State-to-State Kinetic Theory Approach for Transport and Relaxation Processes in Viscous Reacting Gas Flows

E.V. Kustova and E.A. Nagnibeda

Department of Mathematics and Mechanics, Saint Petersburg State University,
198504 Universitetskiy pr., 28, Saint Petersburg, Russia

Abstract. In the paper, the description of non-equilibrium reacting gas flows taking into account detailed vibrational and chemical kinetics is considered on the basis of the kinetic theory methods. The kinetic models for transport and relaxation processes are presented, and peculiar features of transport coefficients in the state-to-state approach for reacting flows are demonstrated. Contribution of different dissipative processes to the diffusion velocity and heat flux is discussed. The state-dependent rate coefficients for vibrational energy transitions, dissociation, recombination and exchange chemical reactions are studied in the zero- and first-order approximations of modified Chapman-Enskog method. Practical applications of proposed models for non-equilibrium gas-dynamics problems are discussed.

INTRODUCTION

During the last decades, state-to-state models of non-equilibrium kinetics received much attention in studies of various gas flows. Simultaneous processes of vibrational relaxation and chemical reactions in high-temperature and high-enthalpy flows frequently lead to substantial violations of quasi-stationary distributions. Under such conditions, the consideration of detailed vibrational-chemical kinetics in a flow is needed, and the equations for the molecular level populations should be coupled to the gas-dynamic equations. State-to-state kinetics was studied originally mainly in spatially homogeneous gases. Then the experience accumulated by physical kinetics was used in studies of fluid-dynamics problems. Detailed non-equilibrium kinetics in different flows was considered by Capitelli, Armenise, Colonna et al; Adamovich, Macheret, Rich; Kustova, Nagnibeda; Shizgal, Lordet; Candler et al; Josyula and other authors (see references in [1]). However, in the most of the papers, the state-to-state description of non-equilibrium kinetics was used only for non-viscous non-conductive flows while for the analysis of heat and mass transfer in viscous flows, weakly non-equilibrium models or multi-temperature ones were traditionally applied. Up to now, in the numerical schemes for viscous flows only the zero-order state-dependent reaction rate coefficients are used.

Important advancement was achieved in the state-to-state transport kinetic theory. For the first time this theory was developed in [2] for diatomic gases. The closed sets of equations for the non-equilibrium distributions and flow parameters were derived as well as algorithms for the calculation of the state-dependent transport coefficients (see also [1]). The state-to-state approach for the flows containing three-atomic CO_2 molecules is proposed in [3].

In the present paper, the main problems of the kinetic theory for non-equilibrium reacting gas flows in the state-to-state approach are analyzed. The attention is focused on the state-to-state description of non-equilibrium kinetics and transport properties in viscous flows; the diffusion velocities and heat flux are considered in details. The first-order corrections to the state-specific rate coefficients of energy transitions and chemical reactions are introduced on the basis of the kinetic theory methods. Main problems and perspectives in the development and applications of the state-to-state kinetic theory models are discussed in the paper.

MACROSCOPIC PARAMETERS AND GOVERNING EQUATIONS

Experimental results on the relaxation times of various processes show that, in a wide temperature range, the equilibration of translational and rotational degrees of freedom proceeds much faster compared to the vibrational relaxation

and chemical reactions. It should be noted that rotational transitions may contribute to the state-to-state vibrational kinetics [4], however in the present work we do not take into account rovibrational exchanges.

Under condition of fast translational-rotational relaxation, the kinetic equations for the distribution functions over molecular velocities **u**, rotational and vibrational energy levels j and i, chemical species c may be written in the form

$$\frac{\partial f_{cij}}{\partial t} + \mathbf{u}_c \cdot \nabla f_{cij} = \frac{1}{\varepsilon} J_{cij}^{rap} + J_{cij}^{sl}, \tag{1}$$

where the integral operator of rapid processes J_{cij}^{rap} describes elastic collisions and rotational energy exchange whereas the operator of slow processes J_{cij}^{sl} represents the vibrational energy exchange and chemical reactions proceeding on the gas-dynamic time scale θ. The small parameter ε in Eqs. (1) is the ratio of the characteristic times of rapid and slow processes. The role of rotational transitions in the state-to-state kinetics is studied in [4].

