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# ON THE DEVELOPMENT OF A KINETIC MODEL FOR A GAS WITH ALLOWANCE FOR NONEQUILIBRIUM PROCESSES

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*The problems of developing a kinetic model of a medium (gas and plasma) are considered from the viewpoint of choice of the most important physicochemical processes. For the problem of a direct shock wave propagating in the atmosphere, kinetic models are selected with allowance for the error in specifying reaction-rate constants. The investigation was performed using an automated system that incorporates structured bases of physicochemical data, a generator of kinetic equations, a complex of programs for direct calculation, and program modules for determining, from a set of admissible solutions, the one satisfying specified criteria.*

1. In the last decade, complex physicochemical phenomena in gas dynamics are simulated using bulky kinetic data bases. Several large systems based on data bases containing thousands of elementary processes (AVOGADRO, CHEMKIN, etc.) are known in the literature. On the one hand, being continuously expanded, such bases become difficult to use, but, on the other hand, the computational possibilities simultaneously increase, making it possible to employ modern effective methods of information processing.

The development of new methods for the mathematical simulation of complex nonequilibrium processes in gas dynamics and formalization of the procedure of generating kinetic equations using physicochemical data bases allow one to perform an effective analysis of the complex mechanism of a chemically reacting and vibrationally relaxing gas. Such purposeful investigation makes it possible to select the most important routes and develop compact models of minimum complexity that adequately describe nonequilibrium processes in a gas.

The present work is a continuation of [1]. Here, in particular, we consider the problems of determining compact mechanisms of the most important routes with allowance for the error in specifying the rate constants of nonequilibrium processes, i.e., the problem of developing kinetic models for inadequately studied objects.

The problem was solved using the automated system described in [2]. The main element of this system is a universal generator that unifies the procedure of formulating the kinetic equations describing the energy relaxation of vibrational modes of polyatomic molecules and chemical transformations of particles. Chemical transformations are considered to mean chemical reactions with allowance for neutral and charged particles (including particles in particular electronic states, for example, excitation and deactivation of particles) and radiative transitions. The universality of the generator implies that kinetic equations can be programmed using symbolic equations of elementary processes in the form of ordinary kinetic formulas. A complete list of the routes considered (with quantitative data on the rate constants) is stored on a computer in the form of a structured base of physicochemical data. Thus, the procedure of formulating kinetic equations by means of the generator is implemented at the information level of mathematical simulation. The information elements (in our case, data on the processes) are stored in formalized form [2] and the data required to solve the problem are selected using specially designed data-base management systems.

The scheme of interaction of the generator with the remaining components of the automated system includes the following elements: structured bases of kinetic data $B_i$, a complex of programs for direct

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calculation of gas-dynamic and relaxation equations $P_k$, and original modules programs $A_j$, which use the direct calculation programs $P_k$ (and, the corresponding data bases $B_i$) as subprograms and are intended for examination of more complex issues of physicochemical gas dynamics than the calculation of direct kinetic problem. In the automated system, such modules $A_j$ are a generator of kinetic models of a medium based on an algorithm of selecting leading processes [1] or a module that permits one to solve variational problems of gas dynamics with allowance for nonequilibrium processes [2]. Thus, using the program components $A_j$, it is possible to find, in a set of admissible solutions, the one that ensures satisfaction of certain specified criteria.

