2

Literature Survey

The present thesis aims to investigate the viability of the LBM for the turbulent flow simulation. The modeling of turbulent flow using LBM has been an active area of research for several years, and multiple attempts are documented in the literature. The literature survey presented in this chapter reviews the studies carried out in the past few years for the benchmark problem of turbulent flow over a bluff body and turbulent flow simulation in a stirred tank reactor. The chapter discusses the various essential aspects and quality results obtained by researchers in recent times.

The remainder of the chapter is organized as follows: Section 2.1 describes the origin of LBM. A brief description on the collision models of LBM is presented in Section 2.2. Section 2.3 reviews the past attempts made to model the turbulent flow using LBM. Section 2.4 summarizes the chapter.

2.1 THE HISTORY OF LBM

The LBM was originated from the LGCA. It is a type of cellular automaton used to simulate fluid flow problems. The dynamics of the LGCA are governed by the principle of discrete kinetics utilizing a discrete lattice and discrete-time, with the local collision rules for the conservation of mass and momentum [Guo and Shu, 2013; Succi *et al.*, 1991]. Later, it was found that LBM can also be derived by using a special standard FD method for the kinetic equation of the discrete velocity distribution function [He and Luo, 1997; Chen and Doolen, 1998]. The first step in this direction was taken by Broadwell [1964] to provide a discrete velocity model for studying the shock structures in a one-dimensional lattice. Here the velocity was chosen in a discrete form, with space and time kept continuous [Benzi *et al.*, 1992]. The full discrete particle velocity model of lattice Boltzmann named HPP primarily coined by Hardy *et al.* [1973, 1976], where space and time both were discretized in a square lattice. The model was used to simulate the particle moving in the axis-parallel direction in a square lattice. However, due to a lack of isotropy in the lattice, the HPP model was found unsuitable to reproduces the non-linear and dissipative terms in the NS equations [Benzi *et al.*, 1992]. In 1986, a group of French and American scientists, Frisch, Hasslacher, and Pomeau (FHP) used the LGCA principles for 2-D hydrodynamics to recover the proper NS equations on a hexagonal lattice. [Frisch *et al.*, 1986]. The model used the LBE in the frame of LGCA to calculate viscosity [Perumal and Dass, 2015]. However, the 3D extension of the FHP model had not shown the required lattice symmetries for the 3D simulations. Further, a 3D model for simulating the NS equations on lattices was proposed by d'Humieres *et al.* [1986] on a four-dimensional (4-D) face-centered-hyper-cubic (FCHC) lattice with all the required symmetries for 3D simulations.

The term lattice in LGCA denotes that one is working on a *d*-dimensional, regular lattice. The word gas implies that gas particles are moving through the lattice. The gas particles are defined by the Boolean variables (0 and 1), residing on a regular lattice node, and the evolution is primarily explained by a set of collision rules that possess suitable conservation laws [Benzi *et al.*, 1992]. The LGCA model has discrete space, time, and particle velocities. A collision and propagation step is included in each iteration of LGCA. However, the LGCA showed significant shortcomings of statistical noise, non-Galilean invariance, an unphysical velocity that is reliant on huge numerical viscosities and pressure, and implementation difficulty in three dimensions [Perumal and Dass, 2015]. McNamara and Zanetti [1988] replaced the particle occupation variables (Boolean variables) with a single-particle distribution function and ignored individual particle motion and particle-particle correlations in the kinetic equations to reduce statistical noise in LBM [Chen and Doolen, 1998]. Afterward, Higuera and Jimenez [1989] made a significant contribution by incorporating the linearized collision operator under the assumption that the particle-distribution function is close to the local equilibrium state [Perumal and Dass, 2015]. This linearized collision operator includes a non-dimensional relaxation time parameter due to the fluid-particle collision, which describes the time taken by the fluid particle to reach equilibrium [Kang and Hassan, 2011].

