An ES-BGK Model for Non-Polytropic Polyatomic Gases

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Abstract

In the study of rarefied polyatomic gases, the ES-BGK model is widely used to represent the collisional term in the Boltzmann equation. However, the standard ES-BGK model struggles with non-polytropic gases, where specific heat depends on temperature. Recently, Kosuge, Kuo, and Aoki (J. Stat. Phys. 177, pp. 209-251 (2019)) proposed an extended model for non-polytropic gases with continuous microscopic energy levels, but it does not satisfy the H-theorem and fails to provide closure of the moment equations via the maximum entropy principle.

To address these shortcomings, we propose a new ES-BGK model for non-polytropic gases, using the kinetic framework of the Borgnakke-Larsen model incorporating continuous energy levels of the molecular internal modes. A key attribute of the proposed ES-BGK model is the internal state density function, which depends solely on the microscopic energy of internal modes, unlike the temperature-dependent formulation in previous studies. This formulation satisfies the H-theorem and allows for the closure of moment equations using the maximum entropy principle, following the procedure of Rational Extended Thermodynamics.

We also present a case study on planar shock waves in carbon dioxide. Our results generally agree with previous studies, except for the internal temperature profile, which is qualitatively distinct and more physically consistent.