**2.** The establishment of thermal equilibrium in a gas is determined by the characteristic relaxation times $\tau_j$ of the nonequilibrium processes considered. These times differ greatly in magnitude and form a hierarchy, which, as a rule, has the form

$$\tau_{\rm col} \leqslant \tau_T \sim \tau_{RR}, \quad \tau_{RT} \leqslant \tau_{VV} \ll \tau_{VT}, \tau_{VV'}, \tau_C, \tau_{CV}, \tag{2.1}$$

where $\tau_{col}$ is the mean time between two collisions, $\tau_T$, $\tau_{RR}$, $\tau_{RT}$, and $\tau_{VV}$ are the characteristic times of establishment of equilibrium for the translational ($T$), rotational ($RR$ and $RT$), and vibrational ($VV$) degrees of freedom [($VV$) denotes energy exchange within a mode], $\tau_{VT}$ and $\tau_{VV'}$ are the characteristic times for vibrational–translational ($VT$) and vibrational–vibrational ($VV'$) energy exchanges between different modes, $\tau_C$ is the chemical reaction time, and $\tau_{CV}$ is the time during which the chemical reaction influences vibrational relaxation. We consider a situation where the characteristic gas-dynamic time $\tau_g$ becomes comparable with, at least, one of the characteristic times $\tau_{VT}$, $\tau_{VV'}$, $\tau_C$, or $\tau_{CV}$. Usually, vibrational modes are modeled by a harmonic oscillator, and it is assumed that within a mode the quantum exchange proceeds much faster than the ($VV'$)-, ($VT$)-energy exchange and chemical reactions [see the hierarchy of times (2.1)]. For most molecules, this assumption is valid at rather low temperatures (several thousand degrees). In this case, lower vibrational levels are primarily excited and the rapid ($VV$) exchange maintains Boltzmann distribution over the levels. In the simulation, we shall assume that the Maxwell velocity distribution is conserved for the translational degrees of freedoms, and the rotational degrees of freedom are in equilibrium with the translational ones. Under these assumptions, the basic nonequilibrium processes considered are chemical transformations of particles and relaxation of the vibrational energies of polyatomic molecules. The kinetic equations describing the indicated processes are given in [1–4], and the generator described above allows one to formulate these equations.

**3.** Solving a particular problem, the researcher can pose the problem of selecting (from the entire set) the most important physicochemical processes [5–9]. In the present paper, to develop a mechanism of the leading routes, we propose to move over from the complex kinetic scheme to a simple one by rejecting insignificant elementary stages. In this case, it is desirable that the initial data base contain all significant processes that model the main phenomena in a gas in full measure. The problem of developing a mechanism of the basic processes is formulated under the assumption that the kinetic data base contains transitions with participation of $C$-, ($VT$)-, ($VV'$)-, and ($CV$)-transitions, and particular problems are solved using the automated system.

To select the leading routes, the researcher specifies conditions of the processes (the element $P_k$) and compiles a general list of particles and elementary stages in the form of a structured data base $B_i$. Use of the generator to formalize the derivation of kinetic equations allows one to create a program module $A_j$ to solve the problem of selecting the leading processes with respect to an arbitrary goal function $\varphi$ [1, 2]. As the function $\varphi$ to be examined, one can take the concentrations of individual components (or the majority of them) (in problems of chemical engineering or ecology), macroscopic gas-dynamic quantities (pressure distribution in studies of the aircraft and spacecraft dynamics or heat flux for heat-exchange problems), etc. In this case, for each value of the threshold accuracy $\varepsilon$, one determines the minimum number of the basic, leading processes that guarantee satisfaction of the accuracy criterion

$$|\varphi_0 - \varphi_*| \leqslant \varepsilon|\varphi_0|. \tag{3.1}$$

Here $\varphi_0$ is the value of $\varphi$ obtained with allowance for the entire set of processes from the initial kinetic data base and $\varphi_*$ is the value of $\varphi$ for a minimum subset of the most important elementary stages.

Building a hierarchy of stages according to their importance for specified criteria makes it possible to solve the problem of selecting the basic routes. The ranging (building a hierarchy) of stages of a complex physicochemical process can be performed by comparing the rates of separate stages [1, 2, 9]. The procedure of determining the weight of the $j$th route in simultaneous course of the $C$-, $(VT)$-, $(VV')$-, and $(CV)$-processes is described in [1, 2].

