29th Congress of the International Council of the Aeronautical Sciences
St. Petersburg, Russia; September 7-12, 2014

ANALYSIS OF THE PREDICTION ABILITY OF REACTION MECHANISMS FOR CFD MODELING OF THE COMBUSTION IN HIGH VELOCITY ENGINES

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Keywords: *supersonic flow, combustion, reaction mechanisms*

Abstract

Comparative analysis of combustion characteristics in supersonic flow of H_2-air mixture with the use of several modern reaction mechanisms has been conducted both for steady and unsteady flows.

1 Introduction

Combustion process in high velocity air-breathing engines is characterized by strong interaction of gasdynamic and chemical processes. This interaction defines both the flow structure and combustion regime formation. The operational conditions in the combustor require the adequate description both of high temperature as well as low temperature ignition. This imposes the strong requirements on the choosing of kinetic mechanisms. In order to highlight the features of ignition and combustion of fuel-air mixture in a high velocity flow it is necessary to apply the detailed reaction mechanisms [1-3]. A great progress in the construction of detailed reaction mechanisms in H_2-air mixture was achieved (see, for example, [4-8]). A few detailed kinetic mechanisms of novel generation describing with rather high accuracy a number set of experimental data on the ignition delay, velocity of laminar flame propagation and time evolution of species concentrations measured with the use of shock tube and flow reactor techniques were built. However, the prediction ability of these detailed kinetic models was tested mostly against the ignition delay. In the combustor of high velocity air-breathing engine, not only this characteristic controls the combustion performance, also the length of energy release zone and combustion completeness become important. As well the unsteady effects must be properly reproduced in such combustors.

In this paper, a comparative analysis of characteristics of combustion in high velocity flow was conducted with the usage of modern reaction mechanisms built by Li et al. [4], O'Conaire et al. [5], Konnov [6], Hong et al. [8] and Starik et al. [9], as well as with the kinetic models of previous generation [1-3]. It is worth noting that the considered mechanisms are frequently utilized in CFD simulations of ignition and combustion of H_2-air mixture in practical devices. The analysis of aforementioned predictive ability of reaction mechanisms has been performed for two combustion regimes, which can take place in the combustor of high velocity air-breathing engine: diffusion mode in pure supersonic flow and the mode with pseudo shock.

2 Diffusion mode of combustion in a supersonic flow

The concrete analysis was conducted for the model combustor in which the gaseous molecular hydrogen was supplied tangentially through 7 pylons sited at the combustor entry. The geometry of model combustor is shown in Fig. 1. Its length is equal to 135 cm and transversal dimension at the inlet section is 13 cm. The pressure, temperature and Mach number of hydrogen jets were the following: P_h=3 atm, T_h=450 K and M_h=2.5. The mass flow rates through all pylons were identical. The following parameters of air flow were

chosen: M_0=3.5, P_0=0.3 atm, at the temperature variation. The temperature in cases considered was equal to T_0=1100, 1300 and 1500 K.

The dynamics of the reacting H_2-air flow was described by the 2D Favre averaged parabolized Navier–Stokes (PNS) equations [10]. Combustion was simulated with the use of quasi-laminar approach. To describe turbulent mixing of air flow and hydrogen jets from pylons, the one-parameter turbulence model [11] specially adapted to compressible jets was utilized in our calculations. It was supposed that turbulent diffusion coefficients were the same for all mixture components and the Lewis number was equal to unity for all species.

The "corrected" boundary conditions on the wall were used for the viscous flow. This makes it possible to use the marching (in longitudinal direction) method that is based on the stationary analog of the Godunov scheme for supersonic flow [12]. The details of the methodology of numerical simulation were reported in [10]. The simplified PNS version of RANS allows one applying the detailed reaction mechanisms and accurate computational grids in the CFD model, which can reproduce properly the processes in mixing layers and formation of oblique shock waves. The computations were performed with the number of nodes equivalent to RANS grid consisting of 350 points in the transversal direction and more than 7000 points in the longitudinal direction.

