

MODELLING RESULTS ON PHYSICAL AND CHEMICAL PROCESSES IN THERMALLY NONEQUILIBRIUM HIGH-TEMPERATURE GAS

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Key words: shock waves, vibration and electronic excitation, dissociation, radiative processes, database, models.

Abstract. The thermally nonequilibrium gases are those in the absence of equilibrium between translational, vibrational, and electronic states of molecules. The main problem in consideration of these gases is the values of coefficients in kinetic equations such as rate constants on vibrational and electronic energy exchange, and on thermally nonequilibrium chemical reactions. The modelling results of these processes consist of the base of original experimental and calculated theoretical data, database on rate constants, as well as bases of intuitive, or empirical, or analytical models for computations of rate constants. The example of original base of protocol and dynamic collision modelling, along with data for processes with excited electronic particles in high temperature air are presented. Reaction mechanism involving electronic atoms and molecules includes processes formation of excited ones, energy exchange, and quenching at collisions and at dissociation and recombination. The role of intensive radiation of atoms and molecules with depopulation of their excited states is noted, and the total heat transfer in gas flow is the result. The radiation effect in front of shock wave with significant translational nonequilibrium is demonstrated. High temperature processes under consideration are important in problems solution on investigations of spacecraft entering Earth and Martian atmospheres at high velocities.

1. INTRODUCTION

The thermally nonequilibrium gases are those in the absence of equilibrium between translational, vibrational and electronic states of molecules. These gases are forming under strong and sharp actions in shock waves and supersonic flows in nozzles and jets, in boundary layers, in intensive combustion, explosion, and radiation. The modelling of thermally nonequilibrium gases is performed in two approximations: with conservation of Boltzmann distribution with quick vibrational energy exchange (two-temperatures gas for T_v , mode kinetics), and in absence of Boltzmann distribution with the description of populations of different vibrational levels (for n_v as molecules concentrations, level kinetics). The main problem in consideration of mode and level kinetics is the values of coefficients in kinetic equations such as rate constants on vibrational and electronic energy exchange, and on chemical reactions. Other operating high-temperature processes are ionization and plasmachemical reactions, which you can see at^{1,2}.

2. BASES OF RESULTS DATA

2.1. Results contents

The values under consideration are the results of modelling of physical and chemical processes, as usually based on experimental and theoretical investigations. The fund of these modelling results consists of three parts:

- fund of original experimental and calculated theoretical information results with textual and graphic presentations, as the *bases of original data*;
- storage (extensive) fund as the *database* with concrete information about values of rate constants on vibration and electronic energy-exchange and chemical reactions;
- logical-algorithmic (intensive) fund as the *bases of models* for computation of rate constants values in one or other approximation.

2.2. Original experimental results: base of protocols

The original detailed results of experimental investigations are conserved by authors. As usual the authors publish only a part of results, which is treated in accordance with their physical assumptions and actual supposed application domain. So a lot of interesting original information is not in use and may be lost. But this information may be required for essentially new processing of original experimental data results. One can recommend to form the base of protocols of all original physical experiments data with its presentation for possible extensive use. These protocols include the structured set of factual data on process: applied facility, investigated gas mixture, method of action on gas, diagnostic procedures, concrete measurement results, and so on.

The demonstrated nomenclature of protocol basic characteristics with concrete examples of applied values in the modelling of oxygen molecules dissociation behind shock wave include (L.B. Ibragimova is the author):

- *experimental set-up*: shock tube with 50 mm inner diameter;
- *testing gas*: molecular oxygen (100 %) at pressure $p_0 = 2.5$ Torr;
- *experimental method*: measurement of radiation intensity I (Volt) in consequence by the light passage crosswise on shock tube;
- *applied equipment*: vacuum monochromator;
- *recorded value*: absorption capacity I/I_0 of O_2 molecules in Schumann–Runge spectral band on wavelength $\lambda = 250$ nm, I_0 is the radiation intensity at the shock wave front;
- *argument of measured value*: time t (mcs) at the passage of shock wave, with decidable capacity $\Delta t = 0.102$ mcs;
- *mean error of experiment result value*: 8 %.

