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Introduction

1.1 BACKGROUND

A fluid can be described as a substance that cannot experience any shearing or tangential force at rest, whereas it starts deforming continuously under the applied shear stress. The popular Navier-Stokes (NS) equations are the fundamental basis of Computational Fluid Dynamics (CFD) to define fluid flow behavior. The fluid flow regimes are characterised by the Reynolds number in laminar, transition, and turbulent flows. The Reynolds number, abbreviated as *Re*, is a dimensionless quantity that represents the ratio of inertial to viscous force. It efficiently suppresses the small perturbations in the fluid flow resulting in the laminar flow regime; however, the larger value of the Reynolds number indicates the low viscous force within the fluid. As a result, it amplifies the perturbations that tend the flow regime from transition to turbulent.

As mentioned in the above para, the most successful and popular way of modeling incompressible flows in CFD is to solve the incompressible NS equations numerically. These equations are sets of second-order non-linear partial differential equations (PDEs) and satisfy the conservation principles of mass, momentum, and energy. The equations are based on the continuum assumption and describe the fluid flow dynamics at the macroscopic scale. The NS equations incorporate diffusive and convective transport of certain variables. The equations are solved with different numerical approaches, such as finite difference (FD) and finite volume (FV) methods. These methods discretize the governing NS equations for the fluid domain. The fluid domain is also discretized (or decomposed) into several sub-domains defined as the computational mesh. It results in algebraic equations that can be solved numerically for each of the sub-domain. The iterative procedures are generally used to solve these algebraic equations to obtain the macroscopic properties of fluid, such as density, velocity, and pressure for each of the mesh points of interest.

Although numerical studies on NS solvers have achieved significant successes, a number of difficulties and challenges remain. Firstly, solving the NS equations is a challenging task due to the non-linear terms in the equations. Secondly, it is not easy to get optimum solutions with the NS solvers for industrial applications, where geometry is much more complex [Hou *et al.*, 2019]. Moreover, the NS equations are particularly suitable for low Knudsen numbers (Kn «1). The Knudsen number is defined as the ratio mean free path of the molecule to the characteristic length of the system. The formulations of NS do not provide the converged solution for the high Knudsen numbers [Raabe, 2004].

From the past three decades, LBM has gained significant popularity as an alternative numerical approach to obtain continuum flow quantities [Aidun and Clausen, 2010a]. It became popular among researchers and scientists due to its wide range of applicability to simulate various chemical and physical processes associated with the fluid flow, multiphase flows [Grunau *et al.*, 1993], immiscible fluids [Gunstensen *et al.*, 1991], heat transfer [Han-Taw and Jae-Yuh, 1993; Ho *et al.*, 2002], and turbulent flows [Jahanshaloo *et al.*, 2013]. The method is initially evolved from the Lattice Gas Cellular Automata (LCGA), considered the fluid as a collection of particles [Sharma *et al.*, 2019]. The method introduced the concept of the averaged distribution function in its solution, which means a single distribution function contains all those fluid particles that are at the same position at the same time moving with the same velocity despite solving the macroscopic flow variable like velocity, density, momentum, and temperature in other CFD solvers. This simplicity in the formulation of the LBM makes it exceedingly easy to code and particularly suitable for massively parallel computation.

The governing mathematical formulation of the lattice Boltzmann equation (LBE) includes the two-step procedure: streaming of the particle distribution functions and their collision. The idea behind the method is that a set of particle distribution functions residing on a lattice node stream to neighboring lattice sites, and collide with particle distribution functions coming from other directions resulting in the exchange of momentum. The net mass and momentum remain conserved during the collision process [Agrawal *et al.*, 2006]. The LBM method is justified by the fact the the collective behavior of many microscopic particles is not especially dependent on the specifics of microscopic processes of the individual molecules underlying the macroscopic dynamics of fluids. The method provides stable and local arithmetic operations for the macroscopic behavior of fluid and recovers NS equations.

