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Kinetic modeling of detonation and effects of negative temperature coefficient

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The kinetic modeling and simulation of reactive flows, especially for those with detonation, are further investigated. From the theoretical side, a new set of hydrodynamic equations are deduced, where the viscous stress tensor and heat flux are replaced by two non-equilibrium quantities that have been defined in our previous work. The two non-equilibrium quantities are referred to as Non-Organised Momentum Flux (NOMF) and Non-Organised Energy Flux (NOEF), respectively, here. The numerical results of viscous stress (heat flux) have a good agreement with those of NOMF (NOEF) near equilibrium state. Around sharp interfaces, the values of NOMF (NOEF) deviate reasonably from those of viscous stress (heat flux). Based on this hydrodynamic model, the relations between the two non-equilibrium quantities and entropy productions are established. Based on the discrete Boltzmann model, four kinds of detonation phenomena with different reaction rates, including Negative Temperature Coefficient (NTC) regime, are simulated and investigated. The differences of the four kinds of detonations are studied from three aspects: hydrodynamic quantities, non-equilibrium quantities and entropy productions. It is found that, the effects of NTC on hydrodynamic quantities are to lower the von-Neumann peaks of density, pressure, and velocity, to broaden the reaction zone, and to subdue the chemical reaction. It may also vanish the peak of temperature. Consequently, the effects of NTC are to widen the non-equilibrium regions and reduce the amplitude of the non-equilibrium effects in the reaction zone. Besides, it is also found that the (local) entropy production has three sources: the chemical reaction, NOEF and NOMF. As for the global entropy production in the system, the portion caused by reaction is much larger than the other two, and the portion caused by NOMF is larger than that by NOEF. Furthermore, the effect of NTC is to widen the region with entropy production caused by reaction and lower the global entropy productions caused by reaction, NOMF and NOEF, which means that NTC drives detonation closer to an isentropic process.

1. Introduction

Detonation is a special case of combustion which is the major energy conversion process and plays a dominant role in the transportation and power generation. It is a kind of chemical reaction phenomenon accompanied with violent energy release [1–4]. The system with detonation can generally be regarded as a kind of chemical reactive flow. The controlled detonation has long been extensively used in various engineering problems. Typical examples are referred to Pulse Detonation Engine [5], Rotating Detonation Engine [6,7], Oblique Detonation ramjet-in-Tube [8], etc.

A detonation process may involve many species of reactants and a large number of reactions. For example, the CH_4/air detonation involves 53 kinds of species and 325 reactions [9,10] and *n*-heptane/air includes 2540 reversible elementary reactions among 556 species [11]. The reaction rate generally varies with the specific reaction. For a practical detonation, the varieties of reactant species, shock strength, local temperature, specific volume, premixing homogeneity may guide the reactions into different chains. Consequently, the final detonation process may show different mechanical and thermodynamical behaviours according to the specific conditions. Therefore, the global reaction

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rate may show non-monotonic dependence on the temperature, even though the reaction rate shows exponential dependence on temperature in common cases, just like what the Arrhenius model describes. In fact, the phenomena related to Negative Temperature Coefficient (NTC) have been observed [11–14]. Physically, the occurrence of NTC may lead to significant different detonation behaviours. To the authors' knowledge, however, its possible effects have not obtained careful investigations.

It has been realised that various non-equilibrium behaviours extensively exist in the combustion and detonation phenomena [15]. But those complicated behaviours and their possible effects have far from been well studied. It has also been well known that the traditional hydrodynamic modeling based on Euler or Navier–Stokes (NS) equations is not enough to describe such complicated non-equilibrium behaviours. The spatial-temporal scales that those complicated non-equilibrium behaviours make effects are much larger than those that the molecular dynamics can access. Under such cases, to investigate the possible effects of the non-equilibrium behaviours, a kinetic model based on the Boltzmann equation becomes preferable.

As a special discretisation of the Boltzmann equation, the Lattice Boltzmann Method (LBM) [16–20] has long been attempted to simulate combustion phenomena [21–28]. The first work was given by Succi et al. [21] in 1997. In those previous studies, the LBM works as a kind of alternative numerical scheme. The combustion systems are described by some kinds of hydrodynamic models.

