Combustion and Flame 196 (2018) 249–254

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

A Lattice-Boltzmann model for low-Mach reactive flows

Yongliang Feng, Muhammad Tayyab, Pierre Boivin*

Aix Marseille Univ, CNRS, Centrale Marseille, M2P2, Marseille, France

ARTICLE INFO

Article history:
Received 22 March 2018
Revised 16 April 2018
Accepted 24 June 2018

Keywords:
Lattice Boltzmann
Reacting flows
Combustion

ABSTRACT

A new Lattice-Boltzmann model for low-Mach reactive flows is presented. Based on standard lattices, the model is easy to implement, and is the first, to the authors' knowledge, to pass the classical freely propagating flame test case as well as the counterflow diffusion flame, with strains up to extinction. For this presentation, simplified transport properties are considered, each species being assigned a separate Lewis number. In addition, the gas mixture is assumed to be calorically perfect. Comparisons with reference solutions show excellent agreement for mass fraction profiles, flame speed in premixed mixtures, as well as maximum temperature dependence with strain rate in counterflow diffusion flames.

1. Introduction

Industries from the aerospace, aeronautic and automotive sectors are increasingly relying on numerical simulation tools. From the occasional use of a research and development department, these tools progressively made it to conception and production departments, where they help to continuously improve designs. The field of low-Mach external aerodynamics and aeroacoustics, have been particularly impacted by the rapid development of Lattice-Boltzmann (LB) methods [1] in the last five to ten years. From industrial benchmarks [2–4], these methods quickly ramped up to full scale applications: full-scale cars [5,6], full-scale aircraft engines [7] and even full-scale aircrafts [8,9], oftentimes with outstanding results.

Combustion modeling in the LB framework, however, remain relatively marginal within the combustion community. A hybrid finite difference lattice Boltzmann model has been presented for the simulation of low Mach number flows with significant density changes by Filippova and Hanel [10] almost twenty years ago. An LB model for combustion modeling was then presented by Yamamoto et al. [11–13] for steady and unsteady reactive flows. About ten years ago, a pressure-based lattice Boltzmann model was presented by Chen et al. for low Mach number combustion simulations by Chen et al. [14,15], based on an incompressible LB model developed earlier by Guo et al. [16]. An entropic lattice Boltzmann model on two-dimensional standard lattice was also presented for compressible thermal flows and extended to combustion applications [17,18]. More recently, detailed kinetics were successfully implemented in the LB framework [19,20].

Thermodynamic closure is one of the key issues in extending the LB capabilities from low-Mach aerodynamics and aeroacoustics to reactive flows, and obtaining satisfactory results in cases with significant thermal expansion is challenging, as indicated by the low-number of combustion models in the LB context. Most of LB models mentioned above for reactive flows were specifically applied under constant pressure, and lack full coupling between thermodynamics and the flow. In particular, because their equilibrium density distribution function only depends on the local density, hydrodynamic pressure and velocity, and not on temperature, these models may fail at setting in motion fluids at rest when heat-release is applied. This aspect is however critical in representing canonical combustion phenomena, such as ignition in a mixing layer, or the dynamics of freely propagating flame in a premixed mixture.

To address this issue, more complex, multi-speed models with aid of finite volume approach were developed for subsonic and supersonic flows [21], including detonations. Alternatively, coupled lattice Boltzmann models on standard lattices have been investigated in low Mach thermal compressible flows [22,23].

The model presented in this work is based on the latter [23] and takes full advantage of the simplicity and practicality of standard lattice models. It is able to deal with multi-component, calorically perfect gas mixtures, and the coupling between the thermodynamics and the flow is two-way. Simplified transport properties are considered, with non-unity Lewis number set for each component. This new LB model for low-Mach reactive flows is presented in the first Section. The second Section validates the model using Cantera [24] as a reference on canonical combustion test cases of premixed and non-premixed combustion.

