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Lattice Boltzmann simulations of heat transfer in flow past a cylinder and in simple porous media



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ABSTRACT

The Lattice Boltzmann method has been further developed for flow and heat transfer computations in terms of two distribution functions. A modified boundary scheme for heat transfer has been proposed for curvilinear fluid–solid interfaces, based on a weighted relaxation time. Weight coefficients depend on the interface location with respect to the regular lattice. The approach has been validated for two cases in a simple and more complex geometry: a non-isothermal flow past a single circular cylinder and in simple porous (granular) media. Computations have been performed with the use of the new boundary scheme for curvilinear interfaces and compared to a standard scheme known from the literature. For the circular cylinder case, results for the local and averaged Nusselt numbers are validated with the outcome of other numerical methods and with experimental data. For the more complex geometry, two configurations are considered: a regular array of square cylinders and a random arrangement of circular cylinders to simulate a granular medium. The results for the Nusselt number are compared, after a suitable volume averaging, with available semi-empirical correlations.

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1. Introduction

Coking is a widely used industrial process to obtain chemically cleaner coal and coking gas. Aside of fluid flow in a granular medium, heat transfer and heterogeneous chemical reactions at the level of coal grains govern the changes of their size and shape as well as devolatilisation with a growing temperature of the medium. The physico-chemical and geometrical complexity of these phenomena imply that more traditional tools and software of computational fluid dynamics (CFD) become prohibitively expensive as far as detailed modelling is concerned. The CFD approach is mostly performed at the macroscale level only, subject to semi-empirical closure relationships [1,2]. Hence the idea of a multiscale approach with a microscopic (single-pore level) computation of representative element of volume (REV), followed by a macroscopic (system-level, unsteady 1D/2D) CFD analysis.

To solve the problem of flow and heat transfer, we have chosen the Lattice Boltzmann method (LBM), also because of its ability to deal with complex and time-varying solid–fluid interfaces, i.e. the boundaries of grains. As a first development step of the approach, we have applied the LBM to simulate fluid flow [3] past a cylinder

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and in a simple granular (or porous) medium. The present work is a logical second step towards the physically-sound description of the process, dealing with non-isothermal flow in the same geometry. As a next-term objective, we will address the thermal dilatation of grains (following a first attempt reported in [4]) and we will include chemical reactions in the medium to finally use resulting closure relationships in a physically sound, macroscale simulation of the coking process.

The LBM is an approach developed in the early 1980s, designed originally as an extension of cellular automata [5] to eliminate a large numerical noise. It is based on the Boltzmann equation [6] with subsequent discretization. The method has proven suitable for simulation of viscous and nearly incompressible fluid flows [7,8] in simple [9,10] and complex geometry [11,12], as well as heat transfer [13,14], also with addition of chemical reactions [15,16]. In those cases, suitable distribution functions (for the density, internal energy or chemical species) with a variety of boundary schemes have been used [7].

In early attempts of solving heat transfer, the single distribution function was used. An important example of a successful implementation of that approach for combustion phenomena was presented by Yamamoto et al. [15]. A brief review of the literature where a single distribution function has been used for heat transfer modelling is offered by Chen and Doolen [8]. Implementations with a single distribution function are still under development: Yuan and Schaefer [17] proposed a thermal LBM for two-phase

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flow and reported a stable, accurate and numerically efficient scheme.

A first proposal for modelling heat transfer with additional internal energy density distribution function (IEDDF) was made by He et al. [13]. Their formulation, although stable and accurate, contained complicated differential terms. A simplified model was presented by Peng et al. [18]. The use of IEDDF brings some issues connected with fluid–solid interfaces. The basic thermal condition was proposed by He et al. [13]; it was successfully applied in 3D by Peng [10]. However, in the case of variable geometry, artefacts are observed during transition of nodes from fluid into solid, as caused by a step change in the relaxation time. The rapid development of the LBM also included improved boundary schemes for heat transfer. A recently published paper [19] presented an interesting attempt to treat curvilinear solid–fluid interfaces on a regular mesh.

In the present work, we build on our experience to date with LBM [3,4] and further develop the approach. We briefly present the main idea of the thermal LBM with two distribution functions: for density and internal energy. We work out a modified numerical boundary scheme for curvilinear fluid–solid interfaces, basing on the On-Site Interpolation-Free (OSIF) scheme for the mass distribution function [3,20]. Apart from the boundary scheme at the interface, also the heat transfer conditions at the inlet and outlet bring a number of implementation issues. In this work we present simulation results with two variants of such conditions. Then, we address heat transfer in a benchmark flow past a circular cylinder and, next, in a general porous medium flow. In the latter case, the LBM results for the Nusselt number are compared with some empirical laws developed for granular/porous media (a regular lay-out of square cylinders and a random layout of circular cylinders).