The program module was used to develop a compact model of kinetics in air behind a direct shock wave propagating at speed $V$ in the atmosphere at altitude $H$. The quantitative physicochemical data in high-temperature air (about a hundred reactions including direct and reverse processes) and details of the calculation were considered in [1]. At high temperatures (several tens of thousands of degrees), nonequilibrium processes in air are characterized by the simultaneous course of vibrational relaxation and dissociation of $N_2$ and $O_2$ molecules. Under these conditions, the rate constants of dissociation $K_d(T, T_v)$ of the molecules are two-temperature and depend on the translational $T$ and vibrational $T_v$ temperatures. As shown in [1], the leading routes required to determine correctly the vibrational and translational temperatures consist of several types of processes ($C$, $VT$ and $CV$). However, the concentrations of the components can be determined with high accuracy using a one-temperature kinetic model that was obtained by substituting the vibrational temperature $T_v$ corresponding to intense dissociation into the formula for $K_d(T, T_v)$. This approximation was used for the one-dimensional flow behind the front of a direct shock wave in an inviscid gas. In particular, the mechanism of the most important reactions describing the concentration of the neutral components $N_2$, $O_2$, NO, N, and O and an electron $e$ is established. It turned out that to calculate the concentrations with a relative accuracy $\varepsilon = 0.3$ behind the wave ($V = 9$ km/sec and $H = 80$ km), it suffices to use the reactions

$$\begin{gathered}
\mathrm{O_2 + M \rightarrow 2O + M\,(M = O, O_2)}, \qquad \mathrm{NO + M \rightarrow N + O + M\,(M = N_2, N)}, \\
\mathrm{O + N_2 \leftrightarrow N + NO}, \qquad \mathrm{N + O_2 \leftrightarrow O + NO}, \qquad \mathrm{O_2 + N_2 \rightarrow 2NO}, \qquad (3.2) \\
\mathrm{N + N \leftrightarrow N_2^+} + e, \qquad \mathrm{O + O \leftrightarrow O_2^+} + e, \qquad \mathrm{N_2 + N^+ \leftrightarrow N_2^+ + N}, \qquad \mathrm{N + O \leftrightarrow NO^+} + e,
\end{gathered}$$

where M is any of the colliding particles.

The kinetic scheme (3.2) is obtained for a wave speed $V = 9$ km/sec. If the velocity $V$ is different, the contributions of the leading processes to the mechanism can change. The change of gas parameters (first of all, temperature) behind the shock wave can lead to a significant change in the characteristic times $\tau_j$ of the elementary stages. In this case, as a rule, the ratio of these times to the characteristic gas-dynamic time $\tau_g$ also changes. Table 1 shows kinetic mechanisms for the most important reactions with variation in the wave speed $V$ ($H = 70$ km). The molar fraction of an electron $\xi_e$ at a threshold accuracy $\varepsilon = 0.5$ was taken as the functional studied. The kinetics was examined in the interval 0–100 cm behind the wave. Reactions that were even once among the leading reactions as the wave speed varied $V$ from 6 up to 10 km/sec are indicated in the column "Process," and the required directions of the reactions are indicated in the columns for the various values of $V$. The change in the content of the basic processes with respect to the functional $\varphi = \xi_e$ for various accuracy $\varepsilon = 0.75$, 0.5, 0.25, 0.1, and 0.05 is shown in Table 2 ($V = 9$ km/sec).

A comparative calculation of the $\xi_e$ behind the shock wave with the complete set of reactions from [1] (solid curves) and the reactions from Table 1 (dashed curves) is shown in Fig. 1. The distance $x$ behind the shock wave ($\log x$ on the plot) is laid off as the abscissa. The numbers at the curves correspond to the speed of the front $V$. In the calculations, a comparison was performed for the mechanism obtained as a result of inclusion of all the reactions from Table 1 into one kinetic data base. This unified mechanism describes the electron concentration more adequately than particular groups of leading reactions at each fixed value of the speed $V$. In particular, for $V = 11$ km/sec, the difference in the results does not exceed 36% (the vertical line in Fig. 1), and for $V = 10$, 9, and 8 km/sec, it does not exceed 18, 16, and 40%, respectively.

