Conclusions and Future Recommendations

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The research work starts with the objective of validating LBM for LES simulation of turbulent flows in various flow domains. In this direction, the thesis contributes to the effect of boundary conditions and discrete velocity models in LBM and effect of baffles on hydrodynamics of stirred tank reactor. The presented research works also depict the advantage of LBM for solving fluid flow problems compare to other traditional CFD solvers. Moreover, a novel highly parallelized LBM-LES solver has been developed for efficient computation on a multi-threaded GPU platform. This chapter highlights the significant conclusions drawn from the current thesis and suggests the scope of future research work in the relevant field of research.

6.1 CONCLUSIONS

The investigations performed in this thesis are categorized into three sections: A) effect of the discrete velocity model, and B) effect of boundary conditions in LBM on turbulent flow simulation past over a bluff body followed by C) effect of baffles on the flow hydrodynamics of stirred tank reactor. The conclusions from each of these studies are summarized in the following paragraphs

6.1.1 Effect of Discrete Velocity Models

In the first study of the thesis, work has been performed to show the effect of various discrete velocity models on the turbulent flow pass over a bluff body. The different 3D discrete velocity models (i.e., D_3Q_{15} , D_3Q_{19} , and D_3Q_{27}) are taken into consideration. The flow domain used in the study is the benchmark flow problem of flow past a square cylinder confined in a rectangular duct. The obtained results provide information about the accuracy and computational efficiency of each discrete velocity model. The results show that D_3Q_{27} provides better accuracy compared to other discrete velocity models for the simulation of turbulent flow past an obstacle in a closed system. However, the model lags in terms of computational efficiency with other velocity models.

6.1.2 Effect of boundary conditions

In the second study of the thesis, the research work investigates the effect of boundary conditions in LBM on turbulent flow behavior past an obstacle. The study presents a comparative analysis of the modified BB and IB methods used to implement no-slip boundary conditions on the boundary nodes of an obstacle (here, a square cylinder). The results obtained for different turbulent statistics are validated with the existing experimental and other numerical results in the literature and show an excellent agreement against them. However, a slight divergence is observed in all the turbulent parameters at the streamwise location near the downstream face of the cylinder, both for the BB and IB method. Moreover, the results also show that the IB method over-predicted the mean drag coefficient (\overline{C}_D) and computationally expensive than the modified BB method.

6.1.3 Effect of baffles on flow hydrodynamics of stirred tank reactor

The thesis further studies the effect of baffles on flow behavior inside the stirred tank reactor. The flow system consists of a stirred tank reactor equipped with 6-blade dual-Rushton impellers. LBM is used to discretize the fluid domain and LES for the modeling of turbulent motions. The influence of cylindrical walls, baffles, and revolving shafts and impellers on the fluid flow is modeled using the IB method. The results are reported for phase averaged velocities and TKE in the presence and absence of baffles. Moreover, the simulations have been performed at three different locations of the placement of impellers on the shaft. The three different locations of the impellers produced three different flow patterns. They can be categorized as parallel flow, merging flow, and diverging flow. The results obtained are well agreed with the experimental data available in the literature. Furthermore, the research finds an interesting fact that in parallel flow, the presence and absence of baffles in the reactor configuration do not impact the flow properties. However, for the other two cases, i.e., merging and diverging flow pattern, the magnitude of both the flow properties, phase-averaged radial velocity, and TKE decrease in the absence of baffles.

6.2 RECOMMENDATIONS FOR FUTURE WORKS

The research work proposed in the present thesis allows formulating future objectives. Some of the recommendations are listed below:

- i. The present thesis investigated the viability of the SRT-LBM model for the turbulent flow simulation. The work shows that SRT-LBM can effectively predict the turbulent flow characteristics in various flow domains, like turbulent flow past over a bluff body confined in a closed system and flow behavior in stirred tank reactor. The work can be extended for applications in other fields, where the turbulent flow plays an important role, such as aerospace engineering, chemical engineering, water resource engineering, ocean engineering, and others.
- ii. The thesis work presented the results with SRT-LBM. The model works well for the high Reynolds number flows, only when some turbulence model can be incorporated in the frame of LBM. As in the present thesis, the LES model is used with LBM for turbulent flow modeling. However, the SRT-LBM model shows instability for high Reynolds number flows when DNS will be used to model turbulence eddies. Thus, alternative LBM models such as MRT, TRT, and others can be used for turbulent flow simulation to resolve the eddies up to the smallest-length scale with DNS.
- iii. In this thesis, a study is reported to show the effect of baffles on the flow hydrodynamics of stirred tank reactors fitted with dual-Rushton impellers. Further, we would like to extend the work for investigating the effect of other reactor components such as blades, impeller geometry, and height to width ratio of the reactor on flow parameters.
- iv. The stirred tank reactors are used for a for a broad range of applications including such as mixing, fermentation, polymerization, chemical reaction kinetics, flocculation, and others [Li *et al.*, 2012]. Moreover, the stirred tank reactor performs various operations such as homogenization, blending of miscible liquid, dispersion of gases or immiscible fluids in liquids, heat and mass transfer, suspension of solid particles, etc. And, all these operations are directly influenced by the flow behavior of the fluid inside the reactor [Kerdouss *et al.*, 2006; Escamilla-Ruíz *et al.*, 2017]. E.g., one of the multiple flow-associated processes, mixing, is utterly dependent on the flow behavior of the fluid. However, in the present thesis work, the study has been performed on stirred tank reactor only for the liquid phase hydrodynamics. This work can be extended to simulate multi-physical processes involved in the stirred tank reactor for its optimization and scale-up.for liquid flow hydrodynamics.