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Gas-Kinetic Unified Algorithm for Multi-Component Monatomic Gas Mixture

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Abstract. In recent decades, gas-kinetic unified algorithm (GKUA) based on Boltzmann model equation has been proposed, which is suitable for the whole regimes gas flows. The original GKUA is designed for single-component gas flows. In this work, we extend GKUA to multi-component monatomic gas mixture flows based on the Andries-Aoki-Perthame (AAP) model. The algorithm are validated by the steady normal shock wave structure problem, the flow around two-dimensional circular cylinder and the pressure/temperature gradient driven microchannel flow problems. Simulation results are in good agreement with those obtained by other methods, which verifies the reliability of the proposed algorithm for the simulation of multi-component monatomic gas mixture. Then, taking the 25N attitude control engine two-dimensional profile as the object, the study of two-dimensional profile nozzle internal and external mixed flow problem is carried out, and the influences of the component concentration ratio and mass ratio on the molecular transport in the engine internal and external mixed flow field are discussed.

AMS subject classifications: 35Q20, 76P05, 82C40

Key words: Gas mixture, gas-kinetic unified algorithm, Boltzmann model equation, vacuum plume, microchannel flow.

1 Introduction

Vacuum plume problem of attitude orbit control engine of in-orbit spacecraft is a cross-regime problem involving continuum flow, rarefied transition flow and free molecular flow. Engine gas is a multi-component gas mixture. In addition to the common characteristics of the general single-component gas flow, the gas flow also involves the interaction between components and between components and solid boundary, producing phenomena such as Baro diffusion and Ghost effect [1,2], and the transport mechanism is

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complex. Multi-component gas mixture flow involves pressure gradient driven, temperature gradient driven and concentration gradient driven. The diffusion and flow of the gas will drive the mass transport and affect the flow [3,4]. At the same time, the chemical compositions and components of gas mixture will affect the gas transport. Therefore, the study of multi-scale flow mechanism of gas mixture is helpful to enrich people's understanding of the basic fluid transfer process, and has important practical significance and application background.

There are two ways to study multi-scale flow of gas mixture. One is the coupling method [5,6] of traditional computational fluid dynamics (CFD) method based on Euler/Navier-Stokes (Euler/N-S) equation and discrete velocity method/direct simulation Monte Carlo (DVM/DSMC) method based on Boltzmann equation. Since it is a coupling method in nature, both the accuracy and stability need to be considered when designing coupling ideas, and the problem of statistical fluctuation caused by DSMC method always exists. The other is a unified method [7–15] based on gas-kinetic theory, which aims to use one method to simulate the multi-scale flow problem in the whole regimes. Among them, Wang et al. [7] developed a unified gas kinetic scheme for two-component gas mixture based on the AAP model [16], and simulated the whole regimes flow problem of two-component gas mixture composed of Hard Sphere (HS) molecules. Zhang et al. [8, 9] developed a discrete unified gas kinetic scheme for two-component gas mixture based on the AAP model and McCormack model [17], and analyzed and compared the two kinetic models. According to Zhang's research, McCormack model is suitable for low velocity or small gradient driven (pressure, temperature, concentration) flow problems, and AAP model can effectively simulate the high-speed flow problem of two-component gas mixture. Wu et al. [10] developed a gas-kinetic unified algorithm for chemical reactions of multi-component gas mixture, and carried out the algorithm verification, and the effect is very good. Xu et al. [13, 14] developed a unified gas-kinetic scheme for multiscale and multicomponent flow transport based on AAP model.

In the past two decades, the gas-kinetic unified algorithm proposed by Li [18–20] for the whole regimes flow of single-component gases has been greatly developed and applied. At present, numerical models and algorithms considering thermodynamic non-equilibrium effects (including rotational energy excitation, continuous energy level vibrational energy excitation and discrete quantum energy level vibrational energy excitation) [21–23] and thermochemical non-equilibrium effects [24] have been developed. Combined with large-scale parallel computing platform [25], it is widely used in microchannel flow [26], external force driven flow [27], high-altitude aircraft flow around [28] and other fields. According to the characteristics of AAP model, which can effectively simulate the high-speed flow problem of two-component gas mixture and has simple structure, and is easy to be extended to multi-component gas mixture, this paper develops a gas-kinetic unified algorithm of multi-component monatomic gas mixture based on AAP model, and applies it to the study of engine vacuum plume problem.

The structure of this paper is arranged as follows: Section I introduces the relevant background, and Section 2 introduces the computable modeling of Boltzmann equation