Furthermore, the LBM depends on the lattice structure of the discrete velocity models for accuracy and stability. The discrete velocity models in LBM notation can be distinguished with D_mQ_n reference, where m represents the domain dimension, and n is the number of directions a particle is restricted to stream. The popular discrete velocity models are: seven velocities (D_2Q_7) and nine velocities (D_2Q_9) LB models for the simulation of two-dimensional (2-D) flows on the 2-D square lattice structure. For the three-dimensional (3-D) flows, fifteen velocities (D_3Q_{15}), nineteen velocities (D_3Q_{19}), and twenty-seven velocities (D_3Q_{27}) models on the cubic lattice structure are quite common. All of the aforementioned LB models include a resting particle in the discrete velocity set [Perumal and Dass, 2015]. In general, LBE models containing a rest particle have higher computational stability. These discrete velocity models play an essential role in obtaining the solutions to fluid flow problems. For example, reductions in the velocity model can significantly decrease the calculation effort but deteriorate the stability and accuracy of the findings. As a result, to achieve a more precise solution, the calculation grids or the number of velocities must be increased.

1.2 RESEARCH MOTIVATION

In the present thesis work, numerical simulations has performed with LBM to examined its viability for the turbulent flow simulation on different geometry cases. The LBM has a number of appealing characteristics that distinguish it from the conventional NS solvers and make it a viable choice for modeling complex turbulent flows.

- The convection term in the governing equation of LBM is linear; however, the NS equations consist of a non-linear convection term that takes a long time to solve numerically.

- The LBM shows isotropic nature to the second order. It means the solution experiences the minimal influence of the orientation of the computational grid. This factor provides an advantage for the simulation of turbulent flow since the turbulent structures are three-dimensional. In other words, if the solution of the numerical scheme is prone to the orientation of the computational grid, it also influenced the direction of turbulent structures [Bespalko, 2011].

- Another advantage of LBM over NS solvers is that the LBE involves local collision operation, compared to the coupled equations in conventional NS solvers, which makes LBM highly parallelizable. This also ensures good scaling performance of computational code with the increasing number of parallel processors and can be used efficiently for parallel computation on a multi-core GPU platform. This advantage is especially useful for modeling turbulent flows, where the computational domain consists of a large number of grid points.

In the literature, many studies have been reported for the turbulent flow simulation using LBM. One of the earliest works in this field was reported by Benzi and Succi [1990] by simulating 2-D forced isotropic turbulence with LBM. Later, Lammers *et al.* [2006] used the direct numerical simulation (DNS) turbulence model to simulate a turbulent plane-channel flow within the incompressible limit ($Re_\tau = 180$) using D_3Q_{19} SRT-LBE. Their results demonstrated excellent agreement with the past DNS and pseudo-spectral data. Another numerical study has been performed by Fernandino *et al.* [2009] using the LES-LBM for the investigation of turbulent fow in an open duct. Chikatamarla *et al.* [2010] used the LBM for the DNS of turbulent fows. Wang *et al.* [2014] presented the comparative study of DNS and LES for the wall-bounded turbulent fow and developed the parallelized computer code suitable to run on multiple GPUs platform. In a recent study Peng *et al.* [2018] presented the DNS results of turbulent flow simulation in a pipe using the LBM.

