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DEVELOPMENT OF A SYSTEMS APPROACH TO THE SOLUTION OF PHYSICOCHEMICAL GASDYNAMICS PROBLEMS

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An automated system for numerical solution of certain problems of physicochemical gasdynamics is developed. The system includes the following main elements: structured physicochemical databases, a generator of kinetic equations of vibrational relaxation and chemical reactions, programs for direct solution of equations of gasdynamics with kinetic equations, a program module for building a compact mechanism of leading processes, and a module for selecting an optimum solution from the set of permissible ones. A variational problem of physicochemical gasdynamics connected with finding the best profile of an ultrasonic nozzle is solved.

The development of methods for solving problems of physicochemical kinetics has led to the necessity of putting these studies on a qualitatively new level and developing methods for forming mathematical models. This approach should not only free the investigator from the painstaking job of setting up kinetic equations but also provide an implementation of a unified direction of the mathematical technology of problem solving – from posing a problem, choosing models, and providing the complete necessary information on physicochemical data, to the promptly formed software complexes suitable for the solution of the problem posed.

A large amount of data characterizing processes which take place in a gaseous medium has been acquired in experimental and theoretical investigations in the field of physicochemical kinetics. They are to some extent systematized and presented in numerous reviews and handbooks [1-4].

A gas flow is usually accompanied by nonequilibrium physicochemical processes (chemical reactions, vibrational and rotational relaxation, etc.) which sometimes can substantially change the pattern of the flow field as compared to a model of an ideal gas with a constant adiabatic exponent.

A number of problems of physicochemical gasdynamics are well described when chemical and plasmochemical reactions and energy relaxation of vibrational levels of polyatomic molecules are taken into account. It is assumed in this case that the Maxwell distribution over velocities is conserved for translational degrees of freedom, rotational degrees of freedom are in equilibrium with the translational ones, the vibrational mode is modeled by a harmonic oscillator, and that energy exchange takes place much faster within each mode than the intermode (VV′) and vibro-translational (VT) exchange and chemical reactions.

A system of kinetic equations describing physicochemical processes in a gas can formally be presented as follows:

$$dc_i/dt = (1/\rho) \sum_{j=1}^{m} (\nu_{ij}^{-} - \nu_{ij}^{+}) W_j, \quad de_i/dt = Q_{VT}^{i} + Q_{VV'}^{i} + Q_{CV}^{i},$$

where c_i are the molar-mass concentrations of chemically reacting components; ρ is the density of the gas mixture; W_j is the rate of the j-th reaction, $e_i = 1/[\exp(\Theta_i/T_i) - 1]$ is the vibrational energy characterizing the average number of vibrational quanta of the i-th type per molecule. The first term on the right-hand side of the change of the vibrational energy Q_{VT}^{i} accounts for the vibro-translational (VT) exchange, the second one, $Q_{VV'}^{i}$, accounts for

