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THERMOCHEMICAL CONVERSION OF HYDROCARBON FUEL FOR THE AJAX CONCEPT

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Abstract

The active heat protection system of hypersonic flight vehicle designed within the framework of concept "AJAX" with an endothermic process of thermochemical hydrocarbon conversion is considered. The study of the interaction between hypersonic airflow and a flight vehicle element is distinguished characteristic areas for which the calculation of gas flow is carried out, the thermochemical reactor characteristics are found.

Fundamentally new concept "AJAX", based on active power interaction between a system and air flowing around it, is considered as one of perspective trends of hypersonic technique¹⁻³. Hypersonic flight vehicle under the concept "AJAX" is an open aerothermodynamic system (Fig.1). The hypersonic airflow kinetic energy assimilated by subsystems of the vehicle is converted to a wide spectrum of useful effects. This approach enables to change understanding all aspects of the further development

of aerospace engineering. The active cooling of construction implements with use of steam reforming of ordinary aviation hydrocarbon fuel, which is the main energy carrier. Hydrogen received as a result of decomposition of hydrocarbons is used for improvement of state variables of fuel mixture. The production of hydrogen and the use of MHD systems for airflow deceleration/acceleration give a possibility to create a ramjet with supersonic combustion. Power-to-weight ratio for such system will exceed significant the same ratio for existing systems. The received electric power can be utilized in systems of plasma flow control to increase lift-to-drag ratio of hypersonic flight vehicle.

Within the framework of the concept "AJAX" the new technologies of hypersonic flight speeds are offered. These technologies allow creating:

1. Active heat protection of hypersonic flight vehicle, based on chemical heat regeneration;
2. Magneto-Plasma-Chemical engine, which uses products of steam reforming of hydrocarbons and exerts energy influence on hypersonic flow;
3. Plasma device for control over aerodynamic characteristics of the airflow around the vehicle.

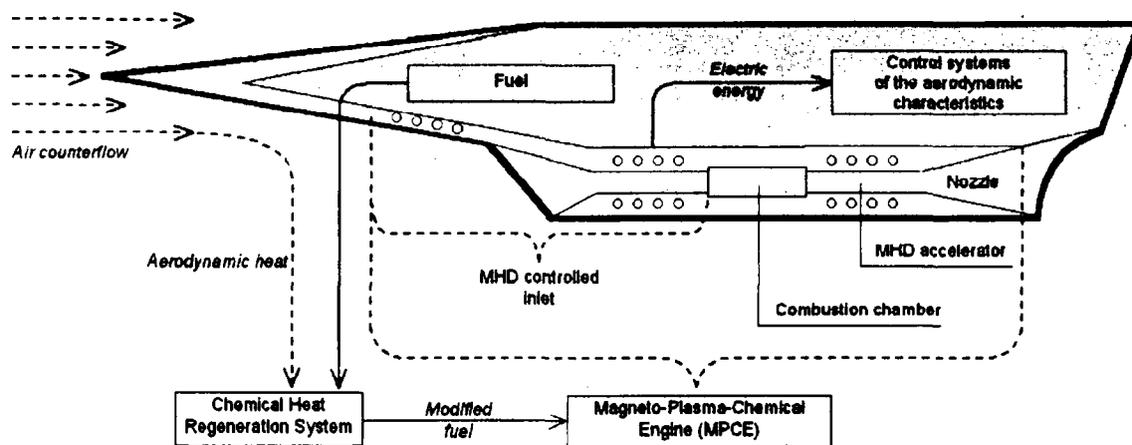


Fig. 1. The schematic diagram of hypersonic flight vehicle

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At the present time several concepts of development of hypersonic aviation are considered. The fuel used is an attribute distinguishing one concept from another. Some characteristics of liquid hydrogen and hydrocarbon fuel are compared in Table 1. Grave drawbacks of liquid hydrogen are small density and low boiling point (cryogenic properties). Preparation time, aerodrome infrastructure, flight safety and some other arguments count in favor of hydrocarbon fuels.