In our runs, combustion efficiency was defined as $\eta = Q_1/Q_0$, where Q_1 is the energy released into the flow due to combustion up to the considered cross-section and Q_0 is the maximal energy, which could be supplied to the flow at the complete mixing of air and fuel and when one global reaction takes place: $2H_2 + O_2 = 2H_2O$. The coefficient of air to fuel equivalence ratio in all considered cases is lower than 1 (fuel-rich mixture), and the value of α decreases from 0.89 to 0.76 when air inlet temperature increases from 1100 K to 1500 K.

The temperature (Fig. 1) and radical OH mass fraction (Fig. 2) fields are presented for "modern" kinetic mechanisms [4-6, 8, 9] and for kinetic mechanisms of previous generation [1, 2] in the case of air inlet temperature T_0=1100 K. It should be noted that the temperature fields predicted by reaction mechanisms of O'Conaire et al. [5], Konnov [6] and modified Jachimowski mechanism [2] are similar, and, at the same time, the predictions of Starik et al. [9] and Hong et al. [8] models are close to one another. For *OH* mass fraction fields, there exist essentially more distinctions in the predictions of the considered reaction mechanisms. However, there are the similar correlations in the predictions for different reaction mechanisms. The analysis showed that the largest ignition delay lengths are provided by Starik et al. [9] and Hong et al. [8] reaction mechanisms as compared to other mechanism predictions. Jachimowski model [1] gives the shortest ignition delay and the highest heat release rate. The comparison of combustion efficiency values predicted by considered kinetic mechanisms for T_0=1100 K is shown in Fig. 7a.

An increase in the air temperature results in the essential decrease of the induction zone length and in the growth of combustion zone length. This is confirmed by the fields of static temperature, mass fraction of *OH* radical and the variation of combustion efficiency along the duct shown in Fig. 3, 4 and 7b, correspondingly, for the case with T_0=1300 K. The reaction mechanisms [4-6, 8, 9] and modified Jachimowski mechanism [2] predict close values of ignition delay. However, the difference in the combustion zone lengths calculated with the use of considered reaction mechanisms remains being noticeable. The most fast increment of combustion efficiency along the duct is predicted by the reaction mechanism of Jachomowski [1], and the smallest rate of combustion efficiency rise and the lowest value of combustion efficiency at the exit of the duct is predicted by reaction mechanism of Li et al. [4] (Fig. 7b). The reaction mechanisms of Konnov [6], Hong et al. [[8]], Starik et al. [9] and modified Jachimowski mechanism [2] provide the values of combustion efficiency close to each other.

Fig. 5 and 6 depict the air temperature and *OH* mass fraction fields at the T_0=1500 K. The combustion efficiency for this case as a function of longitudinal coordinate is presented

in Fig. 7c. It is worth noting that the main tendencies in predictions of lengths of ignition delay and energy release by various reaction mechanisms are identical to these ones in the case with T_0=1300 K. The combustion efficiency curves predicted by Konnov [6] and Hong et al. [8] reaction mechanisms practically coincide as well as those obtained by reaction mechanism Starik et al. [9] and modified Jachimowski reaction mechanism [2] (Fig. 7c). It should be noted that the ignition delay length, length of energy release zone, rate of combustion efficiency rise in the duct predicted by the mechanism of Dimitrov [3] are in good correlation with the predictions of Jachimowski model [1].

Thus, in order to predict the combustion efficiency in a supersonic flow with reasonable accuracy one needs to be very careful in choosing the reaction mechanism. Certainly, processes inside the combustor require further extensive experimental and numerical inspection. The reaction mechanism [9] provides the good consistence with existing experimental data and can be used for the validation of other kinetic models. Because the oxidation and ignition in the H_2-O_2 (air) mixture are determined by the rate of formation of active O and H atoms and OH radicals, it is important to describe properly the evolution of these species. The special attention has been paid to this aspect during the validation of reaction mechanism [9].

