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USE OF A GENERATOR OF KINETIC EQUATIONS FOR SOLVING OPTIMIZATION PROBLEMS OF PHYSICOCHEMICAL GAS DYNAMICS

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A system of numerical solution of some physicochemical gas-dynamics problems is developed. The main elements of the system are a physicochemical database, a generator of kinetic equations of vibrational relaxation and chemical reactions, programs of direct calculation of gas-dynamic equations with kinetic equations, and program units for determining specific solutions of direct calculations.

The system developed is used to solve the variational problem of physicochemical gas dynamics related to the determination of the optimum contour of a supersonic nozzle.

Experimental and theoretical studies on physicochemical kinetics have provided a large body of data characterizing processes occurring in a gas medium; these data are systematized to a certain extent [1–5].

The rapid development of computers and numerical-simulation methods makes it possible to reach a qualitatively new level in solving problems of physicochemical gas-dynamics. This should relieve the researcher of the routine work of formulating kinetic equations and also ensure a unified mathematical line of solving problems — from formulation of a problem, choice of models, and full information on all necessary physicochemical data, to promptly formed program complexes used to solve the formulated problem.

A large number of problems of physicochemical gas dynamics are well described by taking into account chemical and plasma chemical reactions and the energy relaxation of vibrational modes of polyatomic molecules. It is assumed in this case that the Maxwellian speed distribution for the translational degrees of freedom is preserved, the rotational degrees of freedom are in equilibrium with the translational degrees of freedom, the vibrational mode is modeled by a harmonic oscillator, and, within each mode, the energy exchange proceeds much more rapidly than the intermode energy exchange (VV'), the vibrational–translational exchange (VT), and chemical reactions.

The system of kinetic equations describing the physicochemical processes in the gas can be written formally as

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

where c_i is the molar-mass concentration of chemically reacting components, ρ is the gas-mixture density, ν_{ij}^{-} and ν_{ij}^{+} are stoichiometric coefficients, W_j is the rate of the jth reaction, $e_i = 1/[\exp(\Theta_i/T_i) - 1]$ is the vibrational energy characterizing the average number of vibrational quanta of the ith type per one molecule, T_i is the vibrational temperature of the ith mode, and Θ_i is the characteristic vibrational temperature. The first term on the right side of the change in the vibrational energy Q_{VT}^{i} takes into account the vibrational–translational VT exchange, the second term $Q_{VV'}^{i}$ takes into account the intermode VV' exchange, and the third term Q_{CV}^{i} is the change in the vibrational energy due to chemical reactions involving vibrationally excited molecules (CV process). These terms are obtained from the system of microkinetic balance equations as a result of "convolution" (the form of these equations is given in [6, 7]).

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We consider the question of developing a generator of kinetic equations using databases for physicochemical kinetics. Solution of particular gas-dynamic problems with physicochemical transformations implies specification of choice of both gas-dynamic equations (flow through channel, flow behind a shock wave, etc.) and elementary processes. In most cases, however, one has to take into account a large number of chemical reactions and vibrational relaxation processes. In this case, the formulation of kinetic equations of the above-mentioned processes is a laborious problem, and the probability of an error or a slip is high. When one goes over to a new system of physicochemical data in the calculation program with nonformalized kinetics or extends and modifies the already used system, it is necessary to write again the kinetic part.

The necessity of automating the formulation of kinetic equations has led to the development of program generators that formulate the right sides of differential equations describing physicochemical processes. These generators were developed for equations of both chemical kinetics [8] and mode vibrational kinetics [9]. However, a number of problems of physicochemical gas dynamics can be solved only with simultaneous allowance for chemical-kinetic and vibrational-relaxation equations.

In this connection, a universal generator of the right sides of kinetic equations (1) was developed. It takes into account the following processes: chemical and plasma chemical reactions, the vibrational–translational energy exchange (VT process), the vibrational–translational energy exchange (VT processes), the vibrational–vibrational VV' process between different vibrational modes, the CV process with allowance for the effect of chemical reactions on the change in vibrational energy, and transitions with allowance for molecule emission. This generator is universal because the right sides of the kinetic equations are formed by writing symbolic equations of processes as the usual molecular formula. The full list of the processes taken into account together with rate constants is stored as a particular database. Thus, in transformation to another system of kinetic variables, only the name of database is changed.

