock wave that moves to the closed input section. Further, non-stationary shock waves, moving along a DC, can be reflected several times from its ends. Despite the attenuation, the reflected shock waves are a source of entropy growth that is not taken into account when determining the ideal characteristics of PDE. The valve instantly opens when the average pressure of the combustion products in the DC is less than the pressure of the inhibited air and the fuel ideally mixed with it in front of the volume in front of the rotating valve.

The flow of combustion products through the nozzle occurs throughout the entire operation cycle of the PDE. The flow in the expanding part of the nozzle is quasi-stationary and isentropic, and the nozzle exit area is perfectly adjustable. Given the f_0 (the ratio of the area of the nozzle's critical section to the cross-sectional area of the chamber), M_0 and q° , the ratio of the velocities V_{e}/V_0 is obtained as a function of time during the operation period of the PDE chamber. Its integration over the period gives average values of the V_{e}/V_0 and thrust characteristics, taking into account non-stationarity and non-entropy of the flow of combustion products in the detonation chamber.

Figure 2 shows the curves of the V_e/V_0 ratio for the ramjet (Brighton cycle, does not depend on time) and for PDE, calculated according to the ideal thermal efficiency (PDE_{th}) and for several values of f_0 found in the non-stationary model.

Taking into account the non-stationarity of the process in the PDE combustion chamber, we obtain lower tractive characteristics than when using the ideal thermal efficiency. While the larger, the area of the critical section of the nozzle, the worse the thrust characteristics of the engine. On the other hand, the smaller the nozzle throat area, the longer the purging time of the combustion products and the worse the conditions for PDE operation.



Figure 2. V_{e}/V_{0} of an ideal PDE and RAMJET (Brayton cycle) and V_{e}/V_{0} of PDE according to the results of the unsteady calculation

4. Testing and verification of detailed methane-propane mixture combustion reaction kinetics mechanisms

Inaccuracy connected with kinetics mechanism has commonly significant and even crucial influence on reacting flow calculations (including combustion calculations) in comparison with the other applied models. In CFD calculations reaction mechanisms with small amount of components and reactions are mostly used due to computational resources limitations. These mechanisms could reproduce reacting system properties in a short range of thermodynamic parameters. Tendencies to more proper description of reacting system processes and computational resources growth lead to numerous researches devoted to development of reduced kinetics mechanisms specifically for CFD calculations, but most of these works are carried out for pure substances. However, one could note the non-linear effects connected with a small addition of secondary component in pure substance even for alkanes lower homologs: decrease of ignition delay time due to ethane/propane adding to methane is experimentally demonstrated in [7-8]. An attempt to estimate accuracy, which can be achieved with using detailed reaction kinetics for binary methane-propane mixture, is made in current section. As a test case, non-linear effect of ignition time decreasing with adding of propane to pure methane is modelled. At the first stage several detailed kinetics mechanisms are analysed and validated by comparison with experimental data for typical combustion characteristic: ignition delay time.

Main features of selected for consideration detailed kinetics mechanisms are presented in Table 1. Experimental data for methane-propane mixture at high temperatures are included in GriMech 3.0 validation database, comparison is presented for specific temperatures (T=1410 K, 1640 K) and pressures higher than atmospheric (P = 2.5, 7.095atm respectively). A difference between calculation with GriMech 3.0 and experimental data on induction time does not exceed 20%. Inaccuracy values for moderate temperatures and high pressures are significantly higher.

More detailed information on other mechanisms including authors, validation and applicability parameter ranges could be found in references. Table 1 contains also two reduced mechanisms developed based on research of group from National University of Ireland, Galway (version 2010, C4-49).

Mechanism	Components	Amount of components	Amount of reactions	Reference
GRI-Mech 3.0 (1999)	C1-C3	53	325	[9]
UCSD (2016)	C1-C4	68	310	[10]
USC_II (2007)	C1-C7	111	784	[11]
LLNL (2009)	C1-C16			[12]
NUI Galway (2010)	C1-C5	293	2928	[13]
Konnov (2000)	C1-C4, C6	127	1207	[14]

Table 1: Detailed kinetics mechanisms of light alkanes combustion selected for validation

Most common experimental technique of ignition delay time measurements in combustible mixtures is shock tube measurements. Most of experimental data are obtained with this technique which allows obtaining high pressures and temperatures. It is technically more difficult to organize induction time measurements at moderate temperatures T<1100 K and atmospheric pressure in shock tube. It requires combustible mixture residence time increase in working section of shock tube, which leads to tube construction complication and possibility of shock wave breakup and velocity profile alteration in working section due to boundary layer thickening. The ignition delay time for alkanes lower homologs could vary in a wide range: from microseconds typical for combustible mixture temperatures T>1100 K, to seconds – for temperatures $T\sim600..700$ K. It is important for kinetics mechanisms of hydrocarbons oxidation to reproduce the moderate temperatures range T<1050 K which corresponds to negative temperature coefficient (NTC) range, where ignition delay time is decreasing while temperature is increasing.

Lesser amount of experimental data on ignition delay time is obtained with rapid compression machines, flow reactors and constant mixing reactors. Most common approaches for ignition delay time measurements are: maximum radical concentration criteria (CH*, OH*), maximum temperature curve bend, pressure oscillogram alteration. Table 2 includes selected for validation experimental data on ignition delay of methane-propane mixture with experimental conditions and references. Selected data corresponds to measurements in temperature range 963 K<T< 1260 K and pressures P=1 atm and 10.3 atm< P < 43.3 atm. Estimations of experimental uncertainty from references for every data set are given in the notes below the table.