Characteristic	Kerosene	Hydrogen
Chemical formula	C_nH_m	H_2
Molecular weight	-	2.01
Melting point, K	<213	13.86
Boiling point, K	423...573	20.13
Density of liquid, kg/m^3	775-840	70.8
Gas density, kg/m^3	-	0.090
Gas heat capacity, C_p , $kJ/kg \cdot K$	≈ 1.8	14.3
Ignition temperature, K	570	510
Theoretical combustion temperature, K		2300
Stoichiometric ratio on air	14.9	34.5
Mass heating value (lower), MJ/kg	42.9	120.0
Volumetric heating value (lower), MJ/dm^3	34.3	8.51
Cooling capacity (at heating within the specified temperature range, K), MJ/kg	0.93 (293-533)	13.95 (20-922)
* At normal pressure - At boiling point - - At normal temperature and pressure		

Table 1. Comparison of liquid hydrogen and kerosene

Active heat protection of hypersonic flight vehicle in accordance with the concept "Ajax" is based on chemical endothermic transformation of initial hydrocarbon fuel via recuperation of thermal losses generated from the aerodynamic heating of planer and the operation of power plant. This transformation implements in thermochemical reactors (TCR) placed in heat-stressed parts of vehicle, and allows:

to increase cooling capacity of fuel at the expense of physicochemical transformation of initial components;

to ensure cooling of airframe by heat removal via convection and radiation, and also heat absorption

during catalytic reactions directly on the protected surface;

to receive hydrogen-containing fuel mixture fed to the combustor and improving the energy and ecological characteristics of burning.

The flowchart of working process aboard flight vehicle can be represented as it is shown in Fig.2. A part of hydrocarbon fuel and water goes to the feed system, and then into the system of preparation of

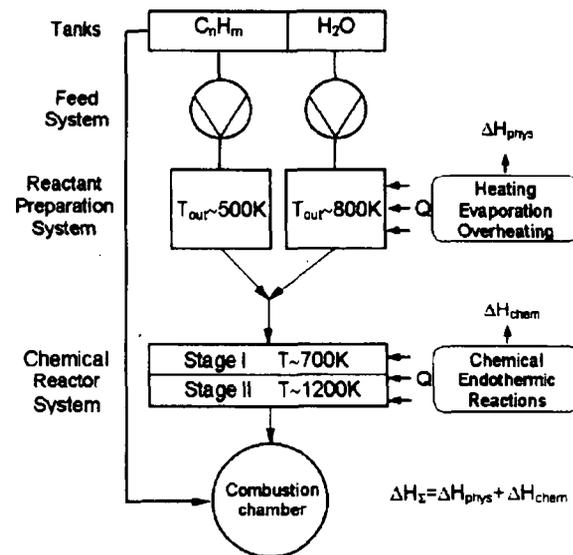
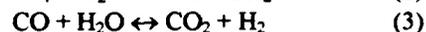


Fig.2. The flowchart of working process in the system of heat protection

reagents. Here they are subjected sequentially to heating, evaporation and overheating up to 300-450 deg C; during the process the energy ΔH_{phys} is absorbed. The suitable heat exchangers are placed in low-temperature part of airframe skin. Then the overheated vapors in a necessary proportion move into the reactor of 1st stage, where they are converted in practically auto-thermal mode. Thereupon, the mixture is formed, where methane is the main component (up to 70-80% of mixture volume):



The reactor of the first stage (gasifier) is made as a separate unit, which can be easily replaced after flight if the catalyst is coked; the latter can be subsequently regenerated. The gas mixture received after the first stage of the process goes into the reactors of 2nd stage located in heat-stressed parts of airframe and engine. High-temperature steam methane reforming with high endothermic effect ($\Delta H_{chem} \sim 10^7$ J/kg) occurs there at 700-900 deg C.