The studies mentioned above confirm that numerous studies have been carried out for the turbulent flow in the frame of LBM. In particular, for the turbulent flow simulation in the 3-D computation domain, the D_3Q_{19} lattice velocity model was primarily adopted by the researchers [Bespalko, 2011; Lammers *et al.*, 2006; Pattison *et al.*, 2009], as it produces higher stable and accurate results comparable to the D_3Q_{15} velocity model [Mayer and Házi, 2006; Mei *et al.*, 2000] and offers better computational efficiency in terms of memory and run time than the D_3Q_{27} velocity model. However, to the best knowledge of the author, the detailed comparison of different discrete velocity models of LBM with the inclusion of turbulence has not been made so far. Very few studies are available in the literature for the comparison of different discrete velocity models. Mei *et al.* [2000] presented a study for the comparison of discrete velocity models for 3D flows with curved boundaries. The results reported the computational efficiency and stability for all the discrete velocity models. The result obtained showed that the D_3Q_{15} velocity is more prone to numerical stability. However, D_3Q_{27} is more computationally expensive, and D_3Q_{19} shown a balance between numerical stability and computational efficiency. Yasuda *et al.* [2014] performed a study to compare the accuracy and computational efficiency of D_3Q_{13} and D_3Q_{19} velocity model using the different (lattice Bhatnagar–Gross–Krook (LBGK), the quasi-equilibrium lattice Boltzmann model (QELBM) and multi-relaxation time (MRT)) collision models of LBM for homogeneous isotropic decaying turbulence. The results reported by Yasuda *et al.* [2014] showed a higher computational performance of D_3Q_{13} velocity model. However, the model suffers from the limitation of less accurate results compared to the D_3Q_{19} velocity model. Later, Yasuda *et al.* [2017] repeated the same study for the homogeneous isotropic decaying turbulence with some more discrete velocity and collision models. The study reported a comprehensive comparison of D_3Q_{13}, D_3Q_{15}, D_3Q_{19}, and D_3Q_{27} velocity models along with QELBM, LBGK, MRT, and ELBM collision models. The obtained results showed that the decrease in the velocities considerably decreases the computational effort, but it provides less accurate results and compromises stability.

Furthermore, the handling of boundary nodes is a critical parameter for flow simulation in simple and complex geometry. Thus, the boundary conditions play a significant role in the CFD and are essential in modeling fluid flow problems. It is because the accuracy, time complexity, and applicability of the numerical method in CFD depend on how the boundary nodes are treated with the relevant boundary condition. Also, the boundary conditions are such an important part of defining a problem that fluid flow behavior shows a completely different flow field because of the implication of different boundary conditions on the boundary nodes, despite the fluid domain being simulated with the same numerical method. A variety of methods are developed for the treatment of stationary and moving boundaries in LBM [Zou and He, 1997; Kao and Yang, 2008; Kang and Hassan, 2011]. The LGCA technique was first considered to determine the boundary conditions at the wall nodes in the LBM. The bounce-back (BB) rule, for example, was utilized to provide a no-slip velocity condition at the boundary walls. The approach is extensively described in the literature [Wolfram, 1986; Lavallee *et al.*, 1991; Cornubert *et al.*, 1991; Ziegler, 1993; Ginzbourg and Adler, 1994]. The idea behind the approach is that the particle distribution functions that propagate along the boundary wall are BB with an appropriate momentum adjustment. The ease of implementing the BB rule for the no-slip boundary condition at the boundary wall supports the notion that the LBM is suitable for modeling fluid flows in complex geometries. However, the method shows first-order numerical accuracy. It degrades the LBM overall accuracy for the interior fluid nodes, where the governing LBE is second-order accurate.

Following that, significant work was expanded in developing more precise boundary conditions than the bounce-back rule. And, the researchers proposed several other methods for the treatment of boundary nodes to enhance the numerical accuracy of the LBM. Noble *et al.* [1995] suggested that a pressure restraint be applied on non-slip walls with hydrodynamic boundary conditions. The BB condition was expanded by Zou and He [1997] for the non-equilibrium component of the particle distribution functions. Ziegler [1993] proposed the half-way bounce-back rule. The method showed that placing the boundary wall at half of the mesh distance of the fluid gives second-order accuracy. The other notable works in this direction are Skordos [1993]; Chen *et al.* [1996]. However, numerous boundary schemes are developed by researchers in the past few years to treat boundary nodes in LBM. A detailed comparison of the impact of these boundary conditions for the wall-bounded turbulent flow is not yet reported in the literature.