2.2 COLLISION MODELS OF LBM

In the past few years, researchers have developed variants of collision models of LBM. The simplified version of the linearized collision operator is the LBGK based on the single-relaxation time (SRT) approximation, which was introduced independently by several authors [Bhatnagar *et al.*, 1954; Qian, 1990; Koelman, 1991; Chen *et al.*, 1991]. The LBGK model recovers the NS equations using the local equilibrium distribution function. The model is also known as the SRT model of LBM. LBGK is the most popular model of the LBM due to its extremely simple formulation. However, the model has several inherent deficiencies, including numerical instability in complex flows at finite Knudsen, K_n or high Reynolds, Re number, and inaccurate boundary conditions [Luo *et al.*, 2011]. As a result, the researchers proposed several other collision models, including the multiple relaxation time (MRT) model [Lallemand and Luo, 2000; d'Humieres, 1994; d'Humières *et al.*, 2001; d'Humières, 2002; Lallemand *et al.*, 2003], two-relaxation time model [Ginzburg *et al.*, 2008b,a; Ginzburg and d'Humieres, 2003]. A detailed description of all these LB models can be found in the review article of Aidun and Clausen [2010b]

2.3 LBM IN TURBULENCE MODELING

This section reviews the studies reported in the literature related to the turbulent flow modeling using LBM. First, attempts are made to address the work done by the researchers using LBM on the benchmark fluid flow problem of turbulent flow over a bluff body. Secondly, the available literature on the turbulent flow simulation in the complex domain of stirred tank reactor using LBM has been reviewed.

2.3.1 Study of Turbulent Flow Simulation over Bluff body

A notable experimental work with the laser-Doppler measurements was conducted by Lyn *et al.* [1995] to explore the ensemble-averaged turbulence features near the wake of a square-cylinder. Another significant contribution in this area was made by Srinivas *et al.* [2006]. Srinivas *et al.* [2006] performed numerical simulation on flow past over a square cylinder at Reynolds number (Re) = 21,400. The authors employed the LES approach to model the turbulence, and a dynamic subgrid-scale stress model was applied to resolve the small-scale turbulent structures. The results for time- and span-averaged axial and transverse velocities at the downstream face of the cylinder were provided. The research work also reported on the distribution of turbulent normal and shear stress. The results were compared with the experimental findings of Lyn *et al.* [1995] and found to be in good agreement. Hamane *et al.* [2015] presented LBM result for two-dimesional turbulent flow around a circular cylinder. SRT-LBM model was used in the simulation. LES model was used to model the turbulent structures. The Smagorinsky

SGS model was adopted for small-scale eddies. The results showed that the small-scale vortices were successfully captured. Wei and Hu [2017] proposed a modified version of LBM and used it to investigate the turbulent flow behavior past over a row of cylinders in 2-D. The results were presented for velocity, vorticity difference, energy density enstrophy spectra. The numerical findings corresponded well with the experimental results of Kellay *et al.* [1998].

Koda and Lien [2015] implemented the LBM on the GPU platform to study the turbulent flow behavior past over a square cylinder confined in a channel. The particular SRT-LBM model was used in the study to discretize the fluid domain. The D_3Q_{19} discrete velocity model was adopted for the 3D computational domain. The authors used the LES method to model the large-scale turbulent structures, and the Smagorisnky SGS model was adopted to resolve the small-scale turbulent motions. The Reynolds number based on the diameter of the cylinder was 3000. The simulations were performed for two different spanwise dimensions. The authors reported that the simulation performed on smaller spanwise dimensions over-predicted the turbulent statistics. However, for other spanwise dimensions, the results were in good agreement with the experimental findings of Nakagawa *et al.* [1999], and the numerical results of Kim *et al.* [2004].

Some other notable works in turbulent flow simulation past over a bluff body include those of Kajzer and Pozorski [2017], Feuchter *et al.* [2019], and An *et al.* [2020]. Although they are more theoretically interesting, there appears to be very little work done on the turbulent flow over a bluff body by LBM.

2.3.2 Study of Stirred Tank Reactor Simulation

This subsection presents a detailed insight into the research studies done in the past years to understand the hydrodynamics of the stirred tank reactor using LBM as a numerical tool. The scope of this review is limited to the studies reported only on the simulation of single (liquid) phase hydrodynamics in stirred tank reactor.

Eggels [1996] took the first step in this direction to visualize the flow behavior in a stirred tank bioreactor using LBM. The author reported the isothermal, single-phase, turbulent flow in a standard configuration stirred tank reactor consisting of a cylindrical vessel fitted with four baffles and a 6-blade disc turbine using a LES turbulence model. The scheme of LBM given by Eggels and Somers [1995] was adopted to discretize the fluid domain. The author presented the use of a new LBM scheme for the turbulent flow simulation. The conventional Smagorinsky model was used in the study with Smagorinsky constant $C_s = 0.1$ to model the subgrid-scale stresses [Smagorinsky, 1963]. The author performed two simulations on largely the same geometry that only differs in some simulation parameters and blade thickness. The results were presented for various turbulent statistics, such as instantaneous and time-averaged vector fields, mean and RMS radial and axial velocity profiles at various radial and impeller midplane locations. The results were validated with the experimental data of Wu and Patterson [1989], and Bakker Bakker [1995]. The results were in good accord with the experimental data. The author concluded that the new LB scheme allows researchers to simulate reactors of different geometries with different impeller shapes. Also, the model is suitable for performing scale-up studies for a single-phase reactor.