The original result of the realized experiment is presented in Figure 1, and in the Table 1, given as the protocol. These data are completed with employment of model of spectral radiation emissivity. Thereafter the application of vibrational energy exchange and chemical reaction models are used. This makes possible to determine the distributions of translational and vibrational temperatures of O_2 molecules versus time, component concentrations, and other data for preparing the values of reaction rate constants. The author result of modelling with application of original protocols is

demonstrated in publication at this conference WEHSFF-2007 (see paper of L.B. Ibragimova et. al).

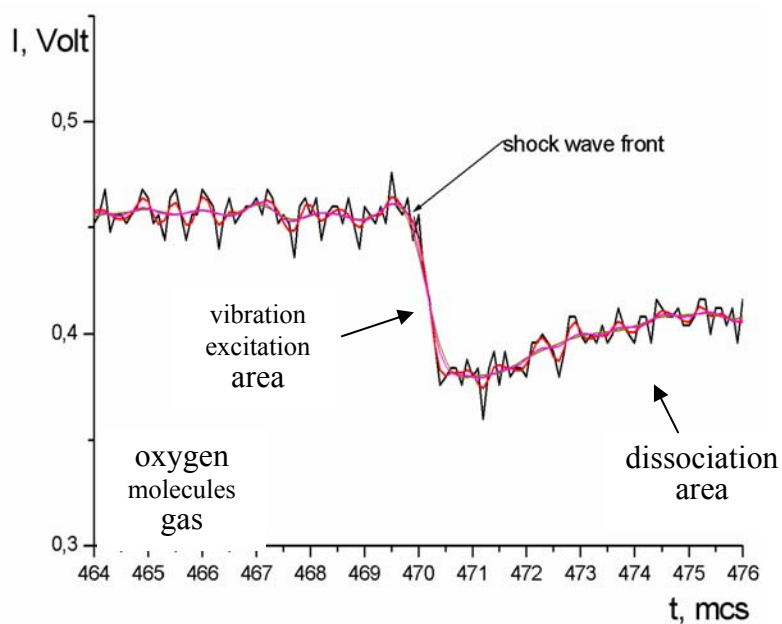


Figure 1. The example of original results on determination of radiation intensity I versus time t in shock wave

t , mcs	I , Volt	t , mcs from shock wave front	I/I_0
469.96	0.4557	0	1
470.06	0.4414	0.1	0.9686
470.16	0.4216	0.2	0.9252
470.26	0.4050	0.3	0.8887
470.36	0.3952	0.4	0.8672
470.47	0.3873	0.51	0.8500
470.54	0.3836	0.58	0.8418
470.78	0.3806	0.82	0.8352
471.16	0.3803	1.2	0.8345
471.39	0.3811	1.43	0.8363
471.56	0.3825	1.60	0.8394
471.69	0.3841	1.73	0.8429
472.05	0.3892	2.09	0.8541
472.45	0.3942	2.49	0.8650
472.89	0.3985	2.93	0.8745
473.49	0.4014	3.53	0.8808
474.03	0.4041	4.07	0.8868
474.63	0.4083	4.67	0.8960
475.00	0.4091	5.04	0.8977
475.54	0.4083	5.58	0.8960
475.99	0.4080	6.03	0.8953

Table 1. The example of base of original data in form of protocol base, which is described in text and demonstrated in Figure 1

The information on original data is the very important and valuable. It can be fruitfully used by the authors and other interested specialists with application of new ideas on process modelling.

2.3. Original theoretical results: dynamic collision modelling

The original results of theoretical modelling of corresponding physical and chemical processes at high temperature are the most well-justified and realistic when they are based on the solution of dynamic collision problems by means of quasiclassical trajectory (QCT) method. These problems are solved for concrete chemical reactions. The realization stages of these problems are followed from models of colliding particles and set of potential energy surfaces for particles interaction to numerical solutions of Hamilton equation under multivariant initial conditions with statistic retrieval. The basic results of trajectory calculations is the reaction cross-sections which represents an average on all orientations of particles in space. The cross-sections values in chemical exchange reaction $\text{CO} + \text{N} \rightarrow \text{CN} + \text{O}$ for different vibrational-rotational (v, j) states of CO molecule in relation to collision energy E_t are displayed in Figure 2, as the example (M.Yu. Pogosbekian is the author).

