Vibrational - Chemical Coupling in High-temperature Air Mixture.

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In the present contribution, kinetic models for vibrational-chemical coupling are proposed for high-temperature air mixture under the conditions of strong deviations from thermodynamic equilibrium. Such conditions occur, for example, on the trajectory of nonexpendable space vehicles in their reentry into the Earth atmosphere, in experiments carried out in high-enthalpy facilities, in supersonic gas flows in nozzles and jets. In these cases, the relaxation time for vibrational degrees of freedom and chemical reactions appear to be comparable with the characteristic time for the variation of basic gas-dynamic parameters of a flow. Therefore, while mathematical modeling of a flow, the equations of gas dynamics and kinetics of non-equilibrium processes should be considered jointly. The set of governing equations for a flow includes not only the conservation equations for the momentum and total energy, but also the equations for chemical and vibrational relaxation. Different models for vibrational- chemical coupling are proposed in a number of papers (see Refs. in [1]). The most rigorous approach is based on the joint consideration of gas dynamic equations and equations for populations of vibrational levels of molecular species and atomic number densities.

In the present paper, the state-to-state approach is used for study of vibrational and chemical kinetics in the space homogeneous 5-component air mixture (N2(i), O2(i), NO(i), N, O) taking into account dissociation, recombination, exchange reactions and vibrational energy transitions. The system containing equations for vibrational distributions and atomic number densities coupled to conservation equations is solved numerically for various test cases. The influence of initial conditions and different reactions on the evolution of molecular level populations, mixture composition, gas temperature and relaxation time is shown.

Along with the state-to-state approximation, non-equilibrium chemical kinetics in the air mixture is studied on the basis of the one-temperature approximation for the space homogeneous case and for the flow behind strong shock waves. The comparison of the mixture composition, gas temperature and heat capacities found in the state-to-state and one-temperature approaches is shown. The results are also compared with ones obtained for binary mixtures of molecules and atoms and using various models of elementary processes. The results may be used for accurate simulations of non-equilibrium air flows.

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References.

1. Nagnibeda, E., Kustova, E.: Nonequilibrium Reacting Gas Flows. Kinetic Theory of Transport and Relaxation Processes. Springer-Verlag, Berlin, Heidelberg , 2009. 252p.