3 Combustion in pseudo shock and in the combustor with near constant Mach number

It is worth noting that for the combustion regimes occurring at high hypersonic flight Mach numbers, the thermal throttling of the flow due to combustion in the duct with supersonic velocity at the combustor entrance, even in the combustor with constant cross section area, is not accompanied by the flow deceleration to sonic value. At the moderate hypersonic flight Mach number, for example, at M_f=6 and supersonic conditions at the exit of engine inlet, the alternative combustion regimes can occur. In the first case, the supersonic at the combustor entrance flow is decelerated due to energy release in the duct of constant cross section area to a small, but greater then 1, supersonic Mach number. Then, this small supersonic Mach number is held in the trailing part of combustor. This regime requires special profiling of the duct. Such combustor is called as iso-Mach combustor. Theoretically, the combustion regime with the flow deceleration to M=1 is considered as very promising because the low level of irreversible losses is expected in this case. At the same time, the other combustion mode named “combustion in pseudo shock” can also take place at these conditions at the combustor entrance. The main features of this combustion mode are the existence of shock train system interacting with boundary layers at the combustor walls with separation regions formation and essential thermal throttling of the duct due to energy release. In this case, the combustion zone contains regions with subsonic velocity inside the duct, and, at the combustor exit section, the transition from subsonic flow to supersonic one occurs. Since the system of shock waves with transition to subsonic flow and separation regions lead to the high level of irreversible losses, the combustion in iso-Mach combustor, at the first look, has some advantages, because, as is supposed, there are no shocks in such a combustor.

It should be noted that the realization of alternative combustion regimes requires the special profiling of combustor shape for each of the regimes. In our analysis, the combustor expansion in area for both combustion regimes was taken identical. The isolator was installed before the combustors, and flow parameters at the entrance of isolator were given identical for both cases. The air to fuel equivalence ratio was close to stoichiometric one. The calculation procedure was following. At the first step, the steady air flow was calculated in the duct. The hydrogen was injected into the air flow through the system of struts, and the unsteady process was simulated. The parameters are such that self ignition is not realized. The pilot flame is used for combustion starting. After combustor starting, the pilot flame is switched off. The flow structure and

details of combustion process are studied after pilot flame switching off.

Numerical simulation was performed on the basis of 2D Favre averaged full Navier-Stokes equations for unsteady turbulent flow of reacting mixture and quasi-laminar approach using CIAM developed code. Two reaction mechanisms developed in [3] and in [9] were applied for analysis. The computational method is based on the implicit version of modified Godunov scheme of higher order accuracy, and details are presented in [10].

It is worth noting that for the iso-Mach combustor with one-stage system of fuel supply the flow stall with disturbances propagation up to the isolator entrance is observed. It is appeared being possible to arrange the stable burning in the combustor using two-stage fuel supply. The Mach number (Fig. 8a) and temperature (Fig. 8b) fields are presented for iso-Mach combustor for the case with two-stage fuel supply. The flow in the expanding part of the combustor remains supersonic with Mach number approximately equal to 1.3. However, the flow structure differs essentially from that for the ideal theoretical scheme with smooth deceleration of supersonic flow without shocks. The principal feature of flow structure is the shock system interacting with boundary layers and separation formation. The Mach number and temperature fields for the second combustor type (combustion in the pseudo shock) are shown in Fig. 9. The large subsonic region and extensive separation zone near the upper wall are observed in the duct. The ejection of fuel by separation region and temperature rise at the head of pseudo shock initiate and support the combustion near the upper wall in the region located upstream of the fuel struts position.

The analysis of reaction mechanisms ([9] and [3]) influence on the flow fields prediction and combustion characteristics was performed. It was shown that this influence is week for combustion in pseudo shock. The following effect of reaction mechanism on the flow in iso-Mach combustor was found. Practically steady state solution was obtained in this case at usage of the reaction mechanism [3]. The pronounced flow oscillations are detected in the region of locations of shock waves and separation zones at the implementation of the kinetic mechanism [9]. These flow oscillations are periodical in time.

4 Conclusion

The analysis of the influence of different reaction mechanisms, chosen for the description of hydrogen-air combustion, on the predictions of flow fields and combustion characteristics was performed. The widely used kinetic mechanisms developed previously and modern were applied for the calculations of different combustion regimes typical for the supersonic flow velocity at the entry of duct.