The current research has also been motivated to visualize the fluid flow behavior, utilizing LBM as a numerical tool in complex geometry. Thus, the simulations to analyze the fluid flow pattern in the stirred tank reactor equipped with dual-Rushton impellers were carried out. For a stirred tank bioreactor, the presence of a high-speed rotating impeller and stationary baffles makes the flow structure highly turbulent. As a result, CFD modeling of turbulent flow in a stirred vessel provides a sufficient amount of useful data to analyze flow behavior, vortex formations, circulation patterns, Reynolds stresses, etc. In addition, the user may easily comprehend the flow-related reactor operations by visualizing all of the above characteristics. Furthermore, one of the multiple flow-associated processes, mixing, is utterly dependent on the fluid flow behavior, which further identifies the possible problems in advance.

1.3 RESEARCH OBJECTIVE AND AND CONTRIBUTIONS

This section describes the major goals of our research and the thesis contributions. The thesis objectives are:

- **Effect of different discrete velocity models of LBM for the turbulent flow simulations:** In the literature, many studies have been reported for the turbulent flow simulation using LBM. Moreover, as mentioned earlier, the LBM depends on the lattice structure of the discrete velocity models. To this end, the first objective of the thesis is to investigates the efficiency of discrete velocity models of LBM for the turbulent flow simulation. And to achieve it, a comparative study with three other 3-D discrete velocity models has been performed for turbulent flow over a bluff body at Re_d = 3000. The study reported the results for various turbulent statistics for all the three discrete velocity models and also presented the computational efficiency of each.

- **Effect of different boundary conditions on the predicted results:** Our objective is to study the effect of different boundary conditions in LBM for the turbulent flow simulation. And, to meet the goal, the impact of two different versions of boundary conditions in LBM used to impose the no-slip condition on the boundary walls is presented. A similar flow configuration of turbulent flow over a bluff body mentioned in the above para is used for comparison.

- **Applications of the developed model to flow in complicated geometries:** As discussed in Section 1.2, CFD plays an essential role in numerous contexts for optimizing reactor design. Thus, the third objective of the present research work is to validate the applicability of the LBM for the modeling of turbulent flow involved in the fluid flow process of stirred tank reactor. A comprehensive study of the stirred tank reactor equipped with a dual Rushton turbine using LBM has been reported in this work. In a stirred tank reactor, it is usually seen that the impeller swirls the whole liquid volume as a homogeneous body in the tank during the stirring processes, resulting in inefficient agitation. The problem can be easily resolved by installing the flat sheet-like structure commonly called 'baffles' on the wall of the reactor tank. The baffles produce shear stresses in the tank, preventing the mass swirling of the liquid volume and using the energy to mix the fluid. The current study presents the flow characteristics in a stirred tank equipped with two six-blade Rushton impeller, and acknowledges the impact of baffles on the flow. Furthermore, the study also shows the effect of baffles with different impeller clearance on the flow characteristics and their influence on mixing.

In addition to the above contributions, the present thesis work also reports the computational efficiency of the LBM algorithm on shared machines. A highly parallel LBM solver is developed using CUDA programming model to execute the simulations on a multi-core GPU architecture.

1.4 THESIS LAYOUT

The remainder of the thesis is structured as follows:

Chapter 2 provides an extensive review of the previous studies carried out on the application of the LBM for simulation of turbulent flow. The chapter mainly discusses the available literature on the use of LBM for the turbulent flow simulation over the bluff body and for investigating liquid phase hydrodynamics in stirred tank reactors.

Chapter 3 provides a detailed description of the methodology used in the present thesis work to study the problems mentioned in the section above. We discuss the governing equations of LBM to discrete the fluid domain, turbulence model, boundary conditions, and the process of parallelization of code on the GPU platform.

Chapter 4 discusses the influence of discrete velocity models of LBM and boundary conditions on the benchmark fluid flow problem of turbulent flow over a bluff body.

Chapter 5 discusses the results obtained from the study to show the effect of baffles on the flow hydrodynamics of dual-Rushton turbine stirred tank bioreactor.

Chapter 6 presents the conclusion of the thesis and recommended list of relevant fields for future work.

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