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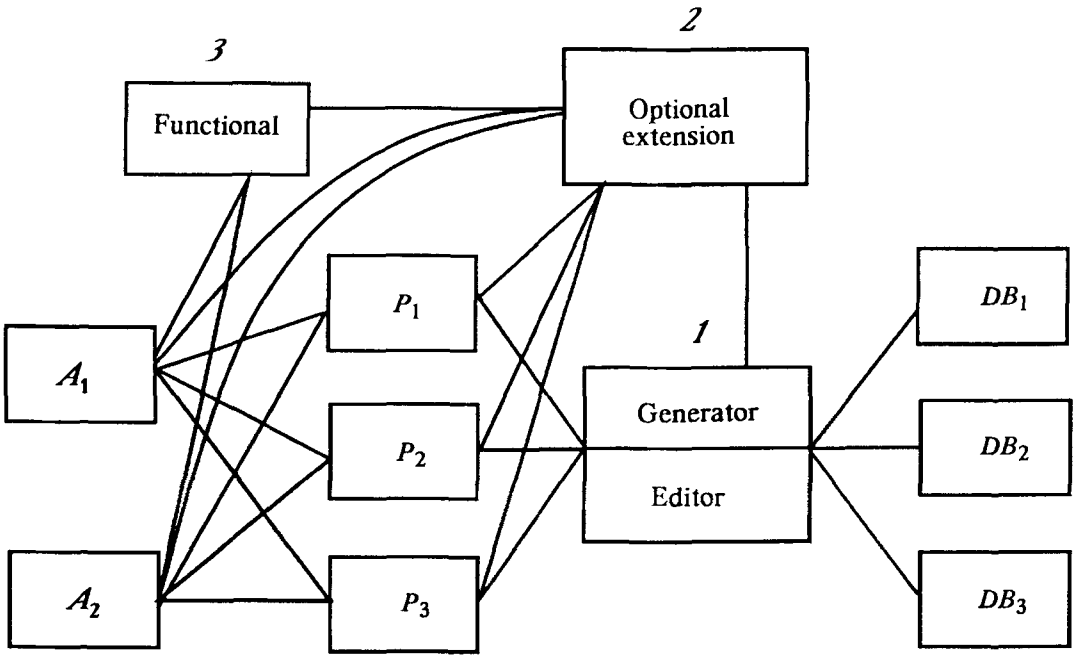

Fig. 1. Flow diagram of interaction of generator of equations of physicochemical kinetics with databases DB_i, programs P_k, and units A_j.

the intermode (VV′) exchange, and Q^i_{CV} is the change in the vibrational energy due to chemical reactions with the participation of vibrationally excited molecules (the CV process). The terms Q^i_{VT}, $Q^i_{VV'}$, and Q^i_{CV} are obtained from a system of microkinetic balance equations by convolution, and their final form can be found in [5, 6].

1. The solution of problems of gasdynamics with physicochemical transformations using a database of the kinetic equations generator implies a particular choice of both gasdynamic equations (flow in a channel, behind a shock wave, etc.) and elementary processes. However, in most cases, one must take into account a considerable number of chemical reactions and channels of vibrational relaxation. Setting up of kinetic equations for the transitions specified is a painstaking job and the probability of error is high. In transition in a program for calculations with unformalized kinetics to a new system of physicochemical data or when extending or modifying a program which is already in use, one must code the equations describing nonequilibrium processes again.

The need for automation of kinetic-equation modeling has led to the development of generators which form the right-hand sides of differential equations describing nonequilibrium processes. Generators of the type have been developed for equations of both chemical kinetics [7] and mode vibrational kinetics [8]. However, the solution of a number of problems of physicochemical gasdynamics is possible only with joint allowance for equations of chemical kinetics and vibrational relaxation.

In this connection, an all-purpose generator of the right-hand sides of kinetic equations was developed which makes it possible to model the following transformations: chemical and plasmochemical reactions (including those involving particles in particular electronic states), radiation transitions, vibro-translational VT energy exchange, vibrational-vibrational VV′ energy exchange between various vibrational modes, and the CV process, taking into account the effect of chemical reactions on the change in the vibrational energy. The universal character of the generator consists in the fact that the right-hand sides of equations describing nonequilibrium processes in a gas are formed on the basis of a symbolic record of processes in the form of a conventional molecular kinetic formula. A complete list of the channels taken into account along with the rate constants is stored in the form of a separate database. Thus, the kinetic equations are formed of the data level of mathematical modeling, when the data elements are stored in the database in a structured form. This form of presentation of the information in the database is necessary for real-time storage and data processing and user-oriented manipulation.

A built-in editor of the generator is used to check the physicochemical database and verify whether it complies with the format adopted.