2. Lattice Boltzmann method

2.1. Governing equations for non-isothermal flow

The Lattice Boltzmann method has by now become a pretty mature approach for simulation of fluid flow phenomena. The basic idea of LBM, with several implementations, is well presented in the book by Succi [7]; a good review of applications for porous media flows has been written by Chen and Doolen [8].

The Boltzmann equation, discretized in time, space (by lattice), and velocity (by distinction of admissible directions identified by *i* subscript, see Fig. 1) on a regular square lattice, describes the evolution of a relevant physical field in terms of its distribution function $f_i(\mathbf{r}, t)$. At the moment, three closely related schemes for LBM can be distinguished. The first one is the single relaxation time (SRT) scheme also known as Bhatnagar–Gross–Krook (BGK) LBM where a microscopic relaxation time is related to the macroscopic fluid viscosity. Another approach developed by d'Humières et al. [21] considers a multiple relaxation time (MRT) scheme; some

additional cost and complexity are balanced by better stability properties and accuracy. A third scheme (TRT, Two Relaxation Times) uses a decomposition of the distribution function as well as relaxation times into anti-symmetric (odd) and symmetric (even) parts, as described in detail by Ginzbourg et al. [22]. In such a hierarchy, the SRT model is placed as a special case of TRT which, in turn, is a special case of the MRT model.

The crucial concept of LBM [5,7] is the discretization of the microscopic velocity vectors, both in direction and magnitude, cf. Fig. 1, for schemes used in 2D or 3D flows (here with 9 or 15 velocities, respectively). It is a matter of experience to choose a valid velocity discretization scheme: for a refined scheme (a higher number of velocity directions), an improved accuracy of the results as well as a better stability can be obtained, along with an adverse impact on CPU time and memory requirements. Also, improving 2D computations with more detailed discretization schemes can be tricky (at interfaces) if one wants to model multiphysics features in a complex geometry.

As far as heat transfer is concerned, a widely used SRT variant, due to instabilities and limitations (constant Prandtl number Pr = 1), has been extended for LBM with two distribution functions by He et al. [13], namely the mass density and the internal energy density distribution functions (IEDDF) with additional relaxation time. That scheme appears to be very stable in comparison with previous work on heat transfer problems [10]. The method described in [13] has been a next step of the SRT LBM development; the main disadvantage of the proposed solution was its complexity (cf. [14]), associated with the occurrence of gradient terms in the evolution equation for IEDDF. A simplified method, elaborated by Peng et al. [18], is widely used and developed also to implement source terms [14] that appear, e.g., with chemical reactions [15].

In the LBM, the flow density and velocity are solved for in terms of the density distribution function f; for an exhaustive description of the method, see [6–8,11,20,23]. The temperature field is found from the IEDDF denoted by g, cf. [14]; the evolution of chemical species, when applicable, is governed by a separate distribution function, cf. [16], etc. The form of all these LB equations is similar [7].

In our case, we proceed with simulation of fluid flow and heat transfer. Here, we explicitly give the LBM equation for the IEDDF g_i (the form of the governing equation for f_i is similar)

$$g_i(\mathbf{r} + \mathbf{e}_i \delta t, t + \delta t) = g_i(\mathbf{r}, t) - \tau_{\theta}^{-1}(g_i - g_i^{\text{eq}}),$$
(1)

where τ_{θ} is the thermal relaxation time and g_i^{eq} represents the equilibrium state of internal energy at (**r**, *t*); it has the following form:

$$\mathbf{g}_{i}^{\mathrm{eq}} = \theta \Omega_{i} \Big[A_{i} + B_{i} \mathbf{e}_{i} \cdot \mathbf{v} + C_{i} (\mathbf{e}_{i} \cdot \mathbf{v})^{2} - D_{i} \mathbf{v}^{2} \Big],$$
(2)

where **v** and θ are the local fluid velocity and temperature, cf. Eq. (4), and the positive coefficients A_i through D_i depend only on



Fig. 1. Examples of discretization of velocity space: in 2D (8 + 1 velocity directions e_i) and 3D (14 + 1 directions).

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