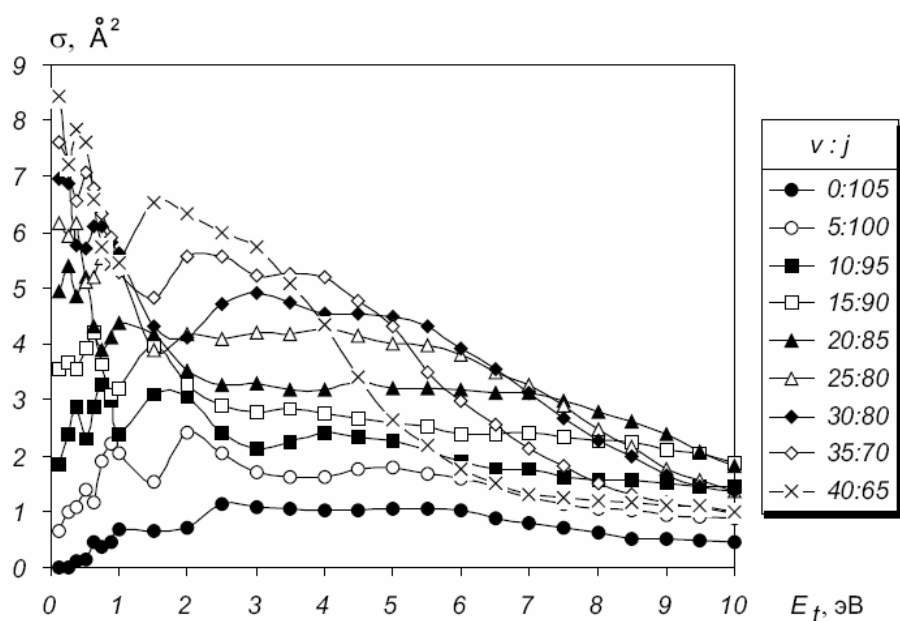


Figure 2. The cross-sections values of chemical exchange reaction $\text{CO} + \text{N} \rightarrow \text{CN} + \text{O}$ (see text)

The final result is the application of integrating procedure for preparing of rate constants as functions of temperature T , vibrational temperature T_v in mode kinetics, and numbers m, n of vibrational levels in level kinetics. The calculations results on concrete processes of vibrational energy exchange and chemical reactions by QCT-method compose the base of calculated data.

These data are used in different ways. The most laborious but prime method is the direct use of these results on rate constants for solution of mode and level kinetics equations³. Another way is the polynomial approximations of calculated results for simplification of equations solution procedure (see^{4,5} for examples). The most suitable and perspective way is the creation of correspondent model on the conceptual description with application of physical notations. The examples of such models for dissociation process are β -model in mode kinetics (see¹ pp.211–213) and Levitsky model and γ -model in level kinetics².

2.4. Database example for processes with the excited electronic particles

The published works provide the creation of databases on kinetics characteristics as the rate constants of physical and chemical processes. This data based on expert analysis of the known results are published in many handbooks and reviews, but information concerning thermally nonequilibrium reactions is limited in these databases. The example of imperfect database is the set of rate constants on processes with the excited electronic states in atoms and molecules. This example is the result of publications examination. It includes the data on excitation, energy exchange, and quenching of electronic states on these processes in high temperature air (V.N. Yarygina is the partner-author). These data present (here, as usual, the electronic states of molecules and atoms are indicated in brackets):

- formation of the excited electronic states as the result of atoms recombination (Table 2) and at particles collisions (Table 3);
- electronic energy exchange at particles collisions (Table 4) and at atom recombination (Table 5);
- quenching of the excited electronic states of atoms and molecules at collisions (Table 6) and at dissociation (Table 7).

The rate constants of these processes are presented by Arrhenius formula

$$k(T) = AT^n \exp(-E_a/kT),$$

or in terms of concrete notation of its value. The asterisks indicate:

- (*) – it is assumed the common efficiency of $N(^4S)$, $O(^3P)$ atoms at collisions with $O_2(b)$ molecule;
- (**) – it is the result of approximation from graph as the origin;
- (***) – the argument of rate constant of the reverse reaction $k^-(T, T_v)$ includes the value of vibrational temperature T_v for nitrogen molecule $N_2(X, v)$.

In specific cases the distinct values of rate constants from different authors are used for identical reaction. These distinctions may be used for estimation of rate constants error.

These data will be useful for solution of kinetic equations with consideration of different electronic states in atoms and molecules in high temperature air.

