Physica A 499 (2018) 40–57

Contents lists available at ScienceDirect

Physica A

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

Mass-conserving advection–diffusion Lattice Boltzmann model for multi-species reacting flows

S.A. Hosseini [a,b,*], N. Darabiha [b], D. Thévenin [a]

[a] Laboratory of Fluid Dynamics and Technical Flows, University of Magdeburg "Otto von Guericke", D-39106 Magdeburg, Germany
[b] Laboratoire EM2C, CNRS, CentraleSupélec, Université Paris-Saclay, 3 rue Joliot Curie, 91192, Gif-sur-Yvette Cedex, France

HIGHLIGHTS

- Derivation of an advection–diffusion Lattice Boltzmann model without the so-called compressibility errors coming from the flow field.
- Derivation of a local expression for a correction to the Fickian diffusion term.
- Use of the lattice Gas kinetic formulation to make the scheme adapted to cases with variable diffusion coefficients.
- Application of the model to 2-D and 3-D cases with detailed chemistry and variable diffusion coefficients.

ARTICLE INFO

Article history:
Received 29 September 2017
Received in revised form 28 January 2018

MSC:
00-01
99-00

Keywords:
Lattice Boltzmann
Reacting flows
Multiple distribution function
Complex chemistry
Combustion
Diffusion
Correction velocity

ABSTRACT

Given the complex geometries usually found in practical applications, the Lattice Boltzmann (LB) method is becoming increasingly attractive. In addition to the simple treatment of intricate geometrical configurations, LB solvers can be implemented on very large parallel clusters with excellent scalability. However, reacting flows and especially combustion lead to additional challenges and have seldom been studied by LB methods. Indeed, overall mass conservation is a pressing issue in modeling multi-component flows. The classical advection–diffusion LB model recovers the species transport equations with the generalized Fick approximation under the assumption of an incompressible flow. However, for flows involving multiple species with different diffusion coefficients and density fluctuations – as is the case with weakly compressible solvers like Lattice Boltzmann –, this approximation is known not to conserve overall mass. In classical CFD, as the Fick approximation does not satisfy the overall mass conservation constraint a diffusion correction velocity is usually introduced. In the present work, a local expression is first derived for this correction velocity in a LB framework. In a second step, the error due to the incompressibility assumption is also accounted for through a modified equilibrium distribution function. Theoretical analyses and simulations show that the proposed scheme performs much better than the conventional advection–diffusion Lattice Boltzmann model in terms of overall mass conservation.

1. Introduction

Many fields of science and engineering involve the transport of multiple reacting species. For such flows, a correct mathematical model describing the interactions between different species is of the utmost importance. A variety of models

* Corresponding author at: Laboratory of Fluid Dynamics and Technical Flows, University of Magdeburg "Otto von Guericke", D-39106 Magdeburg, Germany.
E-mail address: seyed.hosseini@ovgu.de (S.A. Hosseini).

https://doi.org/10.1016/j.physa.2018.01.034
0378-4371/

have been developed to describe such interactions, which can usually be placed in one of the following two categories: (a) single-fluid, or (b) multi-fluid. Although initially developed to solve the Navier–Stokes (NS) equation, Lattice Boltzmann approaches have been extended to a variety of applications and flows [1–3]. This class of solvers can be again classified as either single-fluid or multi-fluid. A variety of so-called multi-fluid models have been developed over the years. Two general classes of multi-component LB models can be distinguished: (1) Models derived from kinetic equations for binary mixtures [4], and (2) models based on pseudo-potentials [5]. The first category mostly relies on kinetic models proposed by Sirovich [6] or by Hamel [7–9] for binary mixtures. Although it has been shown through Chapman–Enskog (CE) expansions that such approaches can recover the full Maxwell–Stefan system of equations, they have usually been limited to binary fluids. Recently, a new kinetic model for multi-component flows has been proposed [10,11]. This model can be applied to any number of species and is shown to recover the Maxwell–Stefan equation. Even though the mathematical formulation allows for multiple species, this model is still not very well adapted to simulations involving a large number of species. This is in part due to the fact that each species distribution function, just like any classical NS solver, has to conserve $D+1$ moments, D being the dimension. This in turn means a large set of velocities per species per node that must be stored in memory.