Then the products of this reaction mixing with fuel from the tank in a certain proportion arrive in the combustor of the power plant. On available cooling capacity $\Delta H_{\Sigma} = \Delta H_{phys} + \Delta H_{chem} \approx 8-10$ MJ/kg the composition of hydrocarbon and water comes nearer to a case of cooling by liquid hydrogen. This circumstance allows viewing application of hydrocarbon fuels with thermochemical conversion to realize cycles, which will be more effective than Brighton cycle, used conventionally in air-breathing engines¹.

One of necessary elements of systems engineering for heat protection and conversion of hydrocarbon fuel is the mathematical modeling of these systems. Some aspects of this work are described below.

Let's consider the scheme of interaction between a heat-protected element of flight vehicle (for example, wing) and hypersonic gas flow shown in Fig.3.

At streamlining a solid body by hypersonic gas flow it is formed a direct shock wave transformed in curvilinear downward along the flow (double line in Fig.3). Processes of dissociation, recombination, ionization, radiation, chemical transformations take place generally in the flow behind the shock wave in gas, and on the body surface. Besides the flow changes downstream from laminar to turbulent. The gas flow enters in thermal and, probably, chemical interaction with streamlined body. The gaseous mixture goes in the TCR channels located in element of flight vehicle. Endothermic reactions with significant thermal effect occur in the mixture. This leads to the cooling of outside surface of the flight vehicle; the latter process, in turn, influences essentially the flow pattern.

At examination of interaction between the hypersonic gas flow and an element of flight vehicle, six areas in reference to the flow and an element can be marked. In area I the use of an approximation of the Boltzman kinetic equation, dependent on particular parameters is possible. For the description of flows in area II it is necessary to use the Navier-Stokes equations. Between areas III and IV there is area of viscous/non-viscous interaction. Obviously, that the study of the flow is very intricate problem even in the simplified statement.

After statement of the task, the algorithms of solution were chosen and extended on interesting class of problems, the computer programs of numerical calculation were developed and debugged and the researches of flat currents in areas III-V were carried out. The programs are made that further they will be used in unified packet for examination of all the pattern "external flow - heat conduction in solid wall - internal current" in self-conjugate statement. In

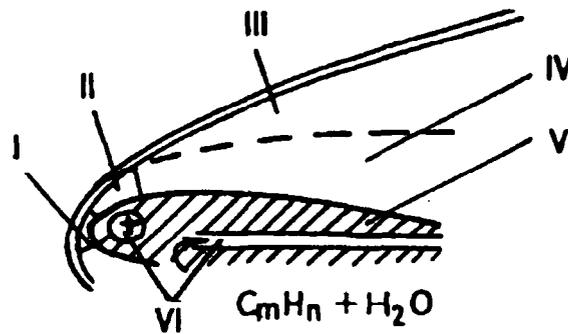


Fig.3. The two-dimensional scheme of interaction between a wing of flight vehicle and hypersonic gas flow:

- I – area near to a frontal point of so-called “molecular current”;
- II – area of “strong interaction”;
- III – area of non-viscous current;
- IV – boundary layer, laminar in the beginning and turbulent at a motion downstream;
- V – solid body, in which the processes are described by the equation of heat conduction;
- VI – subsonic flow of chemically reacting gas mixture in channels of TCR

the present work the interaction interference of the solutions for various areas was accounted to only a small extent: the boundary conditions for the boundary layer (area IV) were received from the solution of the equations of non-viscous current (area III). Therefore the received results for areas III-IV are preliminary, qualitative. For area VI the received results can be viewed as enough good quantitative estimation, if the values of temperature or heat flow on heated surface lay in the explored range of values.

In area III with use of the algorithm of S.K.Godunov⁵ the calculation of flowing around of wing profile under zero angle of attack by stationary chemically inert airflow at Mach 10 is carried out. In calculations the influence of areas I and II on the solution was not taken into account; thus the received results show a degree of gas heating in passing through an oblique shock wave, and also serve as the boundary conditions for area IV.

