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Central-Moment Discrete Boltzmann Method for Reactive Flows

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Abstract. A central-moment discrete Boltzmann method (CDBM) is proposed for reactive flows, accommodating adjustable specific heat ratios and Prandtl numbers. In the framework of CDBM, a unified set of kinetic equations is used to delineate both macroscopic quantities and higher-order central moments. Via these central moments, the nonequilibrium effects that are directly related to the thermal fluctuation beyond conventional hydrodynamic governing equations can be quantified. Moreover, the discrete Boltzmann equation of the CDBM is simpler than that of previous multiple-relaxation-time DBMs, owing to the elimination of the additional term in the DBM. Furthermore, this method is capable of modeling supersonic compressible reactive flows characterized by high Mach numbers. The model is verified through simulations encompassing sound waves, shock waves, thermal Couette flows, regular shock reflections, and supersonic reactive waves.

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1 Introduction

Reactive flows refer to fluid flows with chemical reactions which include a broad range of phenomena, such as flames, detonations, chemical lasers and the earth's atmosphere.

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Applications can be found in the field of transportation, energy generation and materials processing [1]. The research on reactive flows is also a key issue to change the atmospheric pollution, climate change and global warming which are directly relevant to harmful emissions from reactive flows. However, reactive flows are known to be a challenge for numerical simulations due to a large number of coupled physicochemical processes and scales both in time and space [1, 2]. All of the processes, such as the chemical reactions, subsequent heat release, and the fluid dynamics, must be considered simultaneously [1, 2]. In addition, the influence of hydrodynamic and thermodynamic nonequilibrium effects are significant around sharp physical gradients, which are common in violent reacting flows. This increases the complexity of the problem and the difficulty of research, because the nonequilibrium effects always change density, velocity, temperature, etc., in the evolution of fluid systems away from equilibrium, especially in transient and/or extreme conditions [3, 4].

Serving as the cornerstone of kinetic theory, the Boltzmann equation provides the potential to effectively and accurately simulate intricate nonequilibrium flows across a broad spectrum of spatiotemporal scales. In 1997, Succi et al. established the first lattice Boltzmann model (LBM) applied to reactive flows and successfully simulated the methane/air diffusion flame problem in the limit of fast chemistry [5]. Since then, and up until the late 2010s, there are some progress of LBM in combustion research [6–11], but all limited to a simplified case in the absence of a good compressible realization, persistent issues with stability of solvers and the absence of multi-species formulations [12]. As a promising kinetic method, remarkable progresses have been made by using LBM in recent years. For example, in 2019, Hosseini et al. proposed a hybrid lattice Boltzmann-finite difference numerical scheme for the simulation of reacting flows at low Mach number and simulated three-dimensional counter-flow premixed flame [13]. In 2022, Sawant et al. proposed a LBM for compressible reacting multi-species flows recovering the Stefan–Maxwell diffusion closure together with barodiffusion [14]. In 2023, a new finite-volume schemes based on the LBM for simulations of gaseous detonations have been proposed by Gauthier et al. [15]. Despite their progress, most LBMs for combustion are limited to low Mach number reactive flows and all ignore a variety of thermodynamic nonequilibrium effects included in the Boltzmann equation.

In parallel with efforts to develop standard LBMs for reactive flows simulations, other attempts at developing Boltzmann-based models have also made progress, such as discrete Boltzmann method (DBM), which has been developed and successfully used in various complex systems [16–22]. In particular, the DBM introduces higher-order kinetic moments so that hydrodynamic and thermodynamic fields are fully coupled, macroscopic equations can be recovered accurately [23]. Furthermore, the DBM can bring deeper insights into the hydrodynamic and thermodynamic nonequilibrium effects beyond the Navier-Stokes (NS) equations [23]. In 2012, Xu et al. first proposed the idea that the physical quantities and nonequilibrium information of a system can be described and extracted with the help of kinetic moments of distribution functions [24]. In 2013, Yan et al. were pioneers in proposing a DBM for detonations, employing the Lee–Traver reaction