

THE THERMAL NONEQUILIBRIUM PROCESSES IN FULL STATE-TO-STATE LEVEL CHEMICAL KINETICS

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The considerable deviations from Boltzmann distribution over vibrational levels populations of molecules are the result of various strong and sharp actions on a gas, such as shock waves, supersonic nozzle flows and jets, laser irradiation, powerful electrical discharges, intensive combustion, and so on. Under these conditions the most appropriate processes description is provided by a level state-to-state kinetics. Now the main problem in this field is the full level state-to-state kinetics in exchange reactions, for fixed initial states of reagents (m levels) and fixed final states of reaction products (n levels) as well.

Up now, only two models of rate constants, as the coefficients in kinetics equations, describe full level state-to-state kinetics. Starikovskiy vibronic term model is used only for electronic-nonadiabatic processes. The second model is information-theoretical approach, that needs experimental results or calculated data by means of dynamic collision method.

The simulation of full level state-to-state in exchange reactions is successful in solution of the particular dynamic collision problems by means of classical trajectory method, but existing presentations of these full level results are limited to numerical and graphic demonstration without analytical function approximation over gas temperature T and vibrational level numbers m, n .

The recommended formula of rate constant $k(T, m, n)$ for full level state-to-state exchange reactions is presented. The value of this rate constant is dependent on the difference between the energy of vibrational excitation of molecules reagents E_m and reaction products E_n . The model parameters are determined by the calculated results of dynamic collision method for concrete chemical exchange reactions with parallelized supercomputer cluster system.

The application of this model is more useful in solution of full level state-to-state kinetics problems for mixture of components with mechanism included not only chemical exchange reactions, but also dissociation and vibrational-translational energy exchange. The level models of dissociation based on the dynamic collision method and results of generalized Schwarts-Slowsky-Herzfeld theory are used. The specific equilibrium constant in level state-to-state chemical kinetics is being applied for determination of the rate constant of level back reaction when the rate constant of level forward reaction is known as mentioned above.

The example of full level state-to-state kinetics mechanism with these processes in high temperature air mixture is discussed.

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