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COMPLEX OF PROGRAMS FOR IMITATIVE SIMULATION OF ACCELERATION, HEATING, AND MELTING OF PARTICLES IN GAS-DYNAMIC CHANNELS OF TECHNOLOGICAL DEVICES

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This paper describes an interactive complex of programs designed for investigating the processes of acceleration, heating, and melting of particles in the gas-dynamic channels of burners. To illustrate the efficiency of this method, we have investigated the possibility of melting of tungsten particles in the process of their acceleration and heating by combustion products of hydrocarbon fuel in the gas-dynamic channel of the burner with the discharge method of acting on the flow.

Technological devices of flame spraying, abrasive working of surfaces, and jet grinding of solid particles are characterized by the following physical picture of the processes [1]. Particles together with hydrocarbon fuel combustion products are fed into a gas-dynamic channel in which they are accelerated, heated, and, if necessary, melted. An additional acceleration of particles takes place in a free supersonic jet. Carrier gas acceleration in the gas-dynamic channel is realized under the geometric and (or) discharge action on the flow. Completing processes take place in the shock layer formed by the collision of a two-phase jet with the surface being worked or the collision of jets. In investigating the processes of acceleration, heating, and melting of particles by a gas flow, these thermodynamic processes should be considered with regard for the heterogeneous interaction of phases, chemical transformations, phase transitions, etc., proceeding at the high rate and high temperatures attained in combustion of hydrocarbon fuels in air or pure oxygen.

Experimental development and the choice of parameters of technological devices entail problems connected with the difficulties of creating heterogeneous flows and measurement of the parameters of fast high-temperature processes and require considerable material costs. An effective means for reducing working costs and optimizing technological devices and the choice of rational regimes of their operation is offered by the methods of mathematical, mainly numerical, modeling [2–4]. The employment of these methods for modeling processes in technological devices requires an interrelated solution of a large number of individual rather complicated problems, each of which, being a part of a complex problem, can be of interest in itself. This necessitates a rational choice of the gas-dynamic and heat- and mass-exchange processes to be taken into account and the choice of mathematical models describing these processes with the required accuracy. At this stage, the task of the investigations is, on the one hand, the formulation of the physical and mathematical models that allow one to describe the technological process as completely as required for practice. On the other hand, it is necessary to develop effective algorithms and software based on them, which permit calculations on available computers at practically reasonable expenditures of machine time.

Serial calculations and especially adjustment and use, in solving a specific problem, of the already developed software-methodological means requires from the user certain skills and knowledge in the field of programming and mathematical modeling. Users of such programs are, as a rule, specialists in the field of development and improvement of technological processes, who know their specific features and deal mainly with their implementation. They perform investigations of the processes on the basis of the analysis of the relationship between the input (control) and output parameters. The complex of applied programs seems to them to be a kind of a tool of imitative modeling, which permits forming the initial data with allowance for their influence on the proceeding of the technological process, its efficiency, the quality of products of the technological process, etc.

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In this connection, the user should be provided with the possibility of working with the complex of programs in his usual regime, i.e., at the level of input and output data. With an adequate complex of applied programs, a tool for providing this is an interface organized in a certain way enabling the user to work with the program complex with the use of terms and definitions from the subject field of assignment of the complex. This interface together with the auxiliary programs forming the service part of the program complex should make it possible to form and store the initial data, perform current calculations, and process, store, and analyze the calculation data. Owing to the well-developed service part, practical work with the complex does not require from the user any special training in the field of programming and learning of special instructions for working with the complex.

The user works with the complex in the interactive regime and his work is reduced to a certain sequence of operations: problem choice; formation of initial data of the problem in accordance with the presented prototype of their defaults; choice of the form of data presentation from the list of forms of problem-solution processing offered by the complex; problem start for counting; representation of results of the chosen problem solution on the monitor screen in the form of numerical or graphical information depending on the chosen forms of solution processing; organization of storage of current calculation results in the bank of results; matching of obtained calculation results with the results of solving other problems (if any) or with the previously obtained results of the chosen problem at other initial data.