4. At present, the rate constants and sections of physicochemical processes are determined with an error. Sometimes, their values can be described with accuracy up to one or two orders of magnitude, i.e., in this case, a phenomenon that has not been adequately studied is simulated. In this connection, the above results of developing a kinetic model can be related to a small neighborhood of a point in the space of rate constants $K_j$ of the elementary stages (local sensitivity analysis), and, hence, the question of how much these studies are reliable with considerable variation of the constants (global sensitivity analysis) remains open.

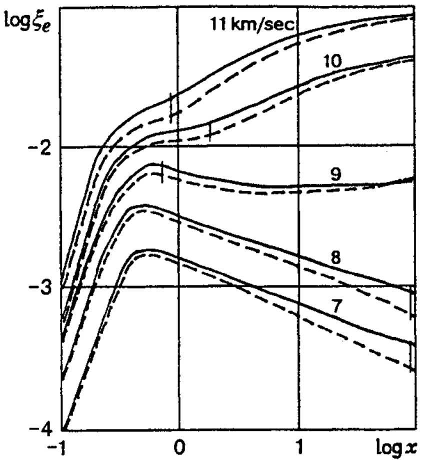

Fig. 1

TABLE 1

*Leading Post-Shock Reactions in Air for Various Velocities V*

| Process | $V$, km/sec | | | | |
|---|---|---|---|---|---|
| | 6 | 7 | 8 | 9 | 10 |
| $O_2 + M = 2O + M (M = O, O_2)$ | → | → | → | → | → |
| $N + O = NO^+ + e$ | ↔ | ↔ | ↔ | ↔ | ↔ |
| $O + N_2 = N + NO$ | ↔ | ↔ | ↔ | → | → |
| $N + N = N_2^+ + e$ | — | — | — | ↔ | ↔ |
| $O + O = O_2^+ + e$ | — | — | — | ↔ | — |
| $N_2 + N^+ = N_2^+ + N$ | — | — | — | — | ↔ |
| $NO + N_2 = N + O + N_2$ | — | — | → | → | → |
| $O + NO = N + O_2$ | → | — | — | — | — |

TABLE 2

*Leading Post-Shock Reactions in Air for Various Accuracy ε*

| Process | $\varepsilon$ | | | | |
|---|---|---|---|---|---|
| | 0.75 | 0.5 | 0.25 | 0.1 | 0.05 |
| $O_2 + M \rightarrow 2O + M$ | $O, O_2$ | $O, O_2$ | $O, O_2$ | $N_2, O, O_2$ | $N_2, O, O_2$ |
| $N + O = NO^+ + e$ | ↔ | ↔ | ↔ | ↔ | ↔ |
| $N + N = N_2^+ + e$ | ↔ | ↔ | ↔ | ↔ | ↔ |
| $O + N_2 = N + NO$ | → | → | ↔ | ↔ | ↔ |
| $O + O = O_2^+ + e$ | — | ↔ | ↔ | ↔ | ↔ |
| $NO + M \rightarrow N + O + M$ | — | $N_2$ | $N_2$ | $N_2, N, O$ | $N_2, N, O, O_2$ |
| $N_2 + N^+ = N_2^+ + N$ | — | — | ↔ | ↔ | ↔ |
| $N_2 + O_2 = 2NO$ | — | — | → | → | → |
| $O + NO = N + O_2$ | — | — | — | ↔ | ↔ |
| $N_2 + M \rightarrow 2N + M$ | — | — | — | $N_2$ | $N_2, O, N$ |
| $N^+ + O = N + O^+$ | — | — | — | — | ↔ |
| $N_2^+ + O = NO + N^+$ | — | — | — | — | → |