The generator incorporates an editor for checking the physicochemical database used. The editor checks correct setting up of the database, verifies satisfaction of the general laws of conservation of mass, charge, and type of particles, and also diagnoses occasional duplication of elementary processes.

The informative logical scheme of interaction of the generator with the remaining components of the system incorporates the following arbitrary elements: physicochemical databases B_i ($i = 1, 2, \ldots$); direct calculation programs P_k ($k = 1, 2, \ldots$) using databases B_i for the formation of kinetic equations; the program units A_j ($j = 1, 2, \ldots$), which use the direct calculation programs P_k (and, accordingly, the databases B_i) as subprograms and are intended for the solution of more complex physicochemical gas-dynamic problems than the calculation of direct kinetic problems. To solve a problem, the program units A_j repeatedly refer to the programs P_k. The specific problem of the unit A_j is also related to a specific type of a certain functional calculated in a particular block. As the units A_j, the system includes the procedure of choosing the leading processes [10] or a procedure that enables one to solve variational problems of gas dynamics with allowance for relaxation processes. Each program P_k incorporates a mini SCDB (system of control of databases), which can copy part of the main database by the specified criteria. The block "nonstandard part" is of certain interest in the system. Entry to this block can be performed from both the generator and the programs P_k and units A_j. The block is referred to when particular fragments of the problem does not fit the standard scheme, an a nonstandard part is constructed additionally in the block. This block of the system is small, as a rule, and is programmed separately for each particular problem.

The system described above was used to solve the variational gas-dynamic problem with physicochemical transformations related to determination of a supersonic nozzle contour that ensures maximum specific power of a CO_2 gas-dynamic laser (GDL). The variational problem was solved by direct numerical methods of searching for an optimum incorporated into this system.

It should be noted that laser technology has reached a new stage of development which is characterized by the use of high-power lasers (10 kW and higher). GDL can be used industrially for welding of thick-walled structures, quenching at great depths, and cutting of high-melting materials. These laser should be compact, have a high-quality beam, and generate radiation with a power of 10–20 kW and higher [11].

The results of optimization of a CO_2 GDL containing CO_2, N_2, and H_2O molecules as a working medium indicate the possibility of obtaining high values of the specific generation power W per unit of gas

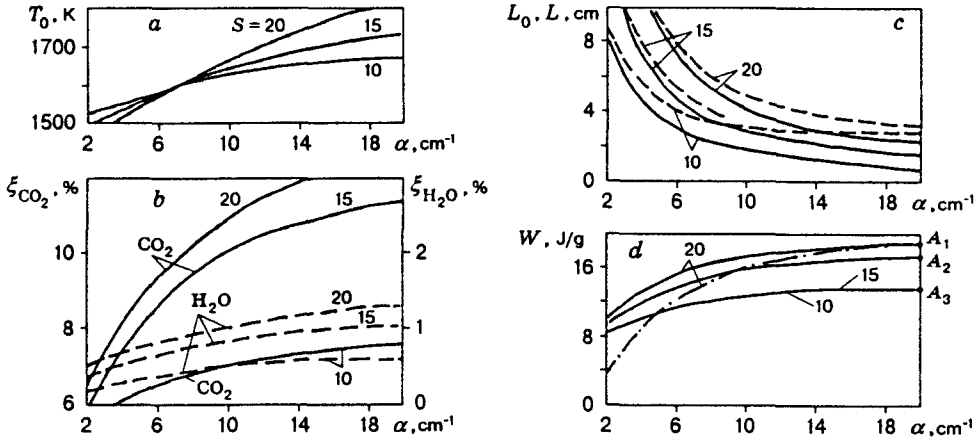

Fig. 1

consumption [12]. However, the thus-obtained optimum parameters do not always satisfy the producer. In particular, in the optimum regime, GDL should have sufficiently high initial temperatures T_0 and a high pressure p_0 at the nozzle-cascade entry, and optimum nozzles should have large divergence angles in the geometrically critical region (at the minimum section of the nozzle). The degree of flow expansion at the nozzle exit is several tens (sometimes more than one hundred) of units.