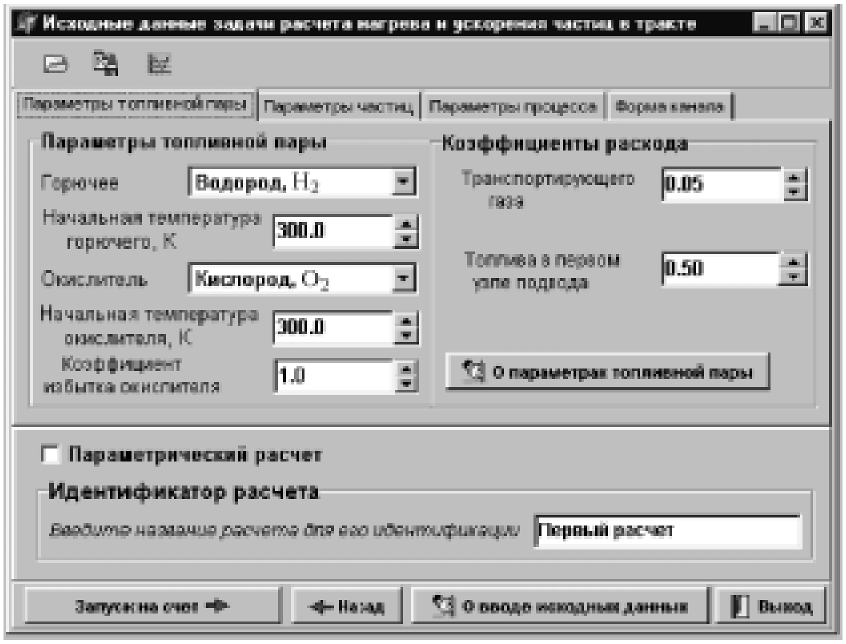
"Two_Phase" Imitative Modeling Program Complex. As a specific example of the software satisfying these requirements, consider the "Two_Phase" program complex [5, 6]. Structurally, the program complex consists of two relatively independent parts. The first part includes applied programs for numerical realization of mathematical models of the processes of acceleration, heating, and melting of particles when they are moving in the gas-dynamic channel and in a supersonic jet leaking onto the substrate. These programs are included in the "Two_Phase" complex in the form of executable EXE-files. The second part is a service shell developed in the Delphi medium as a supplement to Windows.

The programs of the first part are written in the Fortran algorithmic language. The basic elements of the mathematical models used and the algorithms of their numerical realization are given in [1–3]. The two-phase flow in the gas-dynamic channel is described by quasi-one-dimensional equations of the gas dynamics, which take into account the friction and the heat exchange of the two-phase flow with the channel walls, as well as the friction and the heat exchange between the phases. For the flow in a free two-phase jet, two-dimensional equations of the turbulent boundary layer for the gas phase and two-dimensional equations of the hyperbolic type for the dispersed phase are used. Numerical integration of equations is carried out by the matching method along the jet axis. The calculation of the two-phase flow parameters in the shock layer is performed in two stages. First the parameters of the gas phase are calculated by the established method. Then control particles, whose parameters are calculated along their mechanical trajectory, are placed in the gas flow field. In so doing, the influence of the particles on the gas flow parameters is not taken into account.

The second (service) part is a set of visual components (window forms, text windows, command buttons, keys, etc.) and ad hoc software. The window form conforms to the Window operating system. These windows, together with the visual components placed in them, are a tool for choosing problems, forming the initial data, carrying out a comparative analysis of results, storing them and using in Windows applications (Microsoft Word, Excel, etc.). Window forms appear on the screen sequentially as needed in the process of the user's work with the program. On the screen, there appears and is active only that form that enables one to carry out works with the active program necessary for the current stage. Transition to the next form (upon completion of all necessary operations in the current form) or return to the previous form (possibly for making corrections) is done upon pushing proper keys.

Functioning of the window forms and other visual components is provided by programs written in the Object Pascal algorithmic language. Moreover, a constituent of the complex consists of programs realizing the algorithms of preparation of initial data files for the applied program, using the information input by the user into the text windows, and programs providing applied program start, visual representation of obtained results in the form of graphic dependences, tables, etc. These programs maximally use objects of the integrated medium Delphi.