Reactions	A	n	E_a/k	Reference
$N + N + M \rightarrow N_2(A) + M$				s
M=N ₂	8×10^{16}	-0.8	0	[6]
M=N ₂ , O ₂ ,	6.2×10^{14}	0	0	[7]
NO				
M=N, O	1×10^{14}	0	0	[7]
$N + N + M \rightarrow N_2(B) + M$				
M=N ₂ , O ₂ ,	8.7×10^{14}	0	0	[7]
NO				
M=N, O	5.1×10^{15}	0	0	[7]
$O(^3P) + O(^3P) + O_2 \rightarrow$	9.8×10^{15}	-0.41	0	[8]
$O_2(X, a, b) + O_2$				

$O(^3P) + O(^3P) + O \rightarrow O_2(X,a,b) + O$	2.9×10^{16}	-0.41	0	[8]
$N + O + N_2 \rightarrow NO(A) + N_2$	$7.7 \times 10^{13} \cdot (T/300)^{-1.24}$			[6]
$N + O + N_2 \rightarrow NO(B) + N_2$	$1.9 \times 10^{13} \cdot (T/300)^{-1.4}$			[6]
$O + O + O_2 \rightarrow O_2(a) + O_2$	7.0×10^{12}	-0.63	0	[9]
$O + O + O \rightarrow O_2(a) + O$	2.5×10^{13}	-0.63	0	[9]

Table 2. Rate constants on the formation of excited electronic states as the result of atom recombination

Reactions	A	n	E_a/k	References
$N_2(X) + N_2 \rightarrow N_2(A) + N_2$	1.1×10^{12}	-0.5	71600	[6,10]
$N_2(X) + N \rightarrow N_2(A) + N$	1.2×10^{17}	-1.5	71600	[6,10]
$N_2(X) + O_2 \rightarrow N_2(A) + O_2$	6×10^{15}	-1.5	71600	[6]
$N_2(X) + O \rightarrow N_2(A) + O$	7.2×10^{16}	-1.5	71600	[6]
$N_2(X) + NO \rightarrow N_2(A) + NO$	1×10^{12}	-0.5	71600	[10]
$NO(X) + M \rightarrow NO(A) + M$	9.6×10^{12}	-0.5	63510	[10]

Table 3. Also as in Table 2, but at particles collisions

Reactions	A	n	E_a/k	References
$N_2(A) + M \rightarrow N_2(B) + M$	1.2×10^{13}	0	13495	[10]
$NO(X) + N_2(A) \rightarrow NO(A,v) + N_2(X)$	6.02×10^{13}	0	0	[6]
$NO(X) + N_2(A) \rightarrow NO(C,v) + N_2(X)$	5.8×10^{14}	0	0	[6]
$N_2(A) + N_2(A) \rightarrow N_2(B) + N_2(X,v)$	7.4×10^{13}	0	0	[6]
$N_2(A) + N(^4S) \rightleftharpoons N_2(X,v) + N(^3P)$		$k^+ = 2.4 \times 10^{13} (300/T)^{2.3}$		[7] (***)
		$k^-(T, T_v) = 0.1k^+ \exp(1276/T) - 28760/T_v$		
$O_2(a) + O_2(a) \rightarrow O_2(b) + O_2(X)$	4.2×10^{-4}	3.8	-700	[11,12]
— " — " —	5.4×10^7	0	560	[9]
$O_2(b) + O_2(X) \rightarrow O_2(a) + O_2(X)$	2.6×10^2	2.4	281	[7]
— " — " —	2.2×10^7	0.5	0	[9]
— " — " —	2.3×10^7	0	0	[13]
$O_2(b) + N_2(X) \rightarrow O_2(a) + N_2(X)$		$(0.35T + 6.67) \times 10^7$		[11]**
$O_2(b) + O_2(b) \rightarrow O_2(a) + O_2(X)$	2.2×10^7	0.5	0	[9]
$O_2(b) + O(^3P) \rightarrow O_2(a) + O(^3P)$	4.9×10^{10}	0	0	[7,12]
— " — " —	7.3×10^{10}	0.5	0	[9]
$O_2(b) + N(^4S) \rightarrow O_2(a) + N(^4S)$	4.9×10^{10}	0	0	[12]*
$O(^1D) + O_2(X) \rightarrow O(^3P) + O_2(a)$	3.8×10^{12}	0	-67	[12]
— " — " —	9.6×10^{11}	0	-67	[9]
$O(^1D) + O_2(X) \rightarrow O(^3P) + O_2(b)$	1.54×10^{13}	0	-67	[5,9,12]
— " — " —	3.0×10^{13}	0	0	[8]