* Corresponding author.
E-mail addresses: pierre.boivin@polytechnique.edu, pierre.boivin@univ-amu.fr (P. Boivin).

https://doi.org/10.1016/j.combustflame.2018.06.027
0010-2180/

2. Lattice-Boltzmann combustion modeling

Introductory comments: athermal LB method

Lattice Boltzmann methods intend to solve the continuous Boltzmann equation through discretization of space, time, and velocity [1,25,26]. In the so-called *DnQm* model, a *n*-dimensional physical space is filled with a regular lattice (or a Cartesian grid) and velocity space is discretized on a set of lattice tensor $\boldsymbol{E}_{\boldsymbol{m}}^{\boldsymbol{n}} = [\boldsymbol{c}_0, \ldots, \boldsymbol{c}_i, \ldots, \boldsymbol{c}_{m-1}]$. On every lattice node $\boldsymbol{x}$, $f_i(\boldsymbol{x}, t)$ denotes the density distribution of particle with velocity $\boldsymbol{c}_i$, thus the local density ρ and momentum $\rho\boldsymbol{u}$ are defined as $\rho = \Sigma_i f_i$ and $\rho\boldsymbol{u} = \Sigma_i \boldsymbol{c}_i f_i$.

A single time relaxation process is used to model the collision term of Boltzmann equation in this study, which is the so-called Bhatnagar–Gross–Krook (BGK) model [27,28].

$$f_i(\boldsymbol{x} + \boldsymbol{c}\delta t, t + \delta t) - f_i(\boldsymbol{x}, t) = -\frac{1}{\tau}[f_i(\boldsymbol{x}, t) - f_i^{eq}(\boldsymbol{x}, t)], \tag{1}$$

where τ is the relaxation parameter, δt is the time increment and $\delta t = \delta\boldsymbol{x}/\boldsymbol{c}$. $f_i(\boldsymbol{x}, t)$, $f_i(\boldsymbol{x} + \boldsymbol{c}\delta t, t + \delta t)$ are the distribution functions associated with the *i*th discrete velocity $\boldsymbol{c}_i$, and f_i^{eq} is the *i*th equilibrium distribution function given by Qian et al. [1,25]

$$f_i^{eq} = \rho w_i\left[1 + \frac{\boldsymbol{c}_i \cdot \boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i \cdot \boldsymbol{u})^2}{2c_s^4} - \frac{\boldsymbol{u}^2}{2c_s^2}\right], \tag{2}$$

where w_i is the weight coefficient associated to discrete velocity $\boldsymbol{c}_i$ and c_s is sound speed.

Using the Chapman–Enskog multiscale technique [28], the equivalent Navier–Stokes equations can be recovered as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\boldsymbol{u}) = 0, \tag{3}$$

$$\frac{\partial \rho\boldsymbol{u}}{\partial t} + \nabla \cdot (\rho\boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot \left[\rho\nu(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T)\right], \tag{4}$$

where the kinematic viscosity ν is related to the relaxation parameter through

$$\tau = \frac{\nu}{c_s^2\delta t} + \frac{1}{2}. \tag{5}$$

And, the pressure is related to the density by the equation of the state $p = \rho c_s^2$. The equation of state used in this base model is clearly not suitable for reactive flows, as no temperature is considered. The most simple acceptable equation of state for reactive flows is probably the ideal gas law, relating the gas pressure and temperature through

$$p = \rho\bar{r}T, \tag{6}$$

where $\bar{r} = R/\overline{W}$, with R the gas constant, and

$$1/\overline{W} = \sum_k Y_k/W_k,$$

linking the mean molecular weight $\overline{W}$ to the species molecular weights W_k and the species mass fractions Y_k.

A hybrid thermal LB model

Considering the third order Hermite expansion of Maxwell–Boltzmann distribution, one can obtain the equilibrium distribution function in discrete Gauss–Hermite space [26]

$$f_i^{eq} = f_i^{(0)} = \rho w_i\left[1 + \frac{c_{i\alpha}u_\alpha}{c_s^2} + \frac{A_{\alpha\beta}^{(2)}Q_{i\alpha\beta}^{(2)}}{2c_s^4} + \frac{A_{\alpha\beta\gamma}^{(3)}Q_{i\alpha\beta\gamma}^{(3)}}{6c_s^6}\right],$$

$$A_{\alpha\beta}^{(2)} = u_\alpha u_\beta + (\theta - 1)c_s^2\delta_{\alpha\beta},\ Q_{i\alpha\beta}^{(2)} = c_{i\alpha}c_{i\beta} - c_s^2\delta_{\alpha\beta},$$

$$A_{\alpha\beta}^{(3)} = u_\alpha u_\beta u_\gamma + (\theta - 1)c_s^2[u\delta]_{\alpha\beta\gamma},\ Q_{i\alpha\beta}^{(3)} = c_{i\alpha}c_{i\beta}c_{i\gamma} - c_s^2[c\delta]_{\alpha\beta\gamma}, \tag{7}$$

where $[c\delta]_{\alpha\beta\gamma} = c_\alpha\delta_{\beta\gamma} + c_\beta\delta_{\alpha\gamma} + c_\gamma\delta_{\alpha\beta}$, $\delta_{\alpha\beta}$ is the Kronecker symbol and θ is the non-dimensional temperature

$$\theta = \frac{\bar{r}T}{c_s^2} = \frac{RT}{c_s^2}\sum_k \frac{Y_k}{W_k} \tag{8}$$