Table 2: Selected experimental data on ignition delay for binary mixture CH₄+C₃H₈

Mixture	Experimental setup	Fuel-air equivalence ratio, φ	<i>Т</i> , К	P, atm	Measurement method ^a	Reference
CH ₄ +	Flow reactor	0.5, 1.0	963-1137	1	СН	[15] ^{b,c}
C ₃ H ₈	Shock tube	1.0	970-1260	15.1-43.3	P+L	$[8]^{b,c}$
	Shock tube	0.5	1290-1659	10.3-23.8	СН	[7] ^{<i>b,c</i>}

^{*a*}Measurements method: CH – by radical CH radiation, P – by pressure measurements, L – by light radiation (radical is not specified); ^{*b*}Experimental uncertainty: [15] – time measurements error< 30% (by correction data),[8] – direct induction time measurements error are not presented, C_3H_8 concentration measurements error <5%, temperature measurements error ~15 K,[7] – induction time measurements error <10%; ^{*c*}Data from source: [15] – obtained by graph processing, [8], [7] – table data

The results of calculations using the selected mechanisms and the data [7] are shown in Figure 3, the worst data on the error mechanisms LLNL (132.14%) and Konnov (65.44%) are not shown. The top three mechanisms for average error (error for each point calculated by formula $\delta = |\delta_{exp} - \delta_{num}| / \delta_{exp}$) on this set of USC_II are 19.4%, UCSD is 21.58%, and NUI is 21.86%.



Figure 3. Comparison of data [7] with calculations, P = 10.3-23.8 atm, pure methane, $0.05CH_4 + 0.2O_2 + 0.75N_2$, and a mixture of $0.0311CH_4 + 0.0077C_3H_8 + 0.202O_2 + 0.7592N_2$, time in μ s

However, taking into account the range of temperatures and pressures and the presence of pure methane in the data set, all the mechanisms except LLNL show a relatively small error in the determination of induction times. The temperature range T <1100 K is more difficult to model. Such studies in a shock tube were carried out in [8], despite elevated pressures P = 16.2-43.3 atm, the data for moderate temperatures and for small C_3H_8 additives are given from the data the work selected three mixtures with molar ratios of C_3H_8 / CH₄: 1.25%, 2.5%, 5%. A comparison of the calculated and experimental data for this set of experiments is shown in Figure 4. The data of the two mechanisms with the greatest error, as well as in Figure 3 are not shown, these are the mechanisms of LLNL and Gri Mech 3.0. Out of the remaining ones, the best error results are shown by the mechanisms Konnov (68.94%) and UCSD (134.98%).



 $\label{eq:Figure 4. Comparison of data [8] with calculations, P = 16.2-43.3 atm, time in ms, mixtures \\ 0.0845CH_4 + 0.0044C_3H_8 + 0.1913O_2 + 0.7198N_2 \\ 0.0896CH_4 + 0.0023C_3H_8 + 0.1907O_2 + 0.7174N_2 \\ 0.0923CH_4 + 0.0012C_3H_8 + 0.1904O_2 + 0.7161N_2 \\ \end{array}$

The most difficult test for kinetic mechanisms is their data collection [15], in which for atmospheric pressure in a flow reactor for moderate temperatures, the ignition delay times for binary mixtures were measured for various fuel / oxidizer ratios and for different CH₄ / C_3H_8 ratios - 0%, 5%, 10%, 25%, 50%, 75%, 100%.

In this case, the ignition delay times are of the order of a second. A comparison of the calculated and experimental data for the composition of the mixture - 50% CH₄ + 50% C₃H₈ ($\phi = 0.5, 1.0$) is illustrated in Figure 5. GriMech 3.0 shows the best results on this dataset; however, by the average error for all points, UCSD mechanism is comparable with it. The Konnov mechanism on this data set showed the worst results, underestimating the induction times for all mixtures several times, the other mechanisms showed a comparable error.



Figure 5. Comparison of data [15] with calculations, P = 1 atm, time in s, mixtures $CH_4+C_3H_8 + 14O_2 + 52.822N_2 (\phi=0.5) - \text{left},$ $CH_4+C_3H_8 + 7O_2 + 26.41N_2 (\phi=1.0) - \text{right}$

5. Summary

To conclude, the statements of a possible increase in the thrust characteristics of the ABJE by tens of percent due to the use of detonation combustion are unfounded. Even for subsonic and small supersonic Mach numbers of flight, when the ramjet can yield PDE in thrust characteristics, PDE are certainly concede to those of the turbojet engine with deflagration combustion. Therefore, the advantages of ABJE with detonation combustion, if possible, are not in terms of thrust characteristics, but in design simplicity (as for small M_0 in comparison with turbojet engine) or lower heat stress of the engine tract.

The main conclusion for second sub-problem is that even detailed kinetics mechanisms for engine relevant conditions shows for simple binary mixture fuel significant errors. Even qualitatively not all considered in section 4 mechanisms correctly reproduce the decrease in the ignition delay time in methane-propane mixtures. The smallest error, $\sim 50\%$ for 3 experimental data sets, was shown by the UCSD mechanism. Error distribution for all considered reaction mechanisms, as can be expected, is very irregular. The errors values vary from $\sim 10\%$ for high-temperature region and near atmospheric pressure to more than 100% error for low-temperature region.

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