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PROCEEDINGS

Multicomponent Discrete Boltzmann Method for Compressible Reactive Flows with Thermodynamic Nonequilibrium Effects

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ABSTRACT

In many real-world scenarios, such as high-speed combustion processes and re-entry flows in aerospace vehicles, the flow conditions often involve complex interactions between multiple chemical species and energy modes, leading to thermodynamic nonequilibrium effects. Traditional computational fluid dynamics (CFD) methods struggle to accurately capture these phenomena due to their simplifying assumptions regarding equilibrium thermodynamics. To solve this issue, the Multicomponent Discrete Boltzmann Method (MDBM) is proposed as a numerical approach to simulate compressible reactive flows with thermodynamic nonequilibrium effects. Based on kinetic theory, this method can capture the complex interactions between different species and energy modes in reactive flows. The MDBM is capable of handling chemical reactions, mass transfer, and energy exchange between species, making it suitable for a wide range of reactive flow problems. The method is validated through simulations of shock-tube problems and combustion flows, demonstrating its capability to accurately predict thermodynamic nonequilibrium effects in reactive flows. From an academic standpoint, the MDBM contributes to the advancement of CFD methodologies by bridging the gap between continuum-based approaches and molecular dynamics simulations. It provides a more detailed and fundamental understanding of complex fluid dynamics phenomena, which is crucial for developing improved models and theories in fluid mechanics and combustion science. In practical applications, the MDBM has the potential to enhance the design and optimization of various engineering systems. By accurately predicting thermodynamic nonequilibrium effects, engineers can improve the efficiency, safety, and performance of aerospace vehicles, chemical processes, and combustion devices. Overall, the MDBM provides a promising approach for studying complex reactive flows and is crucial for advancing our prediction capabilities in various engineering applications, such as aerospace propulsion, chemical reactors, and combustion systems.

KEYWORDS

Discrete Boltzmann method; reactive flow; nonequilibrium effect; multicomponent

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