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New Kinetic Models in Non-Equilibrium Aerodynamic Problems

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In the paper, non-equilibrium flows of multi-component reacting mixtures are studied on the basis of the kinetic theory methods. Excitation of internal degrees of freedom for mixture molecules and chemical reactions are considered, and different rates of various kinetic processes are taken into account. The adequate choice of accurate kinetic theory models suitable for applications for different aerodynamic problems is discussed.

The important up-to-date problem of the non-equilibrium aerodynamics is the prediction of flow parameters and transport properties on the trajectories of space vehicles in planetary atmospheres or in expanding high-enthalpy flows in nozzles, jets and expanding tubes. When a space body moving with a hypersonic speed enters a planet atmosphere, a rapid gas compression within a thin shock front calls the temperature jump and then, behind a shock front excitation of internal degrees of freedom of gas molecules and chemical reactions start and may essentially impact gas flow parameters and transport properties near the body. Another situation appears in high-enthalpy expanding flows where strongly non-equilibrium conditions originate due to rapid cooling of the flow. In all these cases the relaxation times of some kinetic processes become comparable with the mean time for changing of main gas dynamic parameters. Therefore the gas dynamic equations should be coupled to the equations of non-equilibrium kinetics, and the choice of an adequate kinetic model becomes very important for prediction of flow parameters with a good accuracy. Many studies are devoted to modelling non-equilibrium kinetic processes in shock heated gases in the Earth or Mars atmospheres or in expanding flows in the frame of different approaches. However, estimations of the accuracy for proposed models and limits of their validity under various practically important conditions are not sufficiently discussed in the literature up to the present time. The kinetic theory methods provide a possibility to derive from the kinetic equations for distribution functions the models which describe non-equilibrium flows of multi-component reacting mixtures with a good accuracy and at the same time are suitable for practical applications.

The objective of the present paper is to show new results obtained by the scientific group of Saint-Petersburg State University in the frame of the detailed state-to-state description proposed in the kinetic theory for reacting five-component air flows and for mixtures containing CO_2 molecules as well as using more simple but sufficiently accurate multi-temperature kinetic models also for the air and CO_2 containing mixtures. The results of applications of these models for the flows behind shock waves and in nozzles are presented. Up to recent time, consideration of the flows of air components in the state-to-state approach were limited only by binary mixtures with dissociation whereas the influence of exchange chemical reactions of NO formation on shock heated or expanding air flow parameters was not studied. In the present paper, these effects are considered. The state-to-state and multi-temperature models are applied for shock heated [1, 2] and expanding [3] five-component air flows. The comparison of flow parameters obtained in the most accurate and simplified approaches showed the influence of vibrational distributions on the gas flow parameters and chemical reaction rates.

Another important problem discussed in the paper concerns state-resolved rate coefficients of energy transitions and chemical reactions entering the equations for vibrational level populations. These coefficients are crucial for the correct state-to-state flow simulations. Many models have been developed for the rate coefficients based on analytical theoretical approaches and molecular dynamics. Quasi-classical

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trajectory calculations (QCT) are efficient and accurate but highly computationally consuming, which prevents their direct application in the computational fluid dynamics (CFD). Existing theoretical models have rather narrow limits of applicability, especially if they are based on fitting experimental data. Therefore there is a need in simple but accurate theoretical models suitable for the implementation to the CFD codes. In the paper [4] the idea was to generalize the simple Treanor–Marrone dissociation model [5] by adjusting its parameters on the basis of the recent reliable QCT data from the Phys4Entry database [6]. The advantage of the new model proposed in [4] is that it does not depend on the vibrational ladder and thus can be used with any vibrational spectrum model. A new model proposed in [7] for the rate coefficients of exchange reactions takes into account vibrational excitation not only of reagents but also products of reactions. This effect is rather important for practical simulations.

The models for vibrational energy transitions are also considered in the paper. The model for vibrational relaxation time [8, 9] generalizes the classical Landau-Teller formula for strongly non-equilibrium flows.

Finally, the peculiarities of state-to-state modelling of CO_2 flows [10] are briefly discussed.

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