$O(^1D) + O_2(b) \rightarrow O(^1D) + O_2(X)$	$3 \times 10^{13} (300/T)^{0.1} \exp(-4200/T)$			[7]
$O(^1D) + O_2(a) \rightarrow O(^3P) + O_2(b)$	3.0×10^{13}	0	0	[12]
$O(^1S) + O_2(X) \rightarrow O(^1D) + O_2(b)$	1.0×10^8	0	0	[8]
$O(^1S) + O_2(X) \rightarrow O(^3P) +$ $O_2(A,c,C)$	1.8×10^{12}	0	850	[7]
$O_2(X) + O_2(c) \rightarrow O_2(b) + O_2(X,a,b)$	6.0×10^8	0	0	[8]
$O_2(X) + O_2(C) \rightarrow O_2(X,a,b) +$ $O_2(X,a,b)$	6.0×10^{11}	0	0	[8]
$O_2(X) + O(^1S) \rightarrow O_2(X,a,b) +$ $O(^3P)$	2.4×10^{12}	0	870	[8]

Table 4. Rate constants on the electronic energy exchange at particles collisions

Reactions	A	n	E_a/k	References
$O(^3P) + O(^1D) + O_2 \rightarrow O_2(c)$ + O_2	1.3×10^{15}	-0.41	0	[8]
$O(^3P) + O(^1D) + O \rightarrow O_2(c)$ + O	4×10^{15}	-0.41	0	[8]
$O(^1D) + O(^1D) + O_2 \rightarrow O_2(C)$ + O_2	9×10^{14}	-0.41	0	[8]
$O(^1D) + O(^1D) + O \rightarrow O_2(C)$ + O	2.6×10^{15}	-0.41	0	[8]

Table 5. Also as in Table 4, but at atom recombinations

Reactions	A	n	E_a/k	References
$NO(A) + M \rightarrow NO(X) + M$	5.2×10^{12}	0.5	0	[6]
$NO(B) + M \rightarrow NO(X) + M$	6.4×10^{12}	0.5	0	[6]
$NO(C) + M \rightarrow NO(X) + M$	7.56×10^{12}	0.5	0	[6]
$N_2(A) + N_2(X) \rightarrow N_2(X) +$ $N_2(X)$	$1 \times 10^6 \div 2.7 \times 10^7$			[14,15]
$N(^2D) + N_2 \rightarrow N(^4S) + N_2$	$3.6 \times 10^{10} \div 1.4 \times 10^{11}$			[14,15]
$O_2(a) + O_2 \rightarrow O_2(X) + O_2$	1.02×10^6	0	0	[11,12,16,17]
— " — " —	1.8×10^6	0	0	[18]
— " — " —	$1.2 \times 10^6 \div 2.4 \times 10^6$			[14,15]
— " — " —	1.8×10^6	0	200	[9]
$O_2(a) + O + M \rightarrow O_2(X) +$ $O + M$	3.6×10^{15}	0	0	[19]
$O_2(a) + O_2(a) \rightarrow O_2(X) +$ $O_2(X)$	5.4×10^7	0	560	[9]
— " — " —	1.1×10^7	0	0	[13]
$O_2(a) + O \rightarrow O_2(X) + O$	4.2×10^8	0	0	[11,12,17]
— " — " —	1.2×10^8	0	0	[9]
$O_2(a) + NO \rightarrow O_2(X) + NO$	1.9×10^{10}	0	2030	[20]
$O_2(a) + N_2 \rightarrow O_2(X) + N_2$	1.8×10^3	0	0	[18]
— " — " —	8.4×10^4	0	0	[13]
$O_2(b) + N_2 \rightarrow O_2(X) + N_2$	3.5×10^4	1.6	-428.4	[11,18]
$O_2(b) + O_2 \rightarrow O_2(X) + O_2$	2.6×10^2	2.4	241	[18]