The modification of the Chapman-Enskog method for the Eqs. (1) in the state-to-state approach was proposed in [2] where distribution functions and governing equations were derived in the zero-order and first-order approximations as well as the algorithms for the calculation of transport coefficients. The set of macroscopic parameters in our case includes vibrational level populations of various molecular species n_{ci}, number densities of atomic species $n_{at,c}$, gas velocity **v** and temperature T. The set of governing equations contains the equations of detailed vibrational and chemical kinetics coupled to the conservation equations for the momentum and total energy:

$$\frac{dn_{ci}}{dt} + n_{ci}\nabla \cdot \mathbf{v} + \nabla \cdot (n_{ci}\mathbf{V}_{ci}) = R_{ci}, \qquad c = 1, ..., L, \;\; i = 0, ..., L_c, \tag{2}$$

$$\rho \frac{d\mathbf{v}}{dt} + \nabla \cdot \boldsymbol{P} = 0, \tag{3}$$

$$\rho \frac{dU}{dt} + \nabla \cdot \mathbf{q} + \boldsymbol{P} : \nabla \mathbf{v} = 0. \tag{4}$$

Here L is the number of species, L_c is the number of vibrational levels in species c, U is the total energy per unit mass, $\boldsymbol{P}$ is pressure tensor, **q** is the total heat flux, $\mathbf{V}_{ci}$ are the diffusion velocities. In this case, particles of various chemical species in different vibrational states represent the mixture components, and the corresponding equations contain the diffusion velocities $\mathbf{V}_{ci}$ of molecules at different vibrational states.

The source terms R_{ci} are expressed via the integral operators of slow processes J_{cij}^{sl} and characterize the variation of the vibrational level populations and atomic number densities caused by vibrational energy exchanges and reactions

$$R_{ci} = \sum_j \int J_{cij}^{sl} d\mathbf{u}_c = R_{ci}^{vibr} + R_{ci}^{react}. \tag{5}$$

In the zero-order approximation of the Chapman-Enskog method, $\boldsymbol{P} = p\boldsymbol{I}$ (p is the pressure, $\boldsymbol{I}$ is the unit tensor), $\mathbf{q} = 0$, $\mathbf{V}_{ci} = 0$, and the set of governing equations describes detailed state-to-state vibrational and chemical kinetics in an inviscid non-conductive gas mixture flow in the Euler approximation with Maxwell-Boltzmann distribution over velocities and rotational energies.

TRANSPORT PROPERTIES

In the first order approximation, distribution functions are expressed in terms of the zero-order distribution function $f_{cij}^{(0)}$ and gradients of macroscopic parameters:

$$f_{cij}^{(1)} = f_{cij}^{(0)} \left(-\frac{1}{n}\mathbf{A}_{cij} \cdot \nabla \ln T - \frac{1}{n}\sum_{dk}\mathbf{D}_{cij}^{dk} \cdot \mathbf{d}_{dk} - \frac{1}{n}\boldsymbol{B}_{cij} : \nabla \mathbf{v} - \frac{1}{n}F_{cij}\nabla \cdot \mathbf{v} - \frac{1}{n}G_{cij} \right), \tag{6}$$

where the functions $\mathbf{A}_{cij}$, $\mathbf{D}_{cij}^{dk}$, $\boldsymbol{B}_{cij}$, F_{cij}, G_{cij} are found from the linear integral equations specified by the linearized integral operator for rapid processes [1]. Let us consider transport terms in Eqs. (2)–(4). For the pressure tensor, we obtain

$$\boldsymbol{P} = (p - p_{rel})\boldsymbol{I} - 2\eta\boldsymbol{S} - \zeta\nabla \cdot \mathbf{v}\boldsymbol{I}. \tag{7}$$