To extend the LBM to model and simulate the detonation phenomena with complicated non-equilibrium behaviours, at least two technical bottlenecks must be broken through. The first one is to extend its application range to the cases where the Mach number is larger than 1. The second is that the improved model must be some kinetic model which not only can recover, in the hydrodynamic limit, but also is beyond the traditional NS model. As was shown in recent years, one solution to the first bottleneck is to come back to the Finite-Difference(FD) LBM [29]. In the FD-LBM, the discretisation of the particle velocity space is independent of the discretisations of the space and time. This independence, together with the flexibilities in choosing FD scheme and in discretising the particle velocity space, makes it easier for the numerical system to satisfy the von-Neumann stability condition in the cases with high Mach number compressible flows. The solution to the second bottleneck sees also significant progress in recent years. The LBM has been extended to investigate various non-equilibrium behaviours in complex flows [29–32]. Via such a modeling some new physical insights into the complex flows have been obtained. The observations have also been promoting the development of related methodology. For example, the strength of the non-equilibrium increases in the spinodal decomposition stage and decreases in the domain growth stage. Consequently, it can work as a kind of physical criteria to discriminate the two stages [33]. Different kinds of interfaces, such as material interface and mechanical interface, compressive wave and rarefactive wave, show different specific non-equilibrium properties. Consequently, the Thermodynamic Non-Equilibrium(TNE) can be used to distinguish various interfaces [34]. The TNE behaviours in complex flows have also been used in interface-tracking scheme designs [35]. It has been found that the viscosity (heat conductivity) decreases the local TNE but increases global TNE around the detonation wave [36]. Such an extended lattice Boltzmann kinetic model or discrete Boltzmann model (DBM) should follow more strictly some necessary kinetic moment relations of the local equilibrium distribution function f^{eq}. In a recent study a double-distribution function DBM was proposed, where one distribution function is used to describe the reactant, the other distribution function is used to describe the reaction product [37]. This DBM corresponds to the so-called "two-fluid" hydrodynamic model for combustion.

Entropy production is a highly concerned quantity in both physics and engineering studies. From the physics side, it is helpful for understanding the complex non-equilibrium behaviours. From the engineering side, a process with lower entropy production may have a higher energy transformation efficiency.

The objective of the present work is two-fold. Firstly, we further develop the DBM to investigate various non-equilibrium behaviours in combustion, especially in detonation phenomena, aiming to establish a relation between the TNE and the entropy production. Secondly, via a newly composed reaction function, we investigate the possible influences of the NTC on the behaviour of detonation in hydrodynamic quantities, TNE and entropy productions.

The organisation of the present paper is as below. In Section 2 we present the new form of fluid hydrodynamic equations, and establish the relations between TNE and entropy production, then briefly review the DBM and the newly composed reaction rate function. In Section 3 we validate the model by simulating two classical detonation benchmarks. In Section 4, we simulate four kinds of detonations with different temperature dependent reaction rates, analyze the differences of the four cases, and summarise the effects of NTC on detonation. Section 5 concludes the present paper.

2. Models and methods

2.1. Kinetic and hydrodynamic models, non-equilibrium effects and entropy production

The kinetic model based on Boltzmann equation with chemical reaction has a form as follows:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \Omega + C, \tag{1}$$

where f indicates the distribution function of particle velocity, $\mathbf{v}$ indicates the particle velocity, t is temporal coordinate, Ω and C are the collision term and chemical reaction term, respectively. The equilibrium distribution function of velocity particle in Eq. (1) reads:

$$f^{eq} = \rho \left(\frac{1}{2\pi T}\right)^{D/2} \left(\frac{1}{2n\pi T}\right)^{1/2} \exp\left[-\frac{(\mathbf{v}-\mathbf{u})^2}{2T} - \frac{\eta^2}{2nT}\right]. \tag{2}$$

where ρ indicates density, D indicates spatial dimension and $\mathbf{u}$ is hydrodynamic velocity. η is a free parameter introduced to describe the n extra degrees of freedom corresponding to molecular rotation and/or vibration [38]. The central moment $\mathbf{M}_2^*$, $\mathbf{M}_{3,1}^*$ and thermodynamic non-equilibrium quantities $\boldsymbol{\Delta}_2^*$, $\boldsymbol{\Delta}_{3,1}^*$ are defined as [39]

$$\mathbf{M}_2^*(f) = \int\int f(\mathbf{v}-\mathbf{u})(\mathbf{v}-\mathbf{u})d\mathbf{v}d\eta, \tag{3}$$

$$\mathbf{M}_{3,1}^*(f) = \int\int f(\mathbf{v}-\mathbf{u})\cdot(\mathbf{v}-\mathbf{u})(\mathbf{v}-\mathbf{u})d\mathbf{v}d\eta, \tag{4}$$

$$\boldsymbol{\Delta}_2^* = \mathbf{M}_2^*(f) - \mathbf{M}_2^*(f^{eq}), \tag{5}$$

$$\boldsymbol{\Delta}_{3,1}^* = \mathbf{M}_{3,1}^*(f) - \mathbf{M}_{3,1}^*(f^{eq}). \tag{6}$$

Taking the velocity moment $\int\int d\mathbf{v}d\eta$ of the Eq. (1) gives the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0. \tag{7}$$