**Note.** For dissociation reactions the collision partner M is indicated in the column for $\varepsilon$.

In what follows, we describe implementation of the algorithm of selecting leading processes with allowance for the spread of values of $K_j$ within the specified errors. In this case, the procedure of choosing basic transitions for local sensitivity analysis is an integral part of the synthesis of the mechanism with allowance for the uncertainty of the values of $K_j$. Naturally, the calculated dependences of the component concentrations change with variation in the rate constants of the reactions contained in the initial data base. For processes with a minor contribution, such variation may be insignificant from the viewpoint of satisfaction of criterion (3.1), but for the leading reactions, variation in values of the constants can lead to a change in the content of the mechanism of the basic routes.

Let us vary the temperature dependence of the rate constants $K_j$ of the processes (within the specified errors) in a random fashion (the Monte Carlo method). From local sensitivity analysis, each new set of constants $K_j$ can be put in correspondence to a particular mechanism of the leading processes $R_i$ ($i$ is the test number in the velocity space). For a sufficient number of tests, the combination of all $R_i$ also contains the optimal mechanism of the leading processes with allowance for the error of $K_j$. A uniform distribution between the minimum and maximum values of the constant or a normal distribution with specified parameters

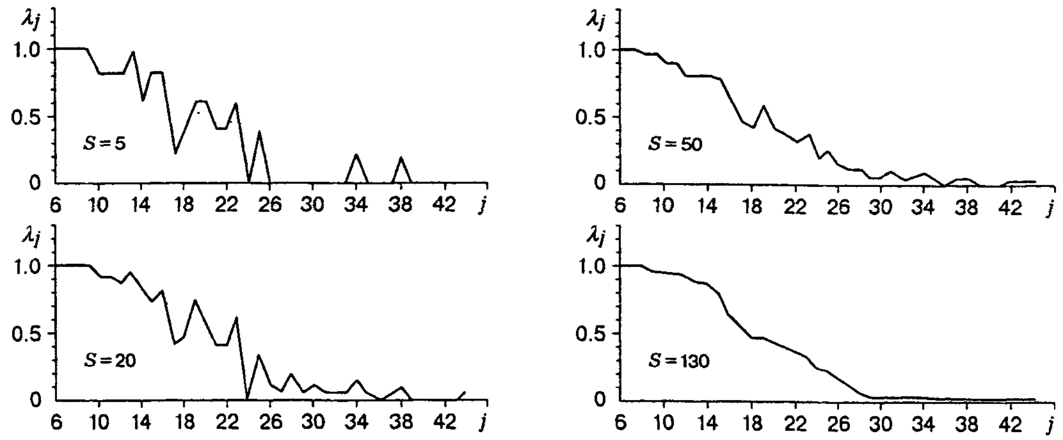

Fig. 2

can be used as the error distribution function. If the kinetic scheme takes into account both the direct and reverse reactions, the value of $K_j$ can be generated only for the direct reaction and the constant of the reverse reaction can be calculated (through the direct reaction constant) using the equilibrium constant.

A great number of publications have been devoted to examining rate constants in high-temperature air. For reactions involving neutral particles, the data on the reaction-rate constants (with errors and expert estimation of the errors) are given in [10]. From the data of [10], it can be concluded that the activation energy $E_a$ for reactions in air is much more accurate than the preexponent. Thus, a random sample of rate constants in air is described by the spread of the preexponent. According to [10], the error in determining the constants for all reactions is within ±300%. However, this estimate is obtained for temperatures not exceeding 20,000 K. Taking into account that the error can increase at $T > 20{,}000$ K, we assumed that the spread of $K_j$ is in the interval

$$K_j^{(p)}/d \leqslant K_j \leqslant dK_j^{(p)}, \tag{4.1}$$

where $K_j^{(p)}$ is the recommended value of the constant and $d = 5$. For reactions involving charged particles and an electron $e$, the rate constants are determined less reliably. In this case, it was assumed that the possible spread of $K_j$ is an order of magnitude on both sides of the recommended $K_j^{(p)}$, i.e., $d = 10$, and the density distribution function between the minimum and maximum values of the constant is uniform. The quantitative data from [1, 10] were used as recommended values of $K_j^{(p)}$.