Here p_{rel} is the relaxation pressure, η and ζ are the coefficients of shear and bulk viscosity. The additional diagonal terms in the stress tensor connected to the bulk viscosity and relaxation pressure appear due to rapid inelastic TR

energy exchange between the translational and rotational degrees of freedom. The existence of the relaxation pressure is caused also by slow processes of vibrational and chemical relaxation proceeding in the gas-dynamic time scale. If all inelastic non-resonant processes occur slow while rapid processes are specified by only elastic (or pure resonant) collisions, bulk viscosity coefficient and relaxation pressure vanish. Such a situation can happen in the case of slow rotational relaxation in a mixture of light molecules. Relaxation pressure is absent also in the case if all kinetic processes occur rapid.

The diffusion velocity $\mathbf{V}_{ci}$ of molecular components c at the vibrational level i is specified by the expression

$$\mathbf{V}_{ci} = -\sum_{dk} D_{cidk}\mathbf{d}_{dk} - D_{Tci}\nabla\ln T, \tag{8}$$

where D_{cidk} and D_{Tci} are the multi-component diffusion and thermal diffusion coefficients for each chemical and vibrational species, $\mathbf{d}_{ci}$ are the corresponding diffusive driving forces depending on the gradients of n_{ci} and pressure.

The total energy flux has the form

$$\mathbf{q} = -\lambda'\nabla T - p\sum_{ci}D_{Tci}\mathbf{d}_{ci} + \sum_{ci}\left(\frac{5}{2}kT + \langle\varepsilon^{ci}\rangle_{rot} + \varepsilon_i^c + \varepsilon_c\right)n_{ci}\mathbf{V}_{ci}, \tag{9}$$

where $\lambda' = \lambda_{tr} + \lambda_{rot}$ is the thermal conductivity coefficient, $\langle\varepsilon^{ci}\rangle_{rot}$, ε_i^c, ε_c are the mean rotational energy, vibrational energy and that of formation. The coefficients λ_{tr} and λ_{rot} are responsible for the energy transfer associated with the elastic collisions and inelastic TR- and RR rotational energy exchanges. In the state-to-state approach, the transport of the vibrational energy is described by the diffusion of vibrationally excited molecules rather than the thermal conductivity. The diffusion of the vibrational energy is simulated by introducing the independent diffusion coefficients for each vibrational state. It should be noted that all transport coefficients are specified by the cross sections of rapid processes excepting the relaxation pressure depending also on the cross sections of slow processes of vibrational relaxation and chemical reactions.

We can notice that the energy flux and diffusion velocities include along with the gradients of temperature and atomic number densities also the gradients of all vibrational level populations. This constitutes the main feature of the heat transfer and diffusion in the state-to-state approach and the fundamental difference between the state-to-state heat flux and diffusion velocities and those obtained on the basis of one-temperature or multi-temperature quasi-stationary distributions.

The transport coefficients can be written in terms of functions $\mathbf{A}_{cij}$, $\mathbf{D}_{cij}^{dk}$, $\mathbf{B}_{cij}$, F_{cij}, G_{cij}:

$$\eta = \frac{kT}{10}[\mathbf{B},\mathbf{B}], \quad \zeta = kT[F,F], \quad p_{rel} = kT[F,G], \quad D_{cidk} = \frac{1}{3n}\left[\mathbf{D}^{ci},\mathbf{D}^{dk}\right], \quad D_{Tci} = \frac{1}{3n}\left[\mathbf{D}^{ci},\mathbf{A}\right], \quad \lambda' = \frac{k}{3}[\mathbf{A},\mathbf{A}]. \tag{10}$$

Here $[A,B]$ are the bracket integrals associated with the linearized operator of rapid processes [1].