— " — " —	2.4×10^6	0.5	0	[9]
— " — " —		$2.4 \times 10^7 \div 6 \times 10^7$		[14,15]
$O_2(b) + O \rightarrow O_2(X) + O$	4.8×10^9	0.5	0	[9]
$O(^1D) + O(^3P) \rightarrow O(^3P) + O(^3P)$	1.92×10^{13}	0	-67	[12]
— " — " —	4.8×10^{12}	0	0	[9,14,15]
$O(^1D) + O_2(X) \rightarrow O(^3P) + O_2(X)$	1.92×10^{13}	0	-67	[12]
— " — " —	3.8×10^{12}	0	-67	[7]
— " — " —	2×10^{11}	0	0	[16]
— " — " —	2.9×10^{12}	0	-67	[9]
$O(^1S) + O_2(b) \rightarrow O(^3P) + O_2(X)$	6.6×10^{13}	0	0	[9]
$O(^1S) + O(^3P) \rightarrow O(^3P) + O(^3P)$	2×10^{13}	0	300	[9]
$O(^1S) + O_2(X) \rightarrow O(^3P) + O_2(X)$	7.8×10^{11}	0	850	[7]
$O(^1D) + N_2 \rightarrow O(^3P) + N_2$		$(-0.00085 \cdot T + 5.17) \cdot 10^{13}$		[21]**

Table 6. Rate constants on the quenching of excited electronic states of atoms and molecules at collisions

Reactions	A	n	E_a/k	References
$O_2(a) + M \rightarrow O(^3P) + O(^3P) + M$	5.4×10^{18}	-1	48008	[12]
$O_2(b) + M \rightarrow O(^3P) + O(^3P) + M$	5.4×10^{18}	-1	40518	[12]
$O(^1S) + O_2(a) \rightarrow O(^3P) + O(^3P) + O(^3P)$	2×10^{13}	0	0	[9]
$N_2(A) + M \rightarrow N + N + M$	2.16×10^{17}	-	41590	[10]
		0.871		
$N_2(B) + M \rightarrow N + N + M$	1.66×10^{16}	-0.9	27840	[10]
$NO(A) + M \rightarrow N + O + M$	4.4×10^{15}	-0.74	11990	[10]

Table 7. Also as in Table 6, but at molecules dissociation

2.5. Bases of models

The deficiency of knowledge on thermally nonequilibrium reactions database leads to the necessity of development of comprehensive information fund for support indicated processes modelling, and for creation and extension of base of models. The existing base of models is the extensive complex, which provides the information-mathematical modelling in the field of physical and chemical kinetics.

The base of models for processes in thermally nonequilibrium dissociation and chemical exchange reactions is provided in terms of logical-algorithmic fund with intuitive, or empirical, or analytical models of reaction rate constants. The detailed description of each model see^{1,2}.

The selection of most suitable models for practical application in the solution of gasdynamics problems is provided by preparing of recommended models in accordance with their reliability, universality and simplicity. The models reliability problem is based on the experimental results and modelling of collision dynamics by means of

QCT method. Experimental results and realization of QCT method are used in model verification and definition of parameters values in empirical models.

Comparison of many models of O_2 , N_2 , Br_2 , I_2 dissociation with experimental results is given in²². In this comparison the relatively good model reliability is demonstrated only in analytical Macheret–Fridman model of two mechanisms dissociation and empirical threshold β -model.

In the widely used simple and universal Park model (see¹ pp.228–231) vibrational temperature T_v contribution is intuitively taken into account by means of substitution of gas temperature T in thermally equilibrium one-temperature rate constant $k(T)$ expression for the effective temperature $T_{eff} = T^s T_v^{1-s}$, where s is the model parameter (author value is $s = 0.7$). The universality of Park model is provided with all well-known information in databases, handbooks, and publications (except data with gas temperature T as constant value). It's very important, that this model can be used for descriptions of chemical reactions mixture with radicals and nonadiabatic processes, including reactions with excited electronic states components; the modelling of these processes using other approaches is not so simple.

The problem in application of Park model is the inadequacy of its reliability by comparison with experimental and calculation results. This problem can be solved by variation of model parameters s under verification procedure on the base of above-mentioned experimental and calculation data. The example of this verification result for reaction $CO + N \rightarrow CN + O$ (as above) for variation of parameter s is presented in Figure 3²³.