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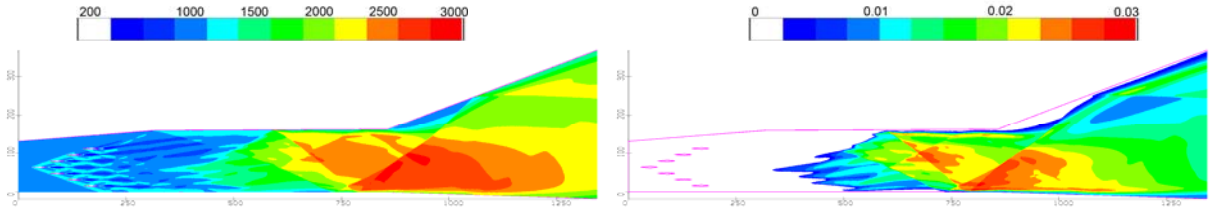

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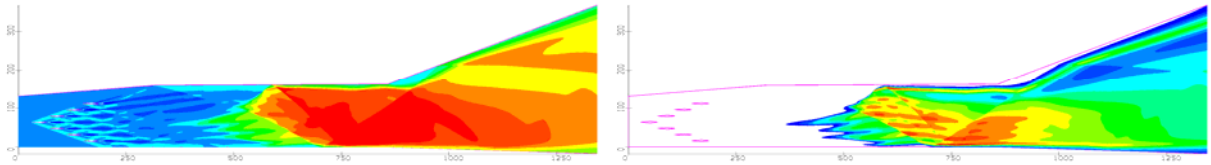

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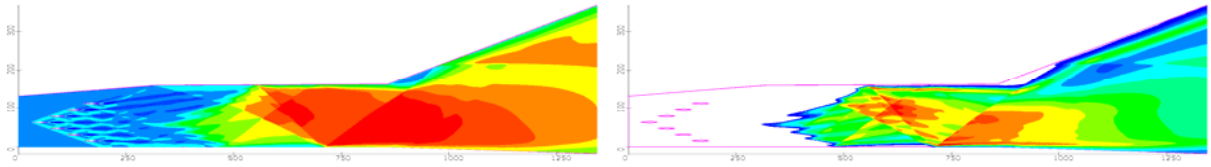

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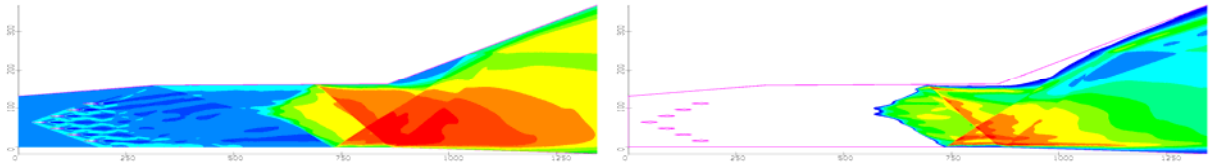

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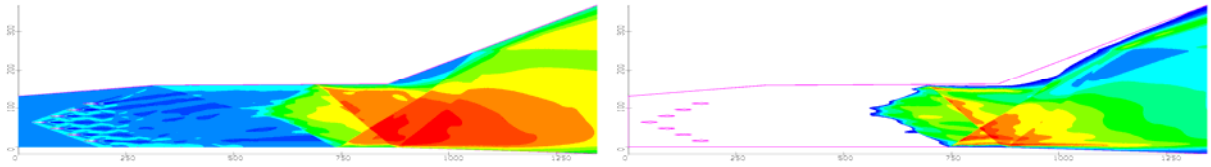

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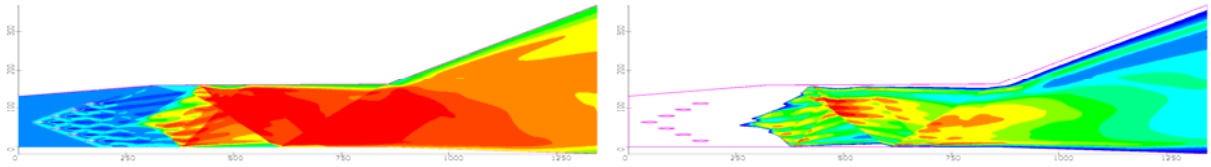
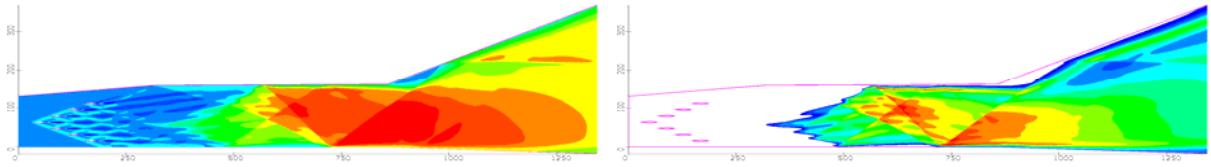