Another work in this direction to study the turbulent flow in a stirred tank reactor was done by Derksen and Van den Akker [1998]. The authors used LES to simulate turbulent flow in a baffled stirred tank reactor of standard configuration with a 6-blade Rushton turbine. LBM proposed by Eggels and Somers [1995] was used as a numerical approach for the simulation of the fluid domain. The simulations were performed up to Reynolds number, $Re = 10000$ on a cubic computational grid of 120^3. An adaptive force field approach proposed by Derksen *et al.* [1997] was adopted for defining the effect of the non-square or rotational objects on the liquid flow field.

The parallel computer code based on Single Instruction Multiple Data (SIMD) was developed to run on the HP-Convex S-Class machine equipped with four processing elements (PE's). The results were presented for the velocity and vorticity components. The wakes were observed behind the impeller blades. Moreover, the two counter-rotating vortices were also seen behind the blades that deliberately dissolved in the turbulent flow as we move away from the impeller region in the radial direction. The power number was calculated to represent the power drawn by the impeller. The power-number versus Reynolds number plot was compared with experimental results of Rushton *et al.* [1950]. The results were consistent with the experimental data. .

Later, Derksen and Van den Akker [1999] performed another LES study to investigate the turbulent flow characteristics in a stirred tank reactor at Reynolds number, $Re = 29000$. The study reported the results for the phase-resolved average flows and different turbulence characteristics. The results were compared with experimental data of Wu and Patterson [1989], and Derksen *et al.* [1998]. The obtained results showed that the maximum radial velocity as a function of radial position was in good agreement with the experimental data. However, the simulations overestimated the maximum tangential velocity by $\sim 15\%$ compared to the experimental results. Also, the authors noticed that the random kinetic energy shows significant deviation from both the experimental results Wu and Patterson [1989]; Derksen *et al.* [1998] at a radial location closer to the impeller. However, the maximum level of kinetic energy achieves a good comparison with the experimental data.

Lu *et al.* [2002] had carried out an LES study for the stirred tank reactor using LBM on a non-uniform grid. The standard configuration of the stirred tank reactor equipped with a 6-blade Rushton turbine and four baffles mounted on the wall of the tank was chosen. Eggels and Somers [1995] LBM model was used as a numerical approach to discretize the fluid domain. A parallel computer code was developed to perform the simulation. The computer program also used the Smagorinsky SGS model to account for the turbulent eddies smaller in length scale compared to the computational lattice size.

In the results, the authors reported the axial profiles of time-averaged radial and tangential velocity components at different radial locations. The results revealed an acceptable agreement with the experimental results of Wu and Patterson [1989]. Moreover, the accuracy of the results was found comparable with the simulated results of Eggels [1996] and Derksen and Van den Akker [1999]. The results also show that the maximum tangential velocities are in better agreement with the experimental results of Wu and Patterson [1989] compared to the results of Eggels [1996] and, Derksen and Van den Akker [1999].

Hartmann *et al.* [2004] studied the turbulent flow within a baffled tank stirred tank reactor powered by a 6-blade Rushton turbine at $Re = 7300$ using the LES and RANS turbulence models. The LBM scheme suggested by Eggels and Somers [1995] was applied to discretize the liquid flow field. Smagorinsky and Voke subgrid-scale models were employed in LES to resolve the small-scale turbulence motions. The influence of the reactor components (i.e., impeller, baffles, and tank wall) on the liquid flow field was represented using an adaptive force-field approach. As a working fluid, silicon oil was used in the investigation with a density of 1039 kg/m^3. To solve the NS equations for the RANS simulation, the CFD algorithm CFX 5.5.1 based on the FV method was used. However, the turbulence was modeled by using the shear-stress-transport (SST) model given by Menter [1994]. The author also conducted the LDA experiment for the validation of simulation results. The results demonstrated excellent agreement for phase-averaged radial velocity obtained from both the RANS and LES models with the experimental findings. However, the RANS findings revealed deviations in the tangential velocity component and overprediction of the tangential velocity component near the center of the impeller tip in all simulated results. In addition, the LES results for the levels and structure of the TKE were more consistent with experimental data in impeller discharge flow than with RANS calculations.