In area IV the equation of two-dimensional laminar compressed boundary layer with non-uniform boundary conditions received from the solution of the Euler equations for area III was solved. It was supposed that there are no chemical reactions and air is unicomponent gas.

The calculations allow us to estimate the contribution of viscous friction at laminar mode of current into the heating of surface of wing profile. The heat-flux distribution q along the upper surface of wing profile of flight vehicle at constant

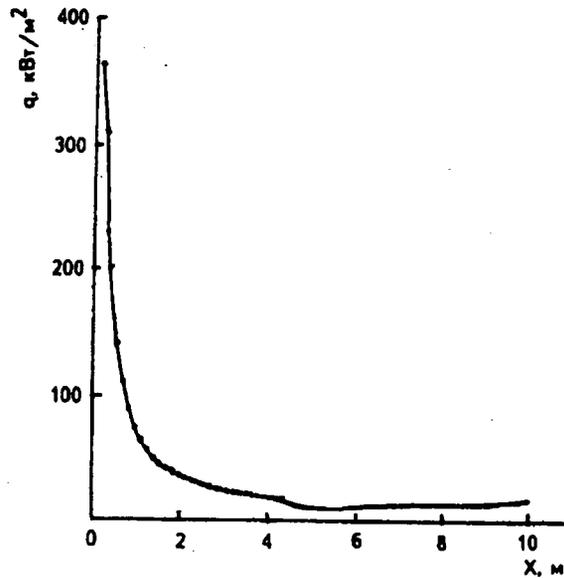


Fig. 4. Heat flow on the upper surface of wing profile

temperature of the surface $T_c = 273$ K is presented in Fig. 4.

The analysis of the received results for areas III and IV allows to make a conclusion that the contribution of viscous friction into a gas heating at laminar flow can reach 25% of total heat energy input into gas.

Flat TCR can be used as a unit of heat protection. This is parallelepiped ($L \gg h$); one of its walls (upper, for definiteness sake) is heated up outside; inner surface of this wall is covered with the catalyst (Fig. 5); the lower wall is heat-insulated. The uniformly intermixed mixture of gaseous

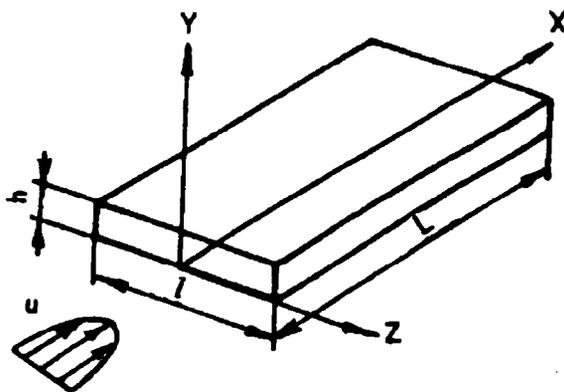


Fig. 5. The scheme of the thermochemical reactor and the coordinate system

hydrocarbon C_mH_n and vapors of water H_2O is fed into the inlet of TCR. The parameters of the mixture are given as follows:

P_{in} the pressure in the mixture, Pa;
 T_{in} the temperature in the mixture, deg C;
 V_{in} the mean flow-rate longitudinal velocity, m/s;
 G_{in} the flow-rate of the mixture, kg/s;
 ρ_{in} the mean density of the mixture, kg/m^3 .

TCR of various types used as units of heat protection of hypersonic flight vehicle should solve two usual tasks:

to provide utilization of heat flows with specific density from 50 kW/m^2 to 1 MW/m^2 , which occur on elements of flight vehicle at motion in atmosphere at Mach 6-10;

to produce hydrogen-containing fuel mixture having a specified chemical composition.