Let us consider the contribution of different processes to diffusion and heat transfer. For the sake of simplicity, we will consider a binary mixture A_2/A. In this case, for the diffusion velocities of molecules at the i-th level $\mathbf{V}_i$ and atoms $\mathbf{V}_a$ we have

$$\mathbf{V}_i = \mathbf{V}_i^{TD} + \mathbf{V}_i^{MD} + \mathbf{V}_i^{DVE}, \qquad \mathbf{V}_a = \mathbf{V}_a^{TD} + \mathbf{V}_a^{MD}. \tag{11}$$

Here, $\mathbf{V}_i^{MD}$, $\mathbf{V}_a^{MD}$, $\mathbf{V}_i^{TD}$, $\mathbf{V}_a^{TD}$, and $\mathbf{V}_i^{DVE}$ are, respectively, the contributions of the mass diffusion, thermal diffusion, and diffusion of vibrational energy

$$\mathbf{V}_i^{MD} = -D_{mm}\mathbf{d}_m - D_{ma}\mathbf{d}_a, \qquad \mathbf{V}_i^{TD} = -D_{Tm}\nabla\ln T, \qquad \mathbf{V}_i^{DVE} = -n\left(\frac{n_m}{D_{mm}} + \frac{n_a}{D_{ma}}\right)^{-1}\nabla\ln\frac{n_i}{n_m},$$

$$\mathbf{V}_a^{MD} = -D_{ma}\mathbf{d}_m - D_{aa}\mathbf{d}_a, \qquad \mathbf{V}_a^{TD} = -D_{Ta}\nabla\ln T. \tag{12}$$

Subscripts "m" and "a" correspond to molecules A_2 and atoms A, respectively. It is obvious that $\mathbf{V}_i^{TD}$, $\mathbf{V}_i^{MD}$ do not depend on the vibrational state i of a molecule and are specified only by its chemical species. These terms formally coincide with the corresponding terms in the relations for the diffusion velocity in the multi-temperature and one-temperature approaches. The difference is determined by the fact that the transport coefficients in these expressions depend on the cross sections of various processes. If we assume, that the diffusion and thermal diffusion coefficients are specified by the cross sections of only elastic collisions, we find

$$\mathbf{V}_i = \mathbf{V}_m^{QS} + \mathbf{V}_i^{DVE}, \tag{13}$$
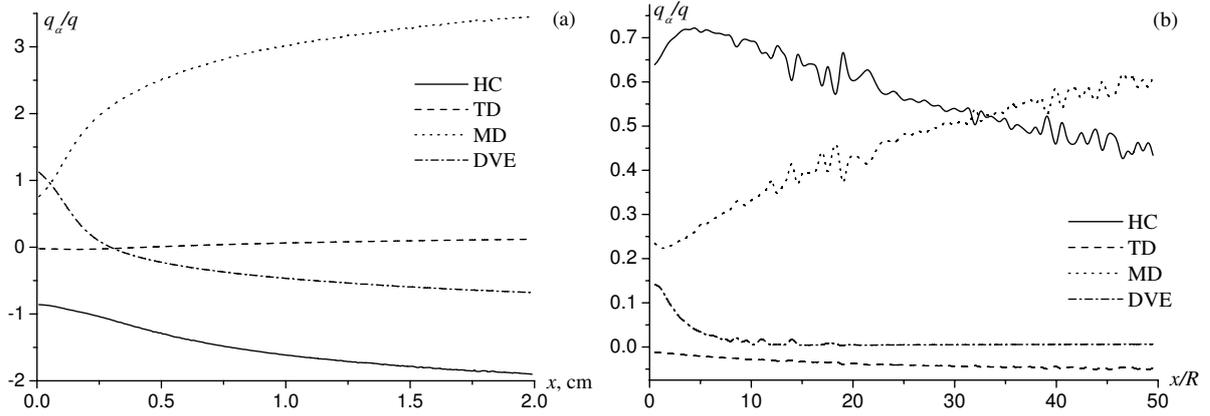
FIGURE 1. Ratio of the heat flux due to various processes (α = HC, TD, MD, DVE) to the total heat flux q (a) behind the shock wave ($T_0 = 293$ K, $p_0 = 100$ Pa, $M_0 = 15$) as a function of the distance x from the front, and (b) in a conic nozzle ($T_* = 7000$ K, $p_* = 100$ atm) as a function of x/R (R is the throat radius).

where $\mathbf{V}_m^{QS}$ is the diffusion velocity of molecules in the quasi-stationary approach, the second term appears only in the state-to-state approach.