Jachimowski (1988)

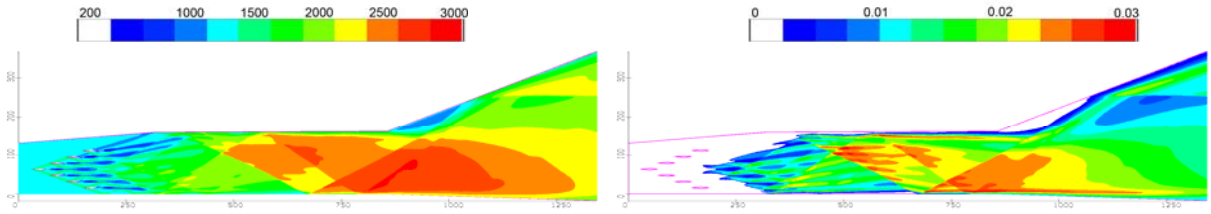


modified Jachimowski (1992)

Case T_0=1100 K

Fig.1. Temperature fields

Fig.2. Mass fraction fields of *OH* radical



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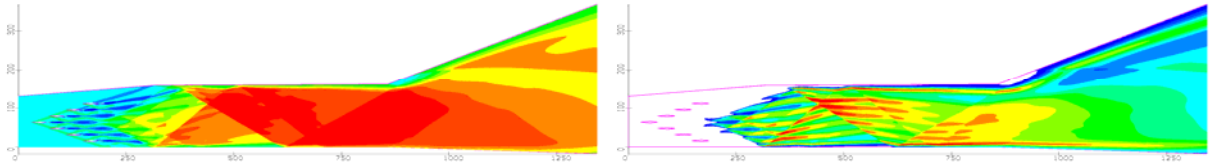
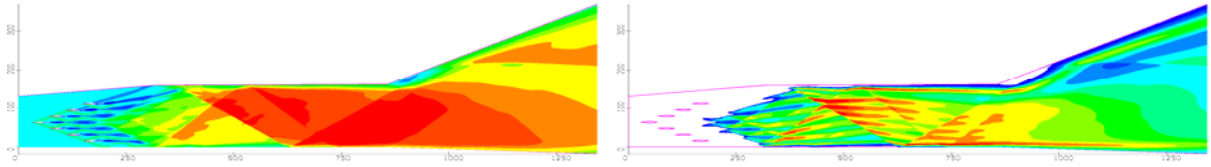


O'Conaire et al. (2004)



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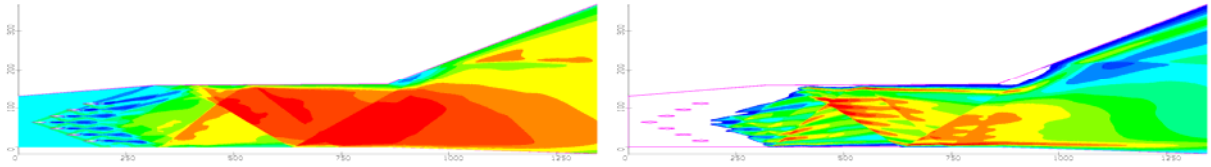

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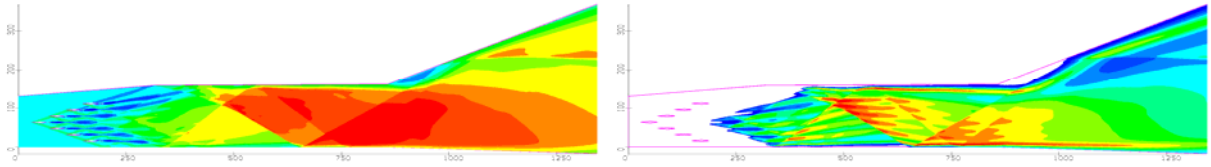