The complex is equipped with a ramified reference system providing the user with: information about its assignment and structure; a brief description of the physical and mathematical formulation of the problems to be solved; description of the possibilities of initial data formation and storage, performing current calculations, and processing and storage of calculation results. The service part of the complex enables the user to work in the interactive dialogue re-



Параметры топливной пары

Горючее: Водород, H_2

Начальная температура горючего, К: 300.0

Окислитель: Кислород, O_2

Начальная температура окислителя, К: 300.0

Коэффициент избытка окислителя: 1.0

Коэффициенты расхода

Транспортирующего газа: 0.05

Топлива в первом узле подвода: 0.50

☐ Параметрический расчет

Идентификатор расчета

Введите название расчета для его идентификации: Первый расчет

Fig. 1. Window form of initial data specification [Исходные данные задачи расчета нагрева и ускорения частиц в тракте = Initial data of problem of calculation of heating and acceleration of particles in channel; Параметры топливной пары = Fuel pair parameters; Параметры частиц = Particle parameters; Параметры процессов = Process parameters; Форма канала = Form of channel; Горючее = Combustible; Коэффициенты расхода = Discharge coefficients; Начальная температура горючего = Initial temperature of combustible; Окислитель = Oxidizer; Начальная температура окислителя = Initial temperature of oxidizer; Кислород = Oxygen; Водород = Hydrogen; Коэффициент избытка окислителя = Excess oxidizer coefficient; Транспортирующего газа = Transporting gas; Топлива в первом узле подвода = Fuel in the first feed unit; О параметрах топливной пары = About fuel pair parameters; Параметрический расчет = Parametric estimate; Идентификатор расчета = Estimate identifier; Введите название расчета для его идентификации = Enter estimate name for its identification; Первый расчет = First estimate; Запуск на счет = Start count; Назад = Back; О вводе исходных данных = About initial data input; Выход = Escape].

gime using terms and definitions from the object region of the complex assignment. As an illustration, Fig. 1 gives one variant of the window form providing initial data specification.

The application of the "Two_Phase" program complex permits investigating the thermal-gas-dynamic processes in the channels of gas-dynamic devices with the aim of providing a more effective use of the chemical energy of the fuel for heating and accelerating particles and choosing rational geometric parameters of gas-dynamic channels and regime parameters of technological devices. The "Two_Phase" complex makes it possible to:

a) estimate the discharge characteristics of the device and the gas-dynamic and thermophysical characteristics of combustion products;

b) estimate the range of change in the dynamic and energy parameters of particles in the gas-dynamic channel, in the jet, and in the shock layer;

c) calculate the distribution of the gas and particle parameters in the gas-dynamic channel, as well as in the flow field of the two-phase jet flowing from it;

d) choose the values of the geometric and regime parameters of the gas-dynamic channel for obtaining maximum values of the energy parameters of particles;

e) calculate the composition of combustion products and their thermodynamic and thermophysical properties;

f) calculate the thermal state of the dispersed phase (temperature field, melt fraction) when it is moving in the gas-dynamic channel, in the free jet, and in the shock layer.

The user can represent calculation results in the form of tables of parameters at the exit from the gas-dynamic channel at various values of the input parameters of the problem; graphs of distributions of gas-dynamic parameters along the gas-dynamic channel or the jet axis; graphs of parametric dependences of flow parameters at the exit from the gas-dynamic channel on the values of one of the input parameters of the problem; fields of isolines of flow parameters in the gas-dynamic channel and (or) the jet.

Evaluation of the Possibility of Melting of Tungsten Particles in the Gas-Dynamic Channel. As an illustration of using the "Two_Phase" program complex, below we give the results of exploring the possibility of melting of tungsten particles upon their acceleration and heating in the gas-dynamic channel of a burner with the discharge method of acting on the flow. These results can be used in developing a technology for spraying refractory coatings. Melting of tungsten particles features commensurability of their melting temperature to the equilibrium stagnation temperature of fuel combustion products. Therefore, melting of tungsten particles in the gas flow is only possible with a certain selection of the fuel pair (combustible–oxidizer) and with an effective organization of the energy exchange between fuel combustion products and particles.