The contribution of several dissipative processes to the heat flux can be also distinguished:

$$\mathbf{q} = \mathbf{q}^{HC} + \mathbf{q}^{MD} + \mathbf{q}^{TD} + \mathbf{q}^{DVE}, \tag{14}$$

where $\mathbf{q}^{HC}$, $\mathbf{q}^{MD}$, $\mathbf{q}^{TD}$, and $\mathbf{q}^{DVE}$ are, respectively, energy fluxes associated with the heat conductivity of translational and rotational degrees of freedom, mass diffusion, thermal diffusion, and the transfer of vibrational energy

$$\mathbf{q}^{HC} = -\lambda' \nabla T, \qquad \mathbf{q}^{MD} = \rho_m h_m \mathbf{V}_m^{MD} + \rho_a h_a \mathbf{V}_a^{MD}, \qquad \mathbf{q}^{TD} = -p\left(D_{Tm}\mathbf{d}_m + D_{Ta}\mathbf{d}_a\right) + \rho_m h_m \mathbf{V}_m^{TD} + \rho_a h_a \mathbf{V}_a^{TD},$$

$$\mathbf{q}^{DVE} = \sum_i \left(\frac{5}{2}kT + \langle \varepsilon_j^i \rangle_{rot} + \varepsilon_i\right) n_i \mathbf{V}_i^{DVE}. \tag{15}$$

We can notice that only $\mathbf{q}^{DVE}$ depends explicitly on the non-equilibrium state-to-state vibrational distributions, while the remaining components in Eq. (14) are similar to the corresponding terms in the expressions for the heat flux in the quasi-stationary approaches.

The expressions given above permit to perform a simple limit transition from the equation for the heat flux in the state-to-state approximation to the corresponding relations in the quasi-stationary approaches. Thus, if in a binary mixture of molecules and atoms the quasi-stationary two-temperature or one-temperature vibrational distribution is established in the zero-order approximation, then, assuming the independence of transport coefficients of the cross sections for inelastic collisions, we can obtain the expression for the heat flux directly substituting the quasi-stationary distribution into the formula for $\mathbf{q}^{DVE}$ in the state-to-state approach. A similar limit transition can also be performed for a multi-component gas mixture.

Fig. 1 shows the contribution of different transport processes in the mixture (N_2,N) to the heat flux variation behind a shock wave and in a nozzle flow along its axis. The contribution of thermal diffusion to the heat flux is small in both flows while mass diffusion of atoms is important in the whole flow region. Diffusion of vibrationally excited molecules plays more important role behind a shock than in a nozzle. Close to the shock front, heat conduction and mass diffusion compensate each other, and the main role in the heat transfer belongs to the diffusion of vibrational states. In an expanding flow, $\mathbf{q}^{DVE}$ is not negligible only close to the throat (but does not exceed 15%).

Detailed transport algorithms given in [1] make it possible to apply accurate state-to-state models for transport properties calculations in different flows. However, up to present time in CFD calculations only simplified transport properties obtained for weak deviations from thermal equilibrium were used. Evaluation of the state-dependent transport coefficients in the flows behind shock waves, in nozzles and in a boundary layer has been done using the approximate way: first, macroscopic parameters were found from simplified fluid-dynamics equations and then implemented to the accurate kinetic theory transport algorithms (see [1]). Self-consistent approach based on the direct

implementation of the state-to-state transport kinetic theory algorithms to the CFD code was performed, for the first time, in [5, 6] for a viscous flow of a binary mixture near a body surface. The comparison of the results obtained in the frame of simplified and self-consistent approaches showed a noticeable difference.