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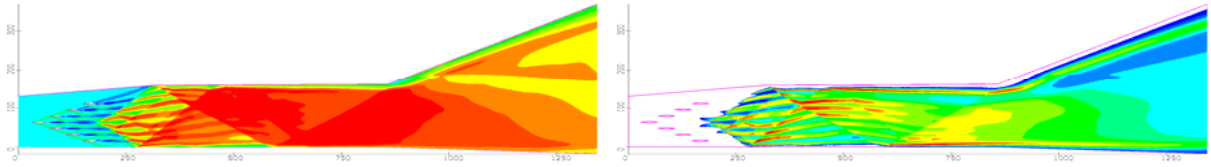
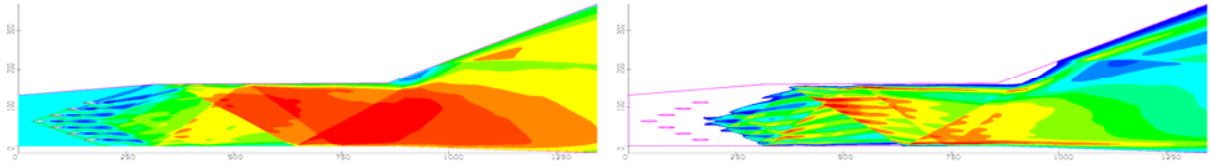


Jachimowski (1988)

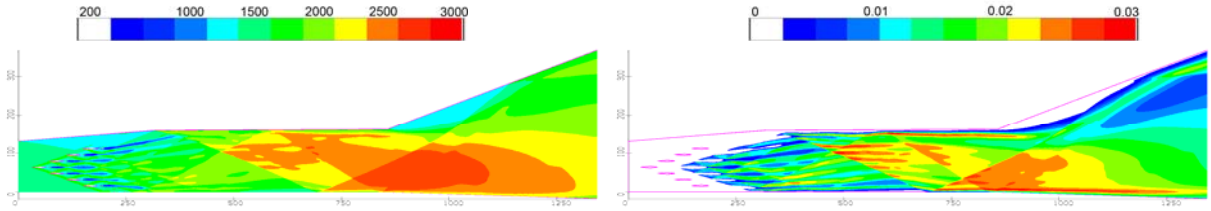


modified Jachimowski (1992)

Case T_0=1300 K

Fig.3. Temperature fields

Fig.4. Mass fraction fields of *OH* radical



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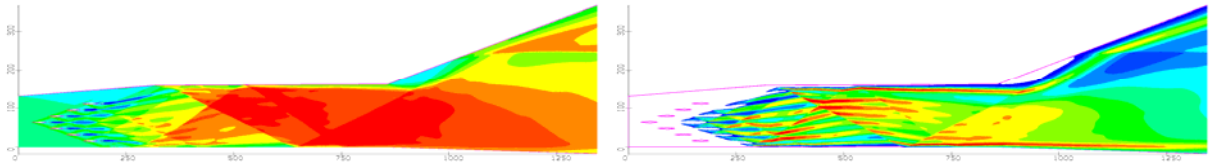

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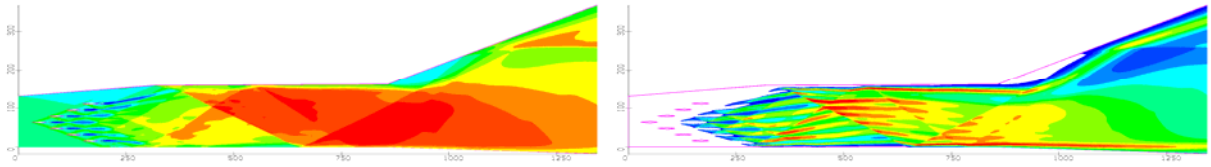

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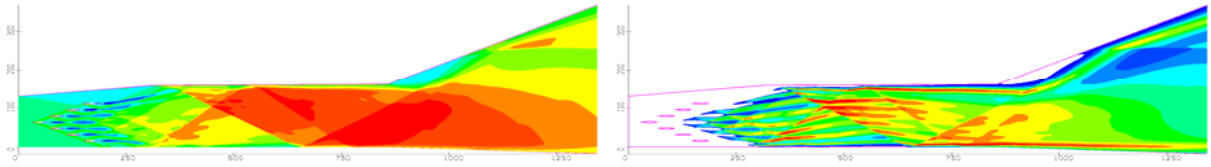

