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Different Approaches to Modeling of Carbon Dioxide Relaxation[1]

ALENA KOSAREVA, OLGA KUNOVA, ELENA KUSTOVA, EKATERINA NAGNIBEDA, Saint-Petersburg State University — Vibrational relaxation of carbon dioxide is studied using strict state-to state (E. Kustova, E. Nagnibeda. AIP Conf. Proc. 2001, I. Armenise, E. Kustova. Chem. Phys. 2014) and simplified multi-temperature approaches (E. Kustova, E. Nagnibeda. Chem. Phys. 2006, A. Kosareva, E. Nagnibeda. J. Phys. Conf. Ser. 2017). The full kinetic scheme considering all vibrational states and different kinds of vibrational energy transitions within and between CO_2 modes is formulated and employed for investigation of 0-D spatially homogeneous relaxation. The analysis of the contributions of different energy transitions to relaxation is presented, and the most efficient and accurate kinetic scheme is determined in the state-to-state approximation. A comparison of the flow parameters obtained using the state-to-state and simplified approximations is made for two typical cases corresponding to a compressed gas (excitation regime) and to an expanding flow (deactivation regime). Reduced-order models are evaluated by comparison with the results of full state-to-state simulations. Possible sources of errors and differences between approaches are identified and ways of improving multi-temperature models are proposed.

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