We studied the problem of determining the leading reactions with respect to the concentrations of the components $N_2$, $O_2$, NO, N, O, and $e$ with accuracy of $\varepsilon = 0.3$ for the case of a shock wave propagating at $V = 9$ km/sec and $H = 80$ km in the atmosphere (see above). The dissociation and recombination reactions for different collision partners M were formally assumed to be different. The main results of the search for the mechanism of the leading processes are shown in Table 3 and Fig. 2. Table 3 give the combination $R_i\,(i = 1, \ldots, S)$ of all reactions of search after $S = 130$ tests in the space of rate constants $K_j$, where $\lambda_j = N_j/S$ is the frequency of localization of the $j$th reaction ($N_j$ is the number of occurrences of the $j$th reaction among the leading reactions after $S$ tests). Table 3 gives 44 reactions ranked according to decreasing frequency $\lambda_j$. For all possible variations in the constants according to (4.1), the remaining reactions do not influence the accuracy of calculation of the components N, O, $N_2$, $O_2$, NO and $e$ in the sense of violation of the threshold condition (3.1). Figure 2 shows the evolution of the distribution function $\lambda_j$ with variation in the number of tests $S$ ($S = 5$, 20, 50, and 130). The reaction number from Table 3 ($j > 5$) is laid off as the abscissa.

The data given in Table 3 and in Fig. 2 allow the following additional analysis to be performed.

1. The function of distribution in $\lambda_j$ converges rather rapidly to its limiting value with increase in the number of tests $S$. First of all, this is true for the most important reactions with frequencies $\lambda_j \sim 1$,

TABLE 3

*Leading Post-Shock Reactions in Air from Global Sensitivity Analysis*

| $j$ | Process | $\lambda_j$ | $j$ | Process | $\lambda_j$ |
|---|---|---|---|---|---|
| 1* | $O_2 + O \to O + O + O$ | 1.0 | 23 | $N + O + N \to NO + N$ | 0.338 |
| 2* | $O_2 + O_2 \to O + O + O_2$ | 1.0 | 24 | $N + N + N \to N_2 + N$ | 0.246 |
| 3* | $O + N_2 \to N + NO$ | 1.0 | 25 | $NO + N^+ \to N_2^+ + O$ | 0.231 |
| 4* | $N + NO \to O + N_2$ | 1.0 | 26 | $NO + O_2 \to N + O + O_2$ | 0.146 |
| 5* | $N + N \to N_2^+ + e$ | 1.0 | 27 | $O_2^+ + N \to NO^+ + O$ | 0.123 |
| 6* | $N_2^+ + e \to N + N$ | 1.0 | 28 | $N + O^+ \to N^+ + O$ | 0.100 |
| 7* | $N_2 + N^+ \to N_2^+ + N$ | 1.0 | 29 | $NO + NO \to N + O + NO$ | 0.085 |
| 8* | $N_2^+ + N \to N_2 + N^+$ | 0.992 | 30 | $NO^+ + N \to N_2^+ + O$ | 0.077 |
| 9* | $NO + N_2 \to N + O + N_2$ | 0.962 | 31 | $N_2 + N \to N + N + N$ | 0.077 |
| 10* | $NO^+ + e \to N + O$ | 0.946 | 32 | $N_2^+ + O \to NO^+ + N$ | 0.062 |
| 11* | $N + O \to NO^+ + e$ | 0.946 | 33 | $N^+ + O \to N + O^+$ | 0.062 |
| 12* | $NO + N \to N + O + N$ | 0.931 | 34 | $N_2 + O \to N + N + O$ | 0.062 |
| 13* | $N + O_2 \to O + NO$ | 0.877 | 35 | $N_2 + O_2 \to N + N + O_2$ | 0.046 |
| 14* | $O + NO \to N + O_2$ | 0.877 | 36 | $O_2^+ + N \to N^+ + O_2$ | 0.039 |
| 15 | $NO + O \to N + O + O$ | 0.800 | 37 | $NO^+ + O \to O_2^+ + N$ | 0.031 |
| 16* | $N_2 + O_2 \to NO + NO$ | 0.623 | 38 | $NO^+ + O_2 \to NO + O_2^+$ | 0.031 |
| 17* | $O + O \to O_2^+ + e$ | 0.554 | 39 | $N_2^+ + O \to O^+ + N_2$ | 0.023 |
| 18* | $O_2^+ + e \to O + O$ | 0.469 | 40 | $N^+ + O_2 \to O_2^+ + N$ | 0.023 |
| 19 | $N_2 + N_2 \to N + N + N_2$ | 0.469 | 41 | $O_2 + Ar \to O + O + Ar$ | 0.023 |
| 20 | $O_2 + N_2 \to O + O + N_2$ | 0.431 | 42 | $O^+ + N_2 \to N_2^+ + O$ | 0.015 |
| 21 | $N_2^+ + O \to NO + N^+$ | 0.408 | 43 | $NO^+ + O \to NO + O^+$ | 0.008 |
| 22 | $NO^+ + N_2 \to NO + N_2^+$ | 0.362 | 44 | $NO + N_2^+ \to NO^+ + N_2$ | 0.008 |