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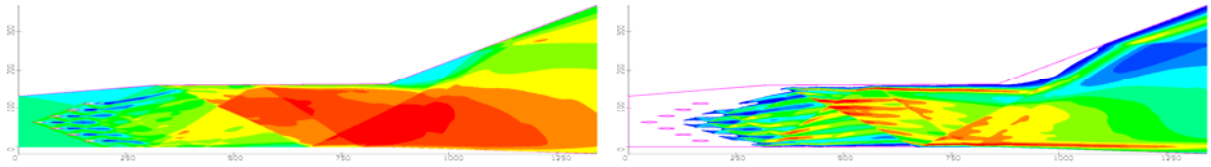

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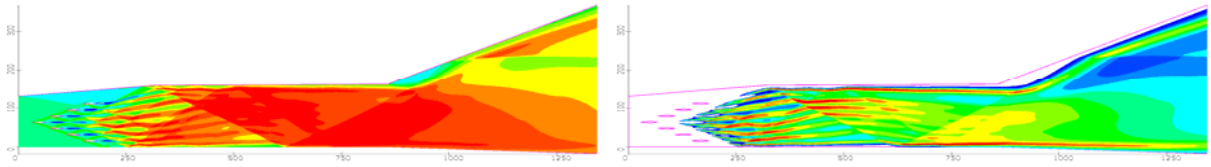
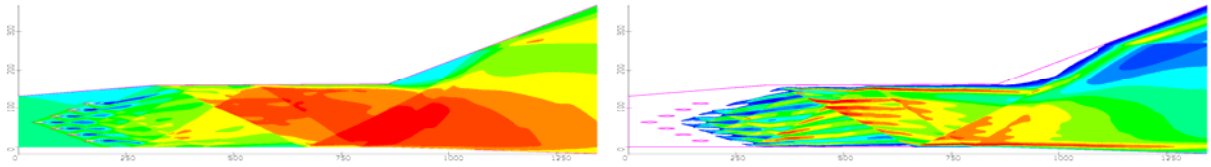


Jachimowski (1988)



Modified Jachimowski (модиф. 1992)