Gillissen and Van den Akker [2012] performed the DNS study to investigate the turbulent flow in a baffled stirred tank reactor equipped with a 6-blade Rushton turbine. The authors compared the obtained results with simulation results of LES and RANS turbulence models and with the experimental data of Laser Doppler Velocimetry (LDV) and Particle Image Velocimetry (PIV) from the literature. The LB scheme of Eggels and Somers [1995] was used for discretizing the liquid flow field. Two DNS cases were performed, one at a coarse grid and the other at a fine grid. Moreover, the authors also performed two simulations with LES to compare the DNS results with LES. In LES1, in order to resolve the small-scale turbulent structure, Smagorinsky SGS with a Smagorinsky constant $C_s = 0.12$ was used. However, in LES2, the Smagorinsky constant was computed dynamically, and the Van Driest wall model was applied. All the simulations were performed at Reynolds number $Re = 7300$. The authors computed the Kolmogorov length scale to verify whether the simulations fully resolve all scales of turbulent eddies. The study revealed that the minimum Kolmogorov length scale in the turbulent wake of the turbine blades was smaller than the grid spacing The authors presented the results for instantaneous vorticity to address this issue, which showed the smooth structures for all the length scale turbulent eddies. The presented results confirmed the well-resolved turbulent flow field. The study also showed that at certain locations, RANS and LES results for the TKE and turbulent energy dissipation rate were consistent with the experimental results compared to the DNS results. The authors suggested that more experimental and numerical work needs to be done to avoid the above-unexpected observation and to accurately predict the turbulent energy dissipation rate close to the turbine.

Shu and Yang [2018] investigated the computational performance of the parallel LBM algorithm on the multi-core GPU architecture for the turbulent flow simulation in a stirred tank reactor. The study was performed on the baffled stirred tank reactor of standard configuration equipped with a 6-blade Rushton impeller at Reynolds number, $Re = 7300$. The MRT scheme of LBM with D_3Q_{19} discrete velocity model was used to discretize the NS equations. LES was used to model the turbulence. However, to resolve the small-scale turbulent structures, three different cases were performed, one with the Smagorinsky SGS model and the other two with Coherent LES model[Kobayashi, 2005]. The immersed boundary (IB) method was used for representing the impact of the reactor components on the fluid domain Kang and Hassan [2011]. The study also performed the three simulation cases on commercial Ansys software.

The results were presented for the axial distribution phase-averaged velocity components and TKE at different radial locations and compared with the data obtained by Hartmann *et al.* [2004] from the laser Doppler anemometry (LDA) experiment and SRT-LBM simulation. The results were in fair agreement with the experimental results. However, it was noticed that results obtained from the coherent LES at reasonable grid resolution for the high turbulence region resolved more than 95% of the total TKE. The results were much better than the Smagorinsky SGS model for reproducing the monotonic decrease of TKE along the radial direction. Furthermore, GPU accelerated LBM simulation on a desktop computer was observed to be computationally efficient compared with conventional CFD solvers. The simulation for the LBM was 1500 times faster than standard CFD simulation at 16 CPU cores, even for the grid resolution of about 8.8 times the Kolmogorov length scale.

2.4 ISSUE AND CHALLENGES

- **Flow over bluff body:** It is discussed in Section 1.1 that LBM is a discrete particle-based method. It consists of the particle distribution functions arranged in a lattice structure of the discrete velocity models. Researchers proposed variants of the discrete velocity models that differ on the dimension of the lattice structure and the number of directions it contains in which the particle distribution functions are restricted to stream. Thus, discrete velocity models of LBM play an essential role in the prediction of flow behavior. Several studies are present in the literature that used different collision and discrete velocity models to perform the simulations. However, the detailed comparison of the effect of discrete velocity models for the turbulent flow behavior past over a bluff body has not been made so far. This is addressed in the present thesis.