The aims of this numerical examination are the follows: determination of potentialities of flat TCR in utilization of heat flows having density up to 1 MW/m^2 ; definition of relation between chemical composition of the resulted fuel mixture and input parameters and limit density of heat flow.

To describe the flow in flat TCR a set of the Navier-Stokes equations in approximation of narrow channel is used. The validity of this model is justified⁶.

For the numerical solution of received set of partial differential equations, the method of generalized sweep⁷ was extended on a case of compressible currents.

The gas mixture going in TCR was considered as uniformly intermixed and heated; therefore T_{in} and the concentration of initial components at the inlet were set constant along the reactor height. The case of equilibrium currents (i.e. infinite high rate of chemical reactions) was explored.

At numerical examination the boundary conditions of 1-st or 2-nd kind on temperature were set. The application of boundary conditions of 1-st kind allows defining heat flow, which is absorbed by a concrete gas mixture at given input parameters. The statement of boundary conditions of 2-nd kind without the solution of conjugate task is physically incorrect in this case; however it allows to estimate level of maximal temperatures in solid body for heat flows of various intensity in combination with parameters determining the current of the gas mixture. Both laminar and turbulent modes of the flow were considered. At turbulent mode conventional "quasi-one-dimensional" approximation was used; in doing so the effective viscosity was determined as the sum of laminar and turbulent viscosities; the latter was calculated by the Prandtl formula in view of interaction between molecular and molar transfers. In calculations all input parameters and geometrical sizes of TCR, boundary conditions

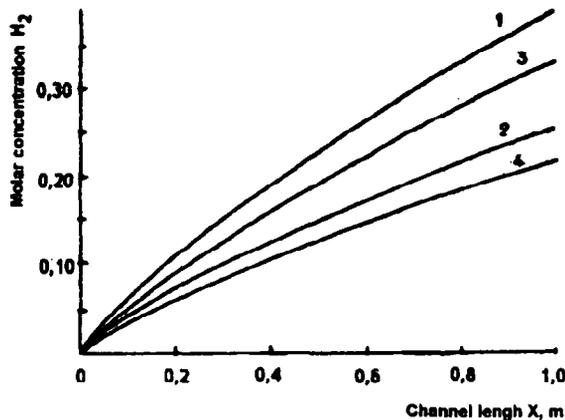


Fig. 6. The distribution of molar concentrations H_2 along the length of the channel. Turbulent chemically-reacting mixture. Parameters of the flow:

$$T_{in} = 400 \text{ deg C}; T_x = 1000 \text{ deg C};$$

$$h = 5.0 \text{ mm}; P = 0.2 \text{ MPa};$$

- 1: $V = 50 \text{ m/s}$, $G = 0.15 \text{ kg/s}$, $H_2O_{in} = 0.425$, $CH_{4in} = 0.575$;
- 2: $V = 50 \text{ m/s}$, $G = 0.15 \text{ kg/s}$, $H_2O_{in} = 0.725$, $CH_{4in} = 0.275$;
- 3: $V = 100 \text{ m/s}$, $G = 0.3 \text{ kg/s}$, $H_2O_{in} = 0.425$, $CH_{4in} = 0.575$;
- 4: $V = 100 \text{ m/s}$, $G = 0.3 \text{ kg/s}$, $H_2O_{in} = 0.725$, $CH_{4in} = 0.275$

for laminar and turbulent modes of current were varied in a wide range.