The interaction of particular programs and databases is shown in Fig. 1. Here DB_1, DB_2, DB_3, ... stand for various databases on physicochemical kinetics; P_1, P_2, P_3, ... are programs for direct calculation which use databases DB_i to form kinetic equations; 1, equation generator with built-in editor; 2, optional extension of automated system (vide infra); A_1, A_2, ... are program modules that use programs for the direct calculation P_k (and databases DB_i, respectively) as subroutines and are developed for the solution of problems of physicochemical gasdynamics more complex than the solution of a direct kinetic problem. In the course of computations, program modules A_j generally call several programs P_k repeatedly. The object under investigation in the module A_j is also connected with the particular form of a certain functional calculated in module 3. The role of A_j is played in the system by a module for choosing leading processes [9] or a model capable of solving variational problems of gasdynamics with regard for relaxation processes. A mini-DBMS is built-in to each of the programs P_k, which, according to criteria given, can copy a portion of the main kinetic database.

Optional extension module 2 is of particular interest. The user can enter this part of the system from both the generator and programs P_k and modules A_j. This system module is called when separate fragments of the algorithm of the solution of the problem do not fit into the standard scheme and nonstandard elements are built-in to module 2.

2. With the use of the system, we, in particular, have solved a variational problem of gasdynamics with physicochemical transformations connected with determining the profile of an ultrasonic nozzle providing the maximum specific power of a gasdynamic CO_2 laser. In this case we used direct methods of the search for an optimum which are built-in to the system described in Section 1.

It should be noted that laser technology is entering new stage of development characterized by the application of high-power (10 kW and higher) lasers. These are powers at which high-speed laser welding and cutting of various metal structures (including thick-walled ones) and composite materials and deep (up to 2 mm) hardening become profitable [10].

The modern laser-based material processing technology utilizes mainly electric-discharge CO_2 lasers, which are effective in solving practical problems requiring powers below 5 kW. However, with increasing power, electric-discharge CO_2 lasers become bulky, difficult to manufacture, and expensive, and the beam quality worsens.

A number of problems facing laser technology can be solved by gasdynamic CO_2 lasers, which, having a power up to 100 kW, are compact, light, simple in design, and reliable in operation. Their power can easily be varied within wide limits. The beam quality of lasers of the type does not change with increasing power from 10 to 100 kW and is close to the best possible [10].

Results of optimization of a gasdynamic CO_2 laser containing CO_2, N_2, and H_2O molecules in the active medium point to the possibility of obtaining high values of lasing power per unit gas consumption W [11]. For example, with the pressure in the mixing chamber $p_0 \approx 1$ MPa, calculations substantiate the possibility of obtaining $W \sim 60$ kJ/kg. However, the optimum parameters is this case cannot always meet requirements of the manufacturer. In particular, in the optimum mode, the gasdynamic laser (GDL) should have a rather high initial temperature T_0 and pressure p_0 at the entrance to the nozzle grid, and optimum nozzles are characterized by large opening angles in the region of the geometrical crisis. The degree of expansion at the exit from the nozzle is about several tens (and sometimes exceeds a hundred).

At larger opening angles in the region of the geometrical crisis of the nozzle with subsequent transition to a plane-parallel gas flow, problems of profiling of the ultrasonic nozzle with the aim of obtaining a shockless gas flow are unavoidable, since the emergence of density jumps can worsen substantially the characteristics of a gasdynamic laser. At a large expansion degree of the gas flow in an ultrasonic nozzle, problems of exhaustion of gases into the atmosphere, e.g., with the help of a diffuser mounted behind the cavity, are unavoidable.

In this connection an investigation of the possibility of operation of a GDL at smaller opening angles and flow expansion degrees in the ultrasonic nozzle, which makes it possible to solve problems connected with profiling of an optimum nozzle, is of considerable interest. This problem, from the theoretical standpoint, should most likely be solved by optimizing the GDL at small values of the above-mentioned parameters. We have presented a formulation of the optimization problem elsewhere [10]. Results of the solution of the problem are presented in Table 1.