REACTION RATE COEFFICIENTS

Now let us consider the source terms R_{ci} in Eqs. (2) expressed as functions of the macroscopic parameters [1]:

$$R_{ci}^{vibr} = \sum_{dki'k'} \left(n_{ci'}n_{dk'}k_{c,i'i}^{d,k'k} - n_{ci}n_{dk}k_{c,ii'}^{d,kk'} \right), \qquad R_{ci}^{react} = R_{ci}^{2\rightleftharpoons 2} + R_{ci}^{2\rightleftharpoons 3},$$

$$R_{ci}^{2\rightleftharpoons 2} = \sum_{dc'd'} \sum_{ki'k'} \left(n_{c'i'}n_{d'k'}k_{c'i',ci}^{d'k',dk} - n_{ci}n_{dk}k_{ci,c'i'}^{dk,d'k'} \right), \qquad R_{ci}^{2\rightleftharpoons 3} = \sum_{dk} n_{dk} \left(n_{c'}n_{f'}k_{rec,ci}^{dk} - n_{ci}k_{ci,diss}^{dk} \right). \tag{16}$$

These expressions contain the rate coefficients for the energy transitions ($k_{c,ii'}^{d,kk'}$), exchange reactions ($k_{ci,c'i'}^{dk,d'k'}$) and dissociation-recombination ($k_{ci,diss}^{dk}$, $k_{rec,ci}^{dk}$):

$$A_{ci} + A_{dk} \rightleftharpoons A_{ci'} + A_{dk'}, \qquad A_{ci} + A_{dk} \rightleftharpoons A_{c'i'} + A_{d'k'}, \qquad A_{ci} + A_{dk} \rightleftharpoons A_{c'} + A_{f'} + A_{dk}. \tag{17}$$

The expressions for the rate coefficients have the following form:

$$k_{(\gamma)} = k_{(\gamma)}^{(0)}(T) + k_{(\gamma)}^{(1)}(n_{ci}, T) + k_{(\gamma)}^{(2)}(n_{ci}, T, \nabla \cdot \mathbf{v}), \tag{18}$$

$k_{(\gamma)}$ for $\gamma = 1, 2, 3, 4$ correspond to the rate coefficients of energy transitions, exchange reactions, recombination and dissociation respectively. The first term defines the zero-order rate coefficients whereas two other terms describe the first-order corrections. For exchange reactions in the zero-order and first-order approximations we have:

$$k_{ci,c'i'}^{dk,d'k'(0)} = \frac{4\pi}{Z_{ci}^{rot}Z_{dk}^{rot}} \left(\frac{m_{cd}}{2\pi kT} \right)^{3/2} \sum_{jlj'l'} \int \exp\left(-\frac{m_{cd}g^2}{2kT} \right) s_j^{ci} s_l^{dk} \exp\left(-\frac{\varepsilon_j^{ci} + \varepsilon_l^{dk}}{kT} \right) g^3 \tilde{\sigma}_{cd,ijkl}^{c'd',i'j'k'l'} dg, \tag{19}$$

$$k_{ci,c'i'}^{dk,d'k'(1)} = -\frac{1}{n} \sum_{jlj'l'} \int \frac{f_{cij}^{(0)} f_{dkl}^{(0)}}{n_{ci}n_{dk}} (G_{cij} + G_{dkl}) g\sigma_{cd,ijkl}^{c'd',i'j'k'l'} d^2\Omega d\mathbf{u}_d d\mathbf{u}_c, \tag{20}$$

$$k_{ci,c'i'}^{dk,d'k'(2)} = -\nabla \cdot \mathbf{v} \frac{1}{n} \sum_{jlj'l'} \int \frac{f_{cij}^{(0)} f_{dkl}^{(0)}}{n_{ci}n_{dk}} (F_{cij} + F_{dkl}) g\sigma_{cd,ijkl}^{c'd',i'j'k'l'} d^2\Omega d\mathbf{u}_d d\mathbf{u}_c. \tag{21}$$