- **Flow simulation in stirred tank reactor:** The studies carried out by the researchers in the past two decades for the investigation of single (liquid)-phase hydrodynamics in the stirred tank reactor using LBM were performed either with the LB scheme proposed by Eggels and Somers [1995] or with the MRT-LBM collision model. Both the models have some advantages and limitations over other collision models of LBM. An advantage of the models is that these models provide better stability for the flow simulation at high Reynolds numbers. The limitations of these models are that despite the models offer higher stability, the algorithms of these models are complex to implement, and the models are less computationally efficient than the SRT-LBM model. Thus, modeling the large-scale reactor with these models is a challenging task and requires high computational power. It emphasizes the importance of using the SRT-LBM model for flow simulation in a large-scale reactor. Thus, in this thesis work, the SRT-LBM model is used to discretize the flow domain. And, LES turbulence model is incorporated in the LBE of the SRT-LBM model to model the turbulent structures.

  Furthermore, a review of previous research studies revealed that most of the works had been done on the stirred tank reactor equipped with a single impeller. However, multiple impellers are usually preferred in the industrial unit for efficient mixing and better productivity. In the past few decades, researchers have used numerous experimental techniques to observe the flow characteristics in stirred tank reactors, such as LDA and particle image velocimetry (PIV). The first experimental study using LDA techniques to observe the flow characteristics in a stirred tank equipped with two-Rushton impellers was performed by Rutherford *et al.* [1996]. This study investigated the flow characteristics, power consumption, and mixing time in the dual Rushton impeller stirred tank reactor at Reynolds number (Re = 40,000). A set of experiments were performed for different spacing between two impellers and at different impeller clearance from the vessel bottom. The other experimental works to understand the flow processes in the stirred tank reactor equipped with dual-impellers are described by Bonvillani *et al.* [2006]; Chunmei *et al.* [2008]; Xinhong *et al.* [2008]. However, relatively fewer numerical studies are available in the literature for a stirred tank reactor fitted with the dual impeller. Some of the works in this direction are presented by Micale *et al.* [1999]; Zadghaffari *et al.* [2009]; Li *et al.* [2012]. Micale *et al.* [1999] reported the numerical results of the flow behavior in the stirred tank reactor fitted with dual-Rushton impellers. The geometric configuration of the stirred tank reactor was similar to that used by Rutherford *et al.* [1996]. The authors used two numerical methods to perform the simulations.: the sliding grid (SG) and the inner-outer (IO) iterative procedure. The presented results showed the comparison between the two numerical approaches and the validation with experimental findings of Rutherford *et al.* [1996]. Zadghaffari *et al.* [2009] performed the numerical simulation on a fully baffled stirred tank reactor with two six-blade Rushton impellers using the sliding mesh (SM) approach. LES was used in the study to model the turbulence eddies. The study also conducted a PIV experiment to validate the simulation results. The authors considered three different speeds of the impeller's rotation in the study, i.e., 224, 300, and 400 rpm. The study reported the results for the flow field, power consumption, and mixing time. Li *et al.* [2012] conducted the PIV experiment and also performed LES simulation on the same geometry used by Rutherford *et al.* [1996] for the merging flow characteristics. The study validated the obtained experimental findings and numerical results with Rutherford *et al.* [1996] and Micale *et al.* [1999].

In this thesis, numerical simulations are carried out using LBM to predict the flow pattern and study the flow properties on a stirred tank reactor of similar configuration to that employed by Rutherford *et al.* [1996] in the experiment. And, to the best knowledge of the author of this work, the comprehensive study of the stirred tank reactor equipped with a dual Rushton turbine using LBM has not yet been reported in the literature. The current study not only presents the flow characteristics in the dual Rushton stirred tank but also acknowledges the impact of baffles on the flow. The study also shows the effect of baffles with different impeller clearance on the flow characteristics and its influence on mixing, which has not been studied so far. The research work reported by Rutherford *et al.* [1996]; Micale *et al.* [1999] are used to validate the results with the experimental observations of Rutherford *et al.* [1996] for the numerous fluid flow properties, including flow averaged velocity and TKE.

2.5 SUMMARY

This chapter provides a detailed review, analysis, and research gaps on the application of LBM in turbulent flow simulation. First, the chapter detailed the development of the LBM and discussed the various types of LBM collision models. Further, the research studies available in the literature for the simulations of turbulent flow over bluff bodies and in stirred tank reactors using LBM have been reviewed. The reviewed studies explored the feasibility of LBM for turbulent flow simulation at various geometrical and simulation parameters. Lastly, the issue and typical challenges in the LBM simulations of turbulent flow over buff bodies and stirred tank reactors are discussed. In a nutshell, the literature survey is described mainly to address the research goals of the thesis. The solutions to the research objectives are discussed in the subsequent chapters.

…