Selected results of calculations demonstrating an overall performance of flat TCR are presented in Fig.6-8. First two figures illustrate the tendency of changing the hydrogen concentration and the wall temperature along the channel. The calculation of heat flux absorbed by TCR 0.15 m in length and 5 mm in height at change of temperature of the mixture at the inlet for two values of mean flow-rate velocity V_{in} is displayed in Fig.8 a,b. From this figure we notice that when the velocity grows the heat

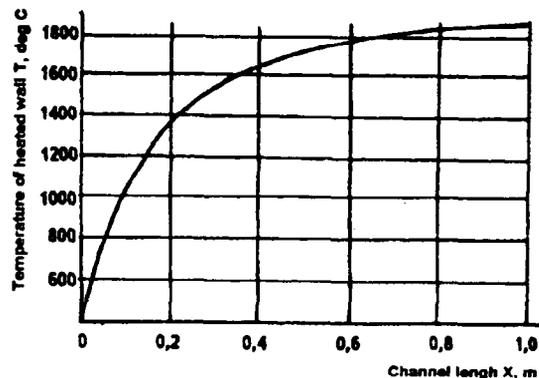


Fig. 7. Relationship between the temperature of heated wall T and the channel length X . Flow is turbulent, mixture is at stoichiometric relation. Flow parameters are as follows:

$$T_{in} = 400 \text{ deg C}, h = 5.0 \text{ mm}, Q_w = 0.3 \text{ MW},$$

$$V_{in} = 49.0 \text{ m/s}, P = 0.3 \text{ MPa}, G = 0.25 \text{ kg/s}.$$

absorption increases; the absorption falls with increase in input temperature. However, in the latter case the degree of methane reforming at the output of the reactor is little higher. This demonstrates role redistribution between convective and "chemical" components during heat removal from protected wall.

Based on the received calculations in approximations of the narrow channel it may be concluded that the flat thermochemical reactors are capable utilize heat flows up to 1 MW/m^2 .

Some design characteristics of thermochemical reactors based on planar catalysts are listed in Table 2.

To obtain the precise quantitative characteristics of TCR we need to research them on the basis of model of three-dimensional turbulent flow of chemically-reacting gas mixture in view of associated heat-mass-exchange.

In conclusion it may be said that the technology described above can find application in various industries using hydrocarbon fuel, such as:

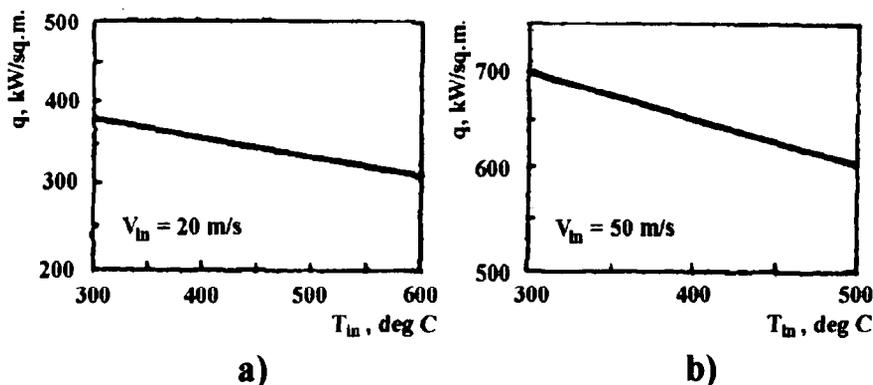


Fig. 8. The heat flow absorbed by the reactor in relation to the mixture velocity at the inlet: a) $V_{in} = 20 \text{ m/s}$; b) $V_{in} = 50 \text{ m/s}$

- transport energetics (internal-combustion, gas-turbine and air-breathing engines);
 - stationary gas-turbine installations on thermal electric generating stations and thermal technical devices (furnaces, dryers etc.);

- devices for transformation and accumulation of heat of nuclear power plant and solar energy;
 - chemical industry (producing of hydrogen, ammonia and other products of organic synthesis).

Heat flow density, MW/m ²	up to 1
Mean flow-rate speed, m/s	1-50
Hydraulic resistance, Pa/m	10 ³
Work temperature, deg C	700-900
Pressure, Pa	up to 5·10 ⁵
Height of flat TCR, mm	2-5
Specific weight of panel made from:	
heat-resistant steel, kg/m ²	≤18
composites, kg/m ²	≤10

Table 2. Calculated characteristics of TCR

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