It is expedient to carry out preselection of the fuel pair using the concepts of stored heat and relative stored heat of combustion products [4]. The stored heat is defined as the difference of values of the specific enthalpy of combustion products calculated at their equilibrium temperature and the melting temperature of particles. The relative stored heat is defined as the ratio of the stored heat to the heat that should be supplied to one kilogram of particles in order to heat them to the melting temperature and melt. In principle, it is equal to the mass of particles that can be heated and melted by one kilogram of combustion products at a completely stagnant flow. From the data on comparison of the parameters of the combustion products of hydrogen, methane, and acetylene in air oxygen given in [4] it follows that for refractories whose melting temperature is above 3000 K, the highest stored heat is possessed by the combustion products of acetylene in oxygen. Estimates of this heat were made proceeding from the following values of the diagnostic variables: pressure in the combustion chamber P_0 = 0.8 MPa; temperature and specific melting heat of tungsten T_m = 3660 K and Q_m = 191 kJ/kg [7–10]; the equilibrium temperature T_e and specific heat capacity $C_{p\mathrm{e}}$ at a constant pressure of combustion products of acetylene in oxygen were, respectively, 3696 K and 10.1 kJ/(kg·K). To heat and completely melt 1 kg of tungsten particles having an initial temperature of 298 K, it is necessary to expend a quantity of heat equal to 812.4 kJ/kg. Proceeding from this, we obtain values of the stored heat of combustion products Q^* = 363.6 kJ/kg and of the relative stored heat m^* = 0.447. Thus, 1 kg of combustion products can melt 0.447 kg of particles in the combustion chamber (at a completely stagnant flow).

In the case of a flow in the gas-dynamic channel of the burner, the flow of combustion products is accelerated, cooling thereby. Therefore, the real relative mass of melted particles will be much smaller. Depending on the mass fraction of particles, the fuel energy may turn out to be insufficient for complete melting of particles. As a parameter on the basis of which estimates of the possibility of particle melting in a high-temperature gas flow can be made, it is expedient to use the concept of the degree of particle melting η. This parameter is defined as the difference of the current specific enthalpy of particles and the specific enthalpy of unmelted particles at the melting temperature divided by the specific melting heat. Values of the parameter $\eta \le 0$ correspond to the solid aggregate state of particles, $0 < \eta < 1$ — to the transient state (partial melt of particles), $\eta = 1$ — to complete melting at a temperature equal to the melting temperature, and $\eta > 1$ — to melting with superheating.

A detailed analysis of the possibility of melting of tungsten particles was performed upon their acceleration and heating in the gas-dynamic channel of combustion products of fuel pairs acetylene + oxygen and hydrogen + oxygen at various combustion chamber pressures and sizes and mass fractions of particles. The characteristics of the gas-dynamic channel are given in [4]. Figure 2 shows the change in the melting ratio of particles of fraction D_p = 10 μm along the gas-dynamic channel at pressures in the combustion chambers P_0 = 0.8, 1.5, and 2.0 MPa for two variants of fuel pairs of acetylene + oxygen and hydrogen + oxygen fuel pairs at a mass fraction of particles K_p = 0.1. From Fig. 2 it is seen that for the acetylene + oxygen fuel pair with increasing combustion chamber pressure P_0 the melting ratio of particles markedly increases. For the hydrogen–oxygen fuel pair, an increase in the combustion chamber pressure has a negligible effect on the melting ratio of particles. Moreover, as is seen from Fig. 2, the hydrogen + oxygen fuel pair does not provide complete melt of particles even at an increased pressure in the combustion chamber. The

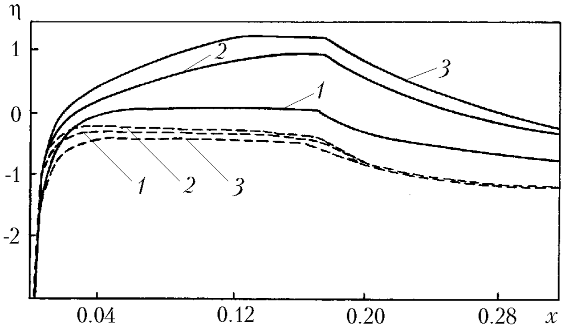
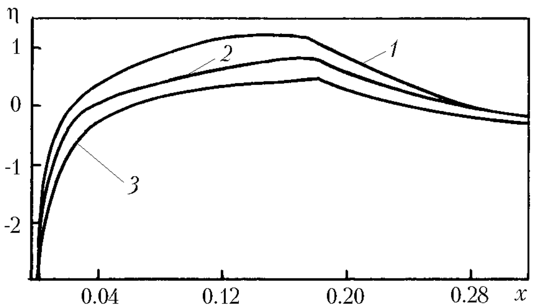


Fig. 2. Change in the melting ratio of particles along the gas-dynamic channel for acetylene + oxygen (solid curves) and hydrogen + oxygen (dashed curves) fuel pairs at combustion chamber pressures: 1) P_0 = 0.8; 2) 1.5; 3) 2.0 MPa. x, m.