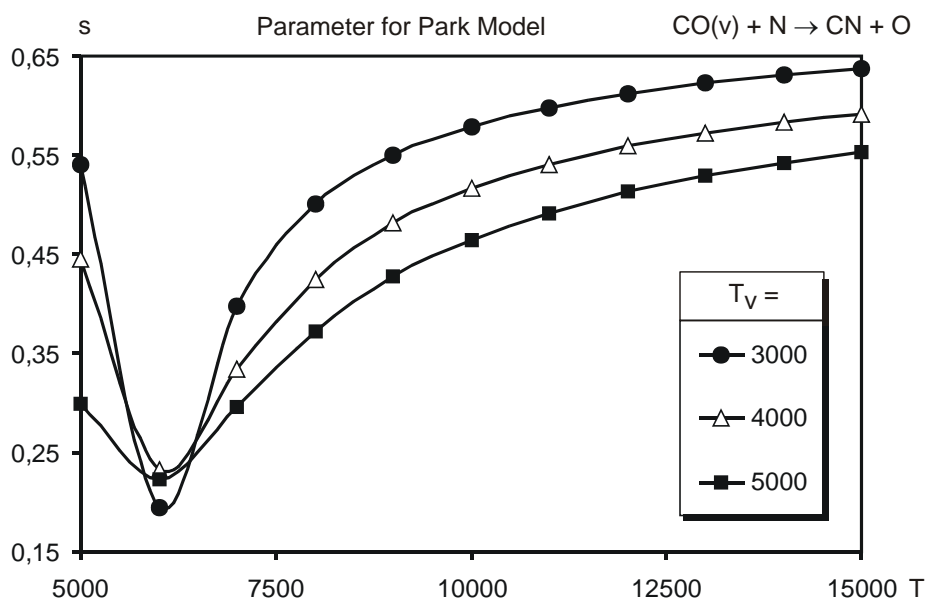


Figure 3. The empirical parameter s in Park model as the function of gas temperature T for three values of vibrational temperature T_v .

In general the variations of model parameters often provide the reliability. The similar procedure is the introduction of temperature dependence of parameter U in Marrone–Treanor model as the characteristic of probability distribution for dissociation from different vibrational levels (see¹ pp.209–211).

The selection of concrete recommended values of parameters and its dependence on temperature and other arguments are interesting for the solutions of kinetic problems and comparison with experimental results.

3. ELECTRONIC-CHEMICAL REACTIONS AND RADIATION

The main process of formation of molecules in the excited electronic states is the atom recombination. This process is considerably more effective than the formation of molecules in the ground electronic state. This result was determined by the authors²⁴ on the base of the formation of CO molecule: the ratio of the recombination rate constants in the excited CO ($A^1\Pi$) and ground CO ($X^1\Sigma$) electronic states can reach about two orders in temperature range $T = 5000 \div 20000$ K. In calculations it was also found that the recombination of CO molecules is more effective for high vibrational states in generalized Marrone – Treanor model for dissociation (see²⁴).

At collisions of molecules in the excited vibrational and electronic states, the transitions from high vibrational levels to the approximately isoenergetic excited electronic states are found to be most rapid (see²⁵). The descriptions of corresponding experimental investigations with the received values of level rate constants at isoenergetic vibrational-electronic energy exchange involving CO molecules are listed in²⁵. These results underline the role of level kinetics in the description of high-temperature gas.

A. Starik and N. Titova^{12,26} studied the models of dissociation of electronic excited molecules in state $O_2(a)$ and models of exchange reactions with molecules $O_2(a)$ and $O_2(b)$. They recommend the application of so-called α -model²⁷, where value α is the coefficient of the excited energy using, as the extension of vibrational energy contribution (see¹, pp.201–206). E. Kustova et al.²⁸ generalize the Marrone – Treanor model (see¹, pp.209–211) for diatomic gases with non-equilibrium electronic-vibration excitation.

Reaction mechanism with the excited electronic atoms and molecules includes processes on energy exchange and quenching at collisions and at dissociation and recombination. The corresponding values of rate constants in high temperature air are given above.

It is well known that the excitation of electronic states leads to intensive radiation of atoms and molecules as a result of distinct radiative transitions for UV and visible radiation, apart from IR radiation due to transitions between vibrational states of molecules. The radiation process has the determining role in depopulation of the excited electronic states of atoms and molecules, and the total heat transfer in gas flows is the result. The detailed descriptions of the models of radiative transfer in gases are presented in S. Surzhikov publications (see^{29,30} and cited there references). The example of the description of physical and chemical processes in shock waves for spacecraft entering Martian and Earth atmospheres at high velocities is also presented in³¹.