In the single-fluid formulation, memory consumption is much lower, and comparable to classical finite-difference methods, as the solver for the species only needs to conserve the zeroth-order moment. In this type of approach, also known as passive scalar, the usual Navier–Stokes equations are used to model the mixture flow field while additional "advection–diffusion–reaction" equations are incorporated to simulate species transport. The scalars – species mass fractions or concentrations in this case – are advected by the flow field and interact with each other through diffusion (non-reactive collision), or chemical reaction. In classical macroscopic models, diffusion usually appears in the transport equation in the form of an additional advection velocity. The diffusion velocity can be computed through the use of the Maxwell–Stefan multicomponent diffusion equations [12]. In cases involving large numbers of species, such as combustion modeling with detailed chemistry, solving the corresponding system of Maxwell–Stefan equations can become very time-consuming. In order to minimize computation time, approximated diffusion velocities are commonly used. Two of the most widely used approximations are [13]: (a) the Fick approximation – as recovered by the classical advection–diffusion lattice Boltzmann model –, and (2) the Hirschfelder and Curtiss model. Although very practical and computationally efficient, both of these approximations lack a fundamental property at the continuum level: total mass conservation [12,14,15]. As such, they can only effectively be applied to flows where all species have the same Lewis number, i.e., the same diffusion coefficients. For applications such as combustion, the previous assumption does not hold in general, small species like atomic hydrogen diffusing much more rapidly than large molecules. In order to conserve mass everywhere and especially in high-gradient areas, such as the flame front, a correction velocity must be introduced [16].

Modeling multi-species reacting flows, especially combustion applications, is an issue of growing importance [17–22]. Most combustion-oriented LB simulations use the passive-scalar approach to model the species. As mentioned earlier the advection–diffusion (AD) model with the Fick approximation does not generally conserve mass at the continuum level. Apart from the overall mass gain/loss introduced by the Fick approximation, it can be shown that, even for unity Lewis numbers, this approach holds only under the incompressibility assumption, by analyzing the macroscopic equation recovered by the AD-LB model. Even for incompressible cases, given that the LB flow solver is weakly compressible, thus allowing for fluctuations in density, the advection–diffusion model must be modified to account for density changes. In view of the growing interest for simulating multi-species reacting flows with the LB approach, developing a correct diffusion model appears to be very important. In the present work, in order to eliminate the continuum-level error coming from the Fick approximation in the diffusion term, an appropriate correction velocity will be derived in the context of the AD-LB model. In order to maintain the locality of the time-evolution operators involved in LB, this so-called correction velocity will be derived using only data from local populations. Furthermore, the error coming from the incompressibility assumption will be corrected by introducing a modified equilibrium distribution function. Finally, to keep the model second-order accurate regardless of the scaling, the error associated with the Fick approximation will be decoupled from numerical dissipation through the lattice gas kinetic scheme approach.

The proposed model is validated by considering three different test-cases of growing complexity. The first test-case is a Gaussian hill subject to a uniform velocity field involving two species with different diffusion coefficients. This test-case shows that the correction velocity introduced in our model effectively removes the non-conservation of mass introduced by the Fick approximation, as the flow field is here strictly incompressible, $\vec{\nabla}\cdot\vec{u}=0$. Second, the effect of the proposed model on the incompressibility error is evaluated by computing a diluted premixed propane/air counter-flow flame. It is shown that the scheme derived in the present work effectively deals with both sources of non-conservation. Finally, a last test-case involving an Ozone/air non-premixed flow with detailed thermo-chemical models is computed in a 3-D configuration to demonstrate the versatility of the developed model.

2. Physical context and conservation at the continuum level

As previously mentioned, the single-fluid approach to model a multi-species flow consists of three main components [12]: (a) Navier–Stokes equations for the mixture, (b) Heat transport equation for the mixture and (c) a set of transport equations for the species. The NS equations can be represented as:

$$\partial_t(\rho\vec{u})+\vec{\nabla}\cdot(\rho\vec{u}\otimes\vec{u})=-(\vec{\nabla}p)\cdot\bar{\bar{I}}+\vec{\nabla}\cdot\left[\mu(\vec{\nabla}\vec{u}+\vec{\nabla}\vec{u}^T)\right], \tag{1}$$