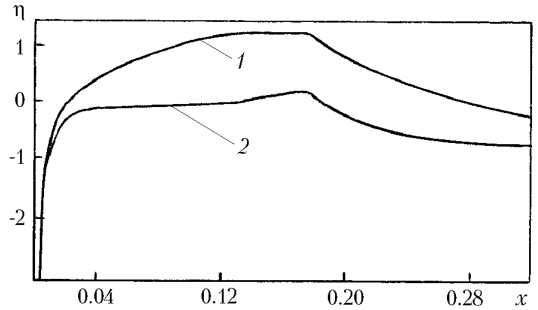


Fig. 3. Change in the melting ratio of particles along the gas-dynamic channel: 1) D_p = 10; 2) 15; 3) 20 μm. x, m.

Fig. 4. Change in the melting ratio melt of particles along the gas-dynamic channel at a mass fraction of particles: 1, K_p = 0; 2, 0.5. x, m.

results presented corroborate the conclusions obtained on the basis of the estimates of the stored heat of combustion products. Thus, to melt tungsten particles in the process of their acceleration and heating in the gas-dynamic channel with the discharge method of acting on the flow, it is necessary to use the acetylene + oxygen fuel pair at an increased pressure in the combustion chamber (as normal pressure, P_0 = 0.8 MPa is taken).

The influence of particle sizes on the relative melting ratio at a mass fraction of particles K_p = 0.1 and a combustion chamber pressure P_0 = 2.0 MPa is shown in Fig. 3. The change in the melting ratio of particles of fraction D_p = 10 μm along the gas-dynamic channel at a combustion chamber pressure P_0 = 2.0 MPa for two values of the coefficient of the mass fraction of particles K_p = 0.1 and 0.5 is illustrated in Fig. 4. A strong dependence of the melting ratio of particles on their mass fraction is observed. It should be noted that with increasing K_p the temperature and velocity of particles in the outlet cross section decrease, and the particle velocity thereby changes insignificantly. The results presented in Fig. 4 show that the melting ratio of particles increases with increasing pressure P_0 in the combustion chamber. The complete melting ratio can be positive on the end of the heating section; however, on the end of the section of supersonic acceleration (of length $L_{s.c}$ = 120 μm) it becomes negative. Therefore, to provide complete melting of particles ($\eta > 0$) at the exit from the gas-dynamic channel, it is necessary to increase the pressure P_0 in the combustion chamber and reduce the length of the section of supersonic acceleration $L_{s.c}$.

CONCLUSIONS

1. Analysis of the results presented permits the conclusion that to provide complete melting of tungsten particles at the exit from the gas-dynamic channel of a burner with the discharge method of acting on the flow, it is necessary to use the acetylene–oxygen fuel pair at a combustion chamber pressure $P_0 \approx$ 2.0 MPa, having minimized the length of the section of supersonic acceleration $L_{s.c}$. Under these conditions, it is possible to completely melt small-fraction particles ($D_p \le 15$ μm) at their relative mass fraction K_p of no more than 0.1. The particles thereby practically

do not influence the gas-dynamic field of the flow in the channel. An increase in the flow rate of particles leads to a decrease in their melt at the exit from the gas-dynamic channel.

2. The results presented in the present paper and in [3, 4] confirm the efficiency of using the "Two_Phase" program complex for imitative modeling of the processes of gas-dynamic acceleration, heating, and melting of particles. The complex comes in the form of a program product and can be disseminated among specialists engaged in the development and use of appropriate technological devices.

NOTATION

C_{pe}, equilibrium specific heat capacity of combustion products at a constant pressure, kJ/(kg·deg); D_p, particle diameter, μm; K_p, mass fraction of particles; $L_{s.c}$, length of the supersonic cylindrical section of the channel, m; m^*, relative stored heat; P_0, static pressure in the combustion chamber, MPa; Q^*, stored heat of combustion products, kJ/kg; Q_m, specific melting heat of tungsten, kJ/kg; T_e, equilibrium temperature of combustion products, K; T_m, melting temperature of tungsten, K; η, melting ratio of particles. Subscripts: e, equilibrium; m, melting; p, particle; s.c, supersonic channel; 0, initial value.

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