Large divergence angles in the geometrically critical region followed by transition to a plane-parallel gas flow inevitably lead to the problem of contouring a supersonic nozzle aimed at producing a shock-free gas flow, because the occurrence of shock waves can significantly deteriorate the characteristics of the gas-dynamic laser. For a large degree of supersonic nozzle gas flow expansion, the problem of discharging waste gases into the atmosphere, for example, by means of a diffuser placed behind the resonator, inevitably arises.

Thus, in practice, in the production of a CO_2 GDL, there are restrictions on the physical parameters of the system, which can decrease the laser power in comparison with "ideal" conditions.

In this connection, it is of interest to study the possibility of GDL operation at smaller divergence angles and a smaller degree of supersonic-nozzle flow expansion, which enable one to solve more successfully the problems related to contouring of an optimum nozzle. Theoretically, it is reasonable to solve this problem by optimization of GDL for low values of these parameters. This problem was formulated in [12]. The results of solution of the above-mentioned problem are given in Fig. 1.

Figure 1 shows the decrease in the specific power W caused by a decrease in the nozzle parameter $\alpha = 2\tan\Theta/h_*$ (i.e., by a decrease in the initial divergence angle Θ or an increase in height of the critical nozzle h_*) and the degree of flow expansion S at the nozzle exit. Here $L = L_0 + L_1$ (L_0 is the length of the supersonic portion of the nozzle and L_1 is the length of the plane-parallel portion of the nozzle) and $S = \text{const}$ for $L_0 \leqslant x \leqslant L_0 + L_1$. In the interval $0 \leqslant x \leqslant L_0$ the contour h is given by a parabola subject to the conditions

$$\frac{h}{h_*} = 1, \quad h_*^{-1}\frac{dh}{dx} = \alpha \quad \text{for} \quad x = 0, \qquad \frac{h}{h_*} = S, \quad \frac{dh}{dx} = 0 \quad \text{for} \quad x = L_0.$$

As the initial variant we considered a gas mixture of 157% CO_2 + 1.55% H_2O + 82.75% N_2 at the initial nozzle-entry temperature $T_0 = 1790$ K. This corresponds to optimization conditions for water vapor for fixed initial pressure $p_0 = 5$ atm. In this case, the optimum nozzle has $\alpha = 21.3$ cm^{-1} and $S = 35$ (for total nozzle length 4.8 cm). For these parameters, calculations show the possibility of obtaining $W = 19.9$ J/g.

In modeling the laser, we assumed that the distance between the mirror and the opposite wall and also the streamwise length of the resonator were 50 cm. The total loss of the beam (for two passages) amounts to 3%. If one seek the optimum of the specific power W by fixing $\alpha = 20$ cm^{-1} but restricting the degree of flow expansion to the conditions $S = 20$, 15, and 10, the maximum value of W decreases only by 4.7, 10.9, and 32.4%, respectively. In Fig. 1d, points A_1, A_2, and A_3 correspond to these values of W. In this case, it is necessary to use the optimum parameters T_0, ξ_i, t, L_0, and L_1, whose numerical values are determined from

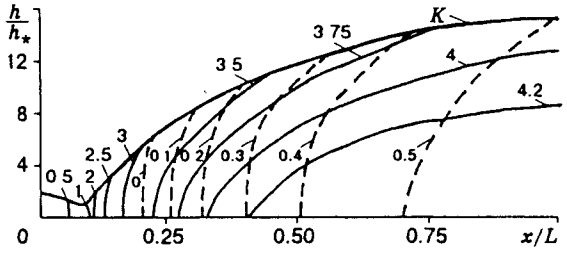

Fig. 2

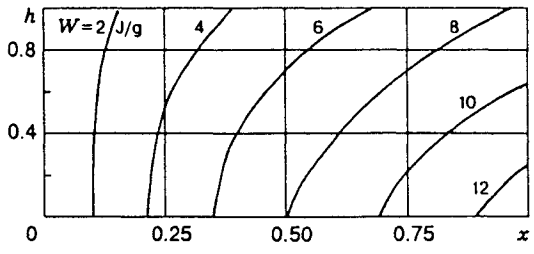

Fig. 3

Fig. 1a–c for $\alpha = 20$ cm^{-1} (ξ_i are the mole fractions of CO_2, H_2O, and N_2 and t is the transmission coefficient of the resonator's mirror).