The interesting appearance of processes in shock waves is the observed radiation effect in front of shock waves. This effect is a result of interaction of gas medium and moving molecules in shock wave (Mott – Smith effect). This causes the significant translational non-equilibrium with high-energy collisions of molecules in front medium, and partially direct dissociation of molecules, excitation of electronic states, ionization, and other processes result by several collisions. The important role of translational non-equilibrium has been determined in experiments^{32–34}, where non-equilibrium radiation peak $NO(\gamma)$ in air shock waves, and Swan bands $CO(4^+)$, $C_2(d)$ in shock waves in

Martian atmosphere mixture were observed (Figure 4; P.V. Kozlov, Yu.V. Romanenko are the partner-authors).

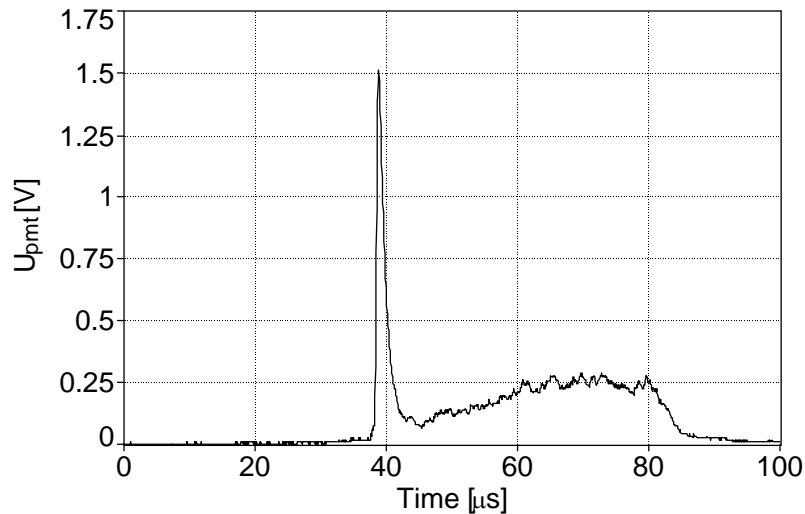


Figure 4. Temporary dependence of one Swan bands C_2 radiation behind the shock wave (SW) front, $\lambda = 4700 \text{ \AA}$, $\Delta\lambda = 78 \text{ \AA}$. Mixture – $CO_2 : N_2 : Ar = 0.096 : 0.003 : 0.901$. Initial pressure $p_1 = 1 \text{ Torr}$, shock wave velocity $V_s = 3.45 \text{ km/s}$. Time is in μs , radiation intensity is in relative values

The modelling of dissociation processes and other chemical reactions in shock wave front was performed in³⁵⁻³⁷. V. Gorelov et al. note the significant concentration peak of NO molecules and penetration of NO molecules into gas before shock wave front³⁸. These precursor phenomena have been fixed for electron concentrations as well as a result of ionization³⁹. So, intensive state-specific radiation near the front of shock waves is the result of strong deviation from Boltzmann distribution.

4. CONCLUSION

Modelling results on physical and chemical processes in thermally nonequilibrium high-temperature gas contain a great body of useful information for applied investigations in different science domains. Their use is provided by application of database and bases of models. The development of protocols of original experimental results is recommended for more effective information utilization. The methods of computer experiments, information-mathematical testing, and comparison with experimental results provide the selection and development of advanced and new models on the base of their simplicity, universality, and reliability for practical applications in the solution of gasdynamics problems.

The created base of models for thermally nonequilibrium reactions provides more realistic representation of real processes, and may be used for fruitful application in flight physics and for solution of practical aerospace problems, e.g. in strong shock waves in air and Martian atmospheres, with combustion and ablation products in boundary layers in flows over body and at nozzles and jets, level spectral radiation, and so on.

5. ACKNOWLEDGEMENTS

Fruitful discussions and collaboration with L.B. Ibragimova, E.G. Kolesnichenko, P.V. Kozlov, E.V. Kustova, E.A. Nagnibeda, M.Yu. Pogosbekian, A.L. Sergievskaya, A.M. Starik, V.N. Yarygina are acknowledged. The author is grateful to T.A. Surzhikova, and N.A. Khrapak for help.

This work was supported by Russian Foundation for Basic Research (grant № 05-08-33438).

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