The moment of equilibrium distribution function on the nearest neighbor type lattices, hereafter referred to as standard lattices (D2Q9, D3Q19, D3Q27, etc.), are then

$$\sum_i f_i^{(0)} = \rho, \tag{9}$$

$$\sum_i f_i^{(0)}c_{i\alpha} = \rho u_\alpha, \tag{10}$$

$$\sum_i f_i^{(0)}c_{i\alpha}c_{i\beta} = \rho\bar{r}T\delta_{\alpha\beta} + \rho u_\alpha u_\beta, \tag{11}$$

$$\sum_i f_i^{(0)}c_{i\alpha}c_{i\beta}c_{i\gamma} = \rho\bar{r}T(u_\alpha\delta_{\beta\gamma} + u_\beta\delta_{\gamma\alpha} + u_\gamma\delta_{\beta\alpha}) + \rho u_\alpha u_\beta u_\gamma + \Psi_{\alpha\beta\gamma}, \tag{12}$$

where $\Psi_{\alpha\beta\gamma}$ is a deviation term due to defect of symmetry of standard lattices for the third order moment. This deviation can be corrected by introduction of an extra force term $s_i = Q_{i\alpha\beta}\frac{\partial}{\partial x_\gamma}\Psi_{\alpha\beta\gamma}$ in the lattice Boltzmann equation. The LB equation with a force term in the second order accuracy scheme is given as [29]

$$f_i(\boldsymbol{x} + \boldsymbol{c}\delta t, t + \delta t) = f_i(\boldsymbol{x}, t) - \tfrac{1}{\tau}[f_i(\boldsymbol{x}, t) - f_i^{eq}(\boldsymbol{x}, t)] + (1 - \tfrac{1}{2\tau})s_i \tag{13}$$

where the external force term s_i reads [23]

$$s_i = Q_{ixx}\frac{\partial}{\partial \boldsymbol{x}}[\rho u_x(1 - \theta - u_x^2)] + Q_{iyy}\frac{\partial}{\partial \boldsymbol{y}}[\rho u_y(1 - \theta - u_y^2)], \tag{14}$$

in two dimensions.

The mass and momentum conservation equations derived through Chapman–Enskog expansion from this model remain unchanged compared to the classical athermal version (3) and (4), with the exception of the equation of state and the relation between the relaxation time and the viscosity (5), which now reads

$$\tau = \frac{\nu}{\theta c_s^2\delta t} + \frac{1}{2}. \tag{15}$$

The approach proposed here is hybrid: coupled with this lattice Boltzmann description, temperature T and mass fractions Y_k equations are solved following a classical finite difference method

$$\frac{\partial T}{\partial t} + u_\alpha\frac{\partial}{\partial x_\alpha}T = \frac{1}{\rho}\frac{\partial}{\partial x_\alpha}\left(\rho D_T\frac{\partial T}{\partial x_\alpha}\right) + \frac{\omega_h}{\rho c_p} \tag{16}$$

$$\frac{\partial Y_k}{\partial t} + u_\alpha\frac{\partial}{\partial x_\alpha}Y_k = \frac{1}{\rho}\frac{\partial}{\partial x_\alpha}\left(\rho D_k\frac{\partial Y_k}{\partial x_\alpha}\right) + \frac{\omega_k}{\rho} \tag{17}$$

D_k and D_T are respectively the *k*th species and thermal diffusivities.

As to simplify the introduction of this model, we assume calorically gases, with a constant mixture heat capacity. Transport properties are specified through constant Prandtl number and constant Schmidt number for each species following [30]

$$D_T = \frac{\nu}{Pr}, \qquad D_k = \frac{\nu}{Sc_k}. \tag{18}$$

Physical and lattice units for length, time, mass and temperature are related through a reference length scale L_0, the physical sound speed c_{sp} for space and time, a reference density ρ_0