where m_{cd} is the reduced mass, Z_{ci}^{rot}, s_j^{ci} are the rotational partition function and statistical weight, $\mathbf{g}$ is the relative velocity, $\tilde{\sigma}_{cd,ijkl}^{c'd',i'j'k'l'}$ is the integral cross section of a collision resulting in a bimolecular reaction. The expressions for the rate coefficients of the remaining processes have the similar form and are given in [1, 7]. It should be noted that the first-order corrections, contrarily to the zero-order coefficients, depend not only on the temperature but also on the vibrational level populations. Moreover they include the term proportional to the velocity divergence $\nabla \cdot \mathbf{v}$ which is absent in a spatially homogeneous gas. The first order terms are expressed via the functions G_{cij} and F_{cij} which specify the bulk viscosity coefficient and relaxation pressure. The terms proportional to $\nabla \cdot \mathbf{v}$ appear in the case if rapid processes are specified by not only elastic (or purely resonant) collisions but also include some inelastic processes.

It should be noted, that in the practical simulations of dynamics of viscous conducting gases, in the equations of non-equilibrium kinetics (in the state-to-state, multi-temperature or one-temperature approaches), the reaction rate coefficients are calculated using the zero-order distribution function. Up to now, no reliable calculations for the first-order reaction rate coefficients are available; such estimates could make it possible to understand the role of the first-order corrections and to justify their neglecting in the complete set of viscous flow governing equations. In our recent study [8], the expressions connecting the first order corrections to the reaction rate coefficients with bulk viscosity and relaxation pressure in the one-temperature approach are proposed. Calculations of these coefficients for compressing and expanding dissociating nitrogen flows [9] showed the importance of the first-order corrections to the reaction

rates particularly for the recombination reaction. Some asymptotic estimates show that the contribution of the first-order corrections to the reaction rates in the boundary layer equations is small. Nonetheless, in the general case this conclusion is not justified, therefore, the calculation for the first-order reaction rate coefficients under different non-equilibrium conditions still presents an important unsolved problem in chemical kinetics.

The state-depending zero-order rate coefficients for bimolecular exchange reactions have been less thoroughly studied than those for dissociation processes. The accurate theoretical approach to this problem primarily requires a calculation for the state-dependent differential cross sections for reactive collisions, and their subsequent averaging over the velocity and rotational energy distributions. In the recent years, quasi-classical trajectory calculations for the cross sections and state-dependent rate coefficients for atmospheric reactions have been carried out by several authors (see Refs in [10, 11, 1]). For the application of the existing results to the problems of non-equilibrium fluid dynamics, the analytical expressions for the dependence of the reaction rate coefficients on the vibrational states of molecules participating in reactions are needed. The existing analytical approximations for numerical results obtained for particular reactions are sufficiently accurate and convenient for practical use; however, their application is restricted by the considered temperature range. Another semi-empirical approach is based on the generalizations of the Treanor-Marrone model to exchange reactions. These models can be used for more general cases, but a lack of experimental data for validation of parameters in these models restricts their applications. Therefore, the development of justified theoretical models for cross sections of reactive collisions and state-dependent rate coefficients for exchange reactions remains a very important problem of the non-equilibrium kinetics.

CONCLUSIONS

The state-to-state models for transport properties and reaction rate coefficients in reacting flows are studied in the paper. The models based on the kinetic theory give the accurate description of a flow and may be used for practical applications. The state-depending transport properties are given in the form which shows including of different processes in multi-component mixtures to diffusion and heat transfer and demonstrates the peculiarities of the state-to-state approximation. The expressions for the zero-order and first order reaction rate coefficients are presented and can be used for the numerical evaluation of the first-order corrections to the rate coefficients which are usually neglected in CFD simulations. The important current problem is direct implementation of accurate kinetic models for transport and reaction rate coefficients to CFD schemes. Consideration of multi-component reacting flows requires further investigations in molecular dynamics and creation of justified models for reactive collisions.

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