**Note.** The asterisk denotes the reactions included in the mechanism (3.2) based on local sensitivity analysis.

and beginning with $S \sim 50$, the distribution function varies mainly in the region of small values of $\lambda_j$. This considerably simplifies practical implementation of the algorithm of synthesis of the leading processes.

2. The quantities $\lambda_j$ can be used to construct a kinetic model describing nonequilibrium processes in a gas. For this, the critical value $\lambda_*$, for example, $\lambda_* \sim 0.1$–$0.2$, is introduced and all reactions for which $\lambda_j < \lambda_*$ are eliminated from the kinetic data base since condition (3.1) is violated at a rather rare combination of the spread of the rate constants $K_j$. The most important reactions with $\lambda_j > \lambda_*$ are at the top of Table 3.

Thus, in the global analysis, the kinetic model of a medium (that satisfies, for example, the condition $\lambda_j > \lambda_* = 0.2$) contains a greater number of processes than the mechanism (3.2) in the local analysis.

The program module for constructing a kinetic mechanism of minimum complexity considerably reduces the number of elementary stages of the complex kinetic scheme and, thus, simplifies the matrix of stoichiometric coefficients. The scheme can be further simplified by using the notions of key components [11] and quasistationary concentrations. The introduction of key components is based on an analysis of the matrix of stoichiometric coefficients of reactions that remained in the base. In addition, the presence of quasiequilibrium blocks in the scheme allows one to reduce the dimension of the system of kinetic equations by expressing some concentrations in terms of others. The kinetic equations describing the leading nonequilibrium processes are less rigid in this case, which is important in numerical calculations. The number of equations can also be decreased using universal relations (the Dalton law, the law of conservation of charge, material balance equations).

We note another important feature of such studies for the solution of variational problems of gas dynamics with allowance for nonequilibrium processes. The list of the determining parameters of optimization includes quantities such as $p^{q-1}l$, where $l$ and $p$ are the characteristic dimension and pressure, $q = 1$ for monomolecular processes, and $q = 2, 3, \ldots$ for processes that take account of double and triple collisions [12]. Thus, the structure of the leading physicochemical routes (in the sense of the number of colliding particles) also specifies the list of determining controllable variables in variational problems.

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