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Uncertainties in Multi-temperature CO₂ Radiation Models

ULYSSE DUBUET, ERWAN PANNIER, CHRISTOPHE LAUX, Laboratoire EM2C, CentraleSupélec, CNRS, Université Paris-Saclay — Multi-temperature distributions are a convenient way to describe nonequilibrium gases close to equilibrium. However, they can require an arbitrary energy partitioning. We present a general method to determine the uncertainties of multi-temperature models. The contribution of each energy mode is calculated in the diagonal basis of the molecular Hamiltonian, and the various possible assignments of the energy terms and groupings of the temperatures are compared. The method is applied to the CO₂ molecule: we determine the nonequilibrium temperature ranges where the calculated nonequilibrium partition functions are insensitive to the assignment or grouping scheme. We then compare the results of this advanced model to the partition functions computed with a simple, uncoupled vibrating rotor (UVR) model. We show that the advanced model only slightly increases the domain of validity compared to the UVR model. We also demonstrate that the uncertainty induced by the assignment of the coupling terms cannot be neglected outside this validity domain. The implications for spectral modeling of nonequilibrium plasma discharges is discussed.

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