Case T_0=1500 K

Fig.5. Temperature fields

Fig.6. Mass fraction fields of *OH* radical

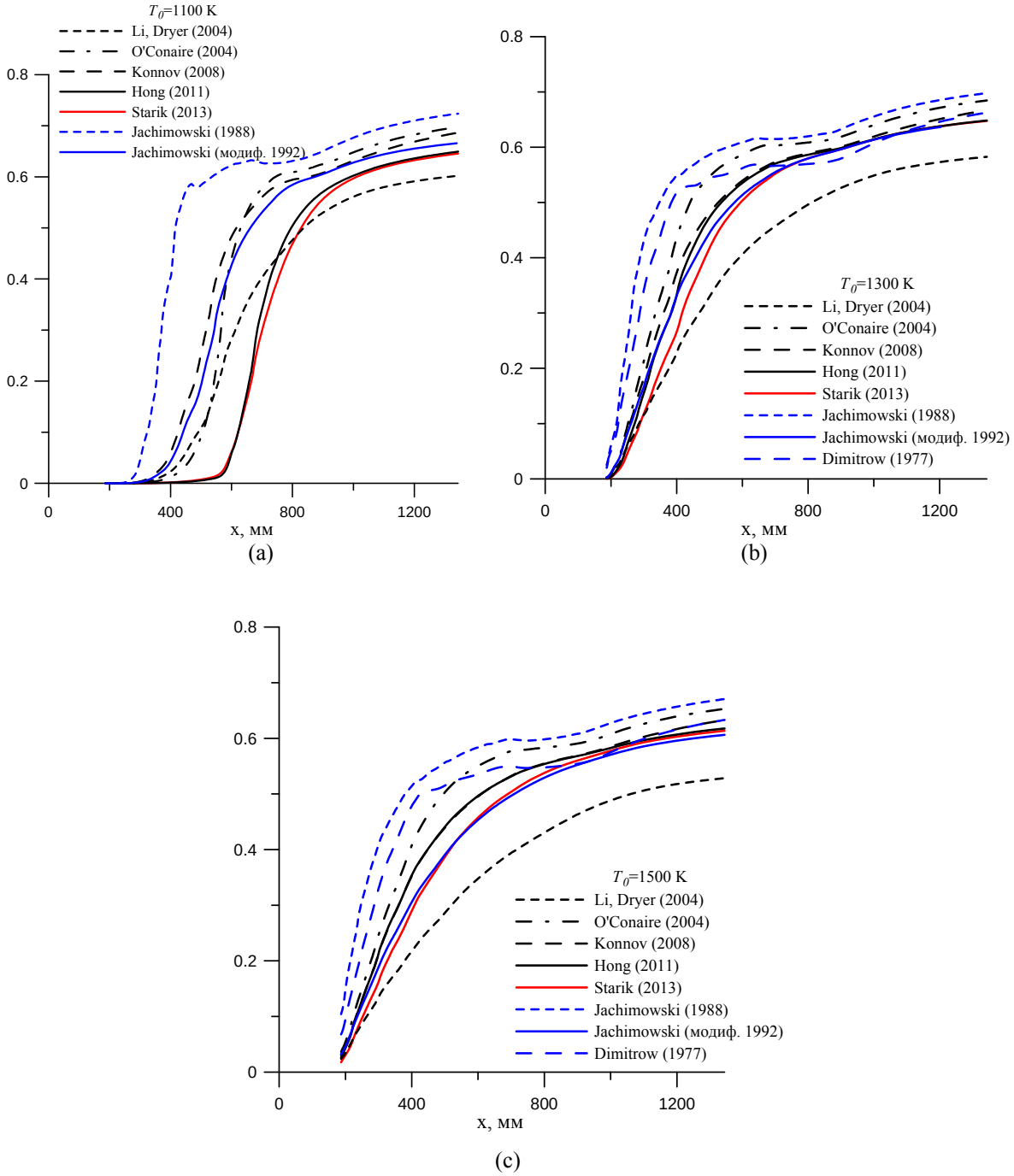
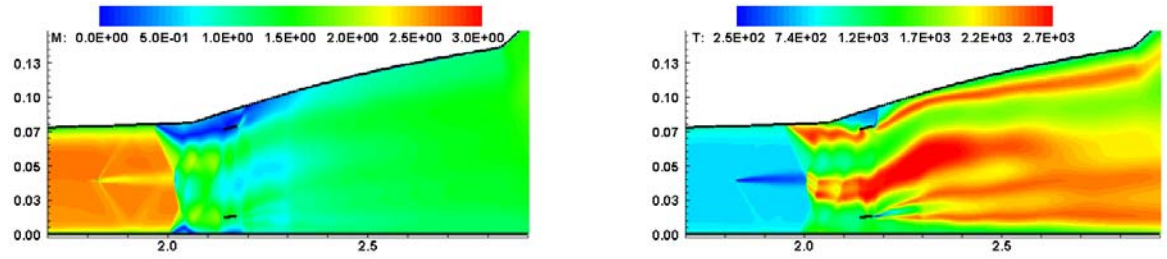
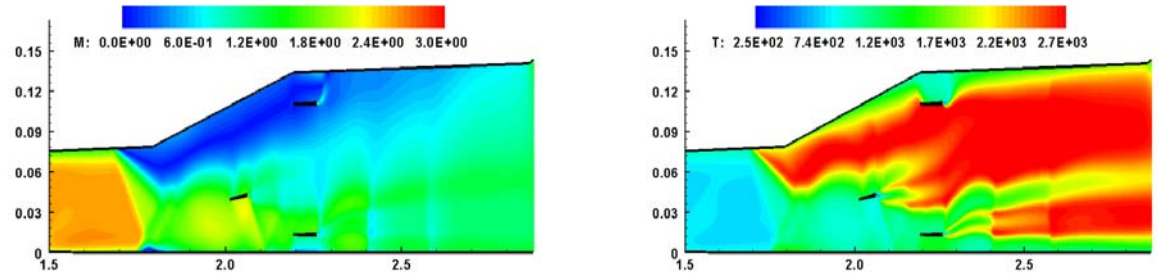


Fig.7. Combustion efficiency η as the function of the duct length
(a) – T_0=1100 K, (b) – T_0=1300 K, (c) – T_0=1500 K



(a) (b)

Fig. 8. Mach number (a) and temperature fields (b) for iso-Mach combustor



(a) (b)

Fig. 9. Mach number (a) and temperature (b) fields for the combustion in pseudo shock

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