TABLE 1. Optimum Values of Parameters in a Gasdynamic CO_2 Laser

n	α, m^{-1}	S	L_0, m	L_1, m	CO_2, %	H_2O, %	T_0, K	t	W, kJ/kg
0	6600	153	0.0455	0.001	10.02	1.75	2330	0.142	64.2
1	6600	50	0.0148	0.031	13.0	0.50	2320	0.157	55.6
2	5000	50	0.0196	0.0264	12.5	0.80	2300	0.152	54.2
3	3500	50	0.028	0.0223	11.00	1.30	2230	0.146	49.2
4	2000	50	0.049	0.013	8.20	1.50	2090	0.133	45.6
5	1000	50	0.098	0.022	5.20	1.25	1910	0.122	38.9
6	750	50	0.131	0.023	4.20	1.10	1850	0.117	36.4
7	500	50	0.196	0.034	3.40	0.85	1805	0.111	32.3

As an initial variant, we considered the gas mixture 10.02% CO_2 + 1.75% H_2O + 88.23% N_2 at T_0 = 2330 K, which corresponds to optimization conditions with the water vapor at a fixed value of initial pressure p_0 = 1 MPa (in a one-dimensional stationary formulation). In this case the first row ($n = 0$) of the table corresponds to the complete list of optimum parameters. The column $\alpha = 2 \tan \theta/h_*$ (with θ being the initial opening angle) determines the nozzle opening in the region of the geometrical crisis. It is followed by three more parameters characterizing the optimum nozzle profile: the expansion degree of the flow at the exit of the nozzle S, the length of the nozzle L_0, and the length of its plane-parallel portion L_1 such that the profile tangent $dh/dx \equiv 0$ when $L_0 \le x \le L_0 + L_1$. Within the interval $0 \le x \le L_0$, the profile h was represented by a parabola with the conditions $h/h_* = S$ and $dh/dx = 0$ at the exit at $x = L_0$. The next two columns in the table list the molar fractions of CO_2 and H_2O (the rest composition is taken by N_2 molecules). Then the initial temperature T_0 at the entrance to the nozzle, the transmission coefficient t of the exit mirror of the cavity, and the maximum lasing power per unit gas consumption W in kJ/kg are listed in the Table. It was assumed that the cavity width across the flow and its length along the flow were both 1 m, and the coefficient of losses per two passes of the beam in the cavity was 0.03. With these parameters, calculations show a possibility to obtain the specific power W = 64.2 kJ/kg.

Information on how the specific power W decreases with a decreasing nozzle parameter $\alpha = 2 \tan \theta/h_*$ (i.e., with decreasing θ or increasing h_*) and expansion degree of the flow at the exit from the nozzle S is presented in the Table (variants $n = 1-7$). If the search for optimum W is carried out with α fixed at 6600 m^{-1} (which corresponds to the variant $n = 0$) but with the constraint $S \le 50$, the maximum value of W decreases by only 15.4% (in the search for an optimum, the quantity S reaches the boundary $S = 50$; see variant $n = 1$ in the Table). In this case, other values of the optimum parameters T_0, ξ_i, t, L_0, and L should be used.

Then nozzles with smaller values of the parameter $\alpha = 2 \tan \theta/h_* < 6600$ m^{-1} were considered, and the problem of finding maximum W with the additional constraint imposed on the expansion degree $S \le 50$ was solved for a fixed set of α (variants $n = 2-7$). Somewhat unexpected results were obtained in the calculations. In particular, when α decreases from 6600 m^{-1} to 500 m^{-1} (by more than an order of magnitude) and the expansion degree S decreases only from 153 to 50 (three times), the optimum value of W decreases only approximately two times. In this case the optimum value of the initial temperature also decreases from 2330 to 1805 K, and the nozzle length grows.

Thus, in the practical manufacture of CO_2 GDLs, instead of nozzles with a large expansion degree and large opening angles (and small values of the critical cross-section), one can use long (0.1–0.2 m) nozzles with an expansion not exceeding 50 and small values of $2 \tan \theta/h_* \le 1000$ m^{-1}. In this case the efficiency of the GDL remains high.