Next, we consider nozzles with smaller values of the parameters α ($\alpha < 20$ cm^{-1}), and solve the problem of searching for the maximum of W with fixed values of the parameter and with additional restrictions on the degree of expansion $S = 20$, 15, and 10. The results of the solution of this problem are given in Fig. 1a–d. where figures at the curves correspond to the variant with the indicated value of the degree of flow expansion. Figure 1a shows the optimum initial temperature T_0, Fig. 1b shows the mole fractions of CO_2 and H_2O molecules, and the fraction of N_2 molecules is determined by subtracting the mole fractions of CO_2 and H_2 from 100%, Fig. 1c shows the nozzle length L_0 (solid curves) and the total length $L = L_0 + L_1$ (dashed curves), and Fig. 1d shows the specific power W. The optimum value of the transmission coefficient of the mirrors t changes in the range of 0.10–0.12 for $S = 20$, in the range of 0.085–0.105 for $S = 15$, and in the range of 0.07–0.075 for $S = 10$. The solution of the problem of searching for the maximum W yields somewhat unexpected results. The value of W gradually decreases as the quantity $\alpha = 2\tan\Theta/h_*$ decreases. For example, as α decreases by an order of magnitude from 20 to 2–3 cm^{-1} and the degree of expansion S decreases from 35 to 10, the optimum value of W decreases only by approximately a factor of two (Fig. 1d). Furthermore, the optimum value of the initial temperature T_0 also decreases from 1790 to 1540 K, and the nozzle length increases. For comparison, the dot-and-dashed curve in Fig. 1d shows the change in W with an immediate decrease in α ($S = 20$; optimization for the parameters T_0, ξ_i, t, L, and L_1 was not performed and they were fixed). For small values of $2\tan\Theta/h_*$, the specific power W can be slightly decreased by simultaneous optimization of the entire set of GDL parameters.

Figure 2 gives the nozzle-parameter distributions calculated under the assumption of a two-dimensional gas flow. The flow field was obtained by solving the inverse problem of a Laval nozzle. As the pressure distribution on the axis, the results of solution of the optimization problem in a one-dimensional formulation for $2\tan\Theta/h_* = 5$ cm^{-1} and $S = 15$ were used. The dimensionless nozzle length is plotted on the abscissa, and the ratio of the nozzle height h to the critical section h_* is plotted on the ordinate. The solid curves correspond to the same Mach numbers (calculated from the effective adiabatic exponent), and the dashed curves correspond to the distribution of the amplification coefficient, in m^{-1}. The height of the minimum nozzle section is $h_* = 2.51$ mm, and the maximum half-angle of the contour is ~32°. The curve denoted by the letter K describes the nozzle contour for $h_* = 2.51$ mm.

Figure 3 shows curves of the same specific power output W from the resonator. The resonator length is plotted on the abscissa and the resonator height is plotted on the ordinate (in relative unites).

The nonuniform radiation-intensity field distribution with allowance for the two-dimensional gas flow leads to a decrease in the power output from the resonator. The total specific power W is 19% smaller than the corresponding power of a one-dimensional flow. If a streamline with minimum critical section $h_* = 2$ and 1.5 mm is chosen as the nozzle contour, the difference in the specific power decreases from 13 to 7.5%, respectively.

Although, for such divergence angles at the nozzle exit and in the resonator, it is not possible to obtain a uniform gas flow, the small values of $\alpha = 2\tan\Theta/h_*$ allows one to use nozzles with a large critical section ($h_* \approx 2.5$ mm). This is important in the design of GDL, since, for the given gas-flow rate, the nozzle cascade

of the laser consists of a smaller number of elements (nozzles), and this, in turn, decreases the loss in the shock waves and in the wake (because of the boundary-layer flow from the nozzle walls) behind the back part of the nozzle cascade. In this case, the losses due to the deterioration of the optical homogeneity of the active medium in the resonator also decrease because of the change in the gas density.

Thus, in manufacturing CO_2 GDL, instead of nozzles with a large degree of expansion and large divergence angles (and small values of the critical section), one can use nozzles with expansion $S < 20$ and small values of the parameter $\alpha = 2\tan\Theta/h_*$ ($\leqslant 10$ cm^{-1}). For small values of the initial nozzle exit pressure ($p_0 \approx 5$ atm), the laser mixture has a relatively low initial temperature ($T_0 \approx 1500$–1700 K). In this case, the GDL efficiency remains low.

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