New Challenges in Modeling Non-equilibrium Carbon Dioxide Flows

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Carbon dioxide is a major species in the Mars and Venus atmospheres, which makes studies of its physical and chemical kinetics of vital importance for space exploration programs [1]. On the other hand, CO_2 is the key indicator of human impact on the Earth environment; development of efficient vibrationally driven techniques of CO_2 conversion requires a deep knowledge of elementary collisional processes and kinetics of excited states [2]. The carbon dioxide molecule has three vibrational modes and, therefore, multiple vibrational relaxation channels including intra- and inter mode transitions; the rates of energy exchanges strongly vary with the temperature and, under certain conditions, differ by several orders of magnitude.

The objective of the present study is to develop self-consistent mathematical models of different complexity to describe non-equilibrium carbon dioxide flows. The models are derived starting from the Boltzmann equation using the kinetic theory methods proposed in [3]. As the first step, kinetic scaling of elementary collision processes is established, based on available experimental data. The collision operator is then naturally split to the terms responsible for the rapid and slow (compared to the gas-dynamic time scale) processes. The generalized Chapman–Enskog method is applied to derive closed sets of flow governing equations in the Euler (inviscid) and Navier–Stokes (viscous) approximations. In each approximation, the model includes constitutive relations for the transport terms and the relaxation terms for multiple intra- and inter-mode vibrational energy exchanges coupled to chemical reactions; algorithms for the transport coefficients evaluation are developed. Three levels of non-equilibrium flow description are discussed: state-to-state, multi-temperature with different temperatures of CO_2 vibrational modes, and one-temperature.

As applications of the developed models, several challenging problems are considered. First, we discuss an issue of large bulk viscosity in CO_2 reported in [4] and later argued in [5, 6]; it is shown that uncoupling rotational and vibrational relaxation results in essential overprediction of the bulk viscosity coefficient under low temperature conditions. Then we study the shock wave structure in carbon dioxide using several continuum approaches [7] and compare it with that obtained on the basis of the model kinetic equation [8]. Finally, we apply the state-to-state model to simulate the vibrational-chemical kinetics, gas dynamics and heat transfer along the stagnation line under Mars entry conditions [9]; the effect of various sets for the state-resolved reaction rate coefficients on the mass and heat fluxes is assessed.

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REFERENCES

[1] P. Reynier, *Progress in Aerospace Sciences* **70**, 1–27 (2014).
[2] A. Fridman, *Plasma Chemistry* (Cambrigde University Press, New York, 2008).
[3] E. Nagnibeda, E. Kustova, *Nonequilibrium Reacting Gas Flows. Kinetic Theory of Transport and Relaxation Processes* (Springer-Verlag, Berlin, Heidelberg, 2009).
[4] M. S. Cramer, *Phys. Fluids* **24**, 066102 (2012).
[5] E. Kustova, M. Mekhonoshina, A. Kosareva, *Phys. Fluids* **31**, 046104 (2019).
[6] Y. Wang, W. Ubachs, W. van de Water, *J. Chem. Phys.* **150**, 154502 (2019).
[7] I. Alekseev, A. Kosareva, E. Kustova, E. Nagnibeda, *AIP Conference Proceedings* **2132**, 060005 (2019).
[8] S. Kosuge, K. Aoki, *Phys. Rev. Fluids* **3**, 023401 (2018).
[9] E. Kustova, A. Savelev, I. Armenise, *J. Phys. Chem. A* **123**, 10529–10542 (2019).