Figure 2 presents distributions of characteristics over the nozzle found in calculations under the assumption of a two-dimensional character of the flow. The flow field is obtained as a result of solving an inverse problem for a Laval nozzle. Data from the solution of the optimization problem in a one-dimensional formulation at $2 \tan \theta/h_* = 1000$ m^{-1} were used as a pressure distribution over the axis. The x-axis represents the dimensionless nozzle length x^1. Solid curves correspond to Mach numbers M (calculated from the effective adiabatic exponent), and

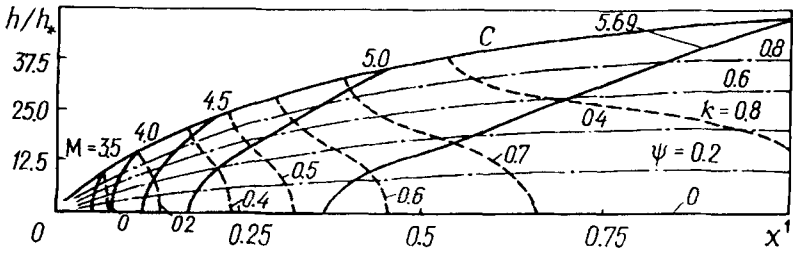

Fig. 2. Values of Mach number M (solid curves), optical amplification coefficient k (dashed curves), and flow function (dash-dot curves) in an ultrasonic nozzle of a gasdynamic CO_2 laser. Curve C presents the nozzle profile. Initial conditions correspond to variant $n = 5$ from Table 1.

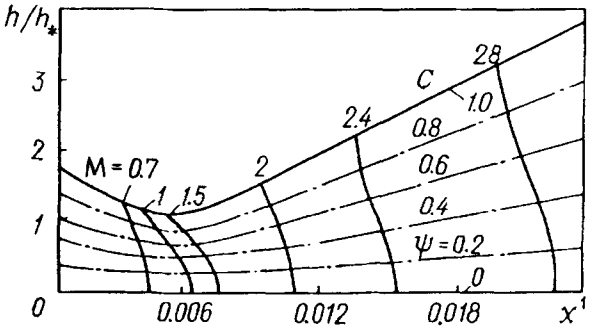

Fig. 3. Values of Mach number M (solid curves) and flow function (dashed curves) in an ultrasonic nozzle of a gasdynamic CO_2 laser in the region of the geometric crisis. Curve C presents the nozzle profile. Initial conditions correspond to variant $n = 5$ from Table 1.

dashed curves correspond to the distribution of the amplification coefficient k, m^{-1}, and these curves are crossed by dash-dot flow curves. Numbers near the flow curves correspond to relative values of the flow function ψ. The value of ψ that determines the nozzle profile is taken as unity. The nozzle height at the minimum cross-section $h_* = 0.00123$ m, and the maximum halfangle of the shape is $\sim 32^\circ$. It is evident that a rather uniform field is obtained at the exit from the nozzle, and the uniform character of the gas flow is conserved in the cavity. Flow lines and isolines of the Mach number in the region of the geometric crisis are presented in Fig. 3. A certain nonuniformity is observed in the field of emission intensity when the gas flows through the cavity. However, the total specific power W is exceeded by the corresponding value for one-dimensional flow by only 6%.

Thus, the automated system developed for the solution of problems of physicochemical gasdynamics, which includes a kinetic-equation generator, makes it possible to solve rather complex problems of reacting gas flow.

NOTATION

T, translational gas temperature; T_i, vibrational temperature of the i-th mode; VT, vibro-translational energy exchange; VV′, vibro-vibrational energy exchange between various modes; CV, chemical effect on vibrational relaxation; γ_i, molar fraction of the i-th component; Θ_i, characteristic vibrational temperature of the i-th mode; Q^i_{VT}, Q^i_{VV}, and Q^i_{CV}, change of vibrational energy due to VT and VV′ exchange and CV process, respectively; ν^+_{ij} and ν^-_{ij}, stoichiometric coefficients; T_0 and p_0, initial temperature and pressure at entrance of nozzle; h and h_* nozzle height at its arbitrary and critical cross-sections; x, distance along nozzle axis; ψ, flow function.

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