Multi-species multi-phase simulation of medium sized bioreactor with LES using Lattice-Boltzmann Equations

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Bioreactors are widely used in the industry to provide suitable environments for various bio-chemical processes. Primary concerns for these reactors are adequate mass transfer (e.g. O2 in, CO2 out), bubble holdup, heat transfer for temperature control, impeller power input, turbulence parameters and overall uniform mixing [1]. While reactor size of about 250m^3 is common in the industry, laboratory experiments and simulations have been confined to reactors of less than 1000L [2], [3]. Generally, operation parameters from designs in laboratory show inferior product yield, increased cell lysis and by-product formation [4], when used for operating full scale reactors. This is primarily due to the poor mixing at large scales. Various strategies have been used to utilize these scale down reactors for prediction of crucial parameters in a full-scale industrial reactor [5]. Using these methods, a recent investigation of the metabolic response of E. coli and production of the recombinant pre-proinsulin in presence of dissolved oxygen tension (DOT) revealed that relatively large losses were incurred due to the transients and formation of unwanted by-products. These methods recreate the transient behaviour by switching the working fluid between well mixed and “frozen” reactor states. Though these methods offer an in-depth analysis of a full scale reactor, they provide little input for design improvement.

Physical processes that occur in a stirred bioreactor are complex. A typical stirred reactor is a baffled cylindrical vessel with 3-4 turbines for mixing, with air sparger at the bottom (e.g. for introducing O2) of the tank. Different blade configurations are used to enhance mixing of the turbulent fluid with optimal power input to the impeller [6]. Ingredients to control PH value and other phenomenon like foaming, are added and expected to mix homogenously during the fermentation process. It is a multispecies, multiphase, turbulent flow with a rotating impeller. The bubbles introduced at the bottom break into smaller ones due to the shear induced by the rapid rotation of the impeller, and when the conditions permit, coalesce into larger ones. The size and speed of bubble injection also influences the optimal rotation speed of the impeller, and hence the required power [6]. Indeed, gas hold up in a reactor is one of the important design parameters.

Although experiments have been used very effectively to measure important flow features and design large reactors, advancement in computational techniques have allowed the use of CFD to study the flow more effectively. Computer simulations are more suited for designing since required parameters like geometry and volume of the reactor, type of blades of the turbine, rotation speed of the impeller can be easily modified. Mishra and Joshi [7] use CFD and experiments to analyse the flow pattern using a mix of two impeller of disc-turbine (DT) and pitched-blade down flow turbine (PTD) types. Recently, Ahmed et al [8] compare experiments and computations on a 5L dual-turbine aerated reactor and provide detailed flow parameters. Panneerselvam et al. [9] compare experiments and simulations on single turbine aerated reactor with Rushton turbines and with pitched turbine blades. Kerdouss et al. [10] simulated dual turbine aerated 40L reactor with commercial software ANSYS Fluent.

Sungkorn et al. [11], [12], developed a CFD code based on Lattice Boltzmann scheme to simulate a single turbine aerated reactor in Newtonian and non-Newtonian mediums. Turbulence was modelled using LES with Smagorinsky-Lilly subgrid model and van-Driest wall damping function. The boundary for the reactor and the rotating parts (the impeller and its shaft) are treated with immersed boundary method (IBM). The motion of bubbles is computed using Lagrangian tracking taking into account various forces like gravity, stress gradients, drag and lift and added mass. The interaction of the phases is achieved by two-way coupling introduced by Deen [13]. Reader is referred to Sungkorn et al. [11], [12] for more details.

We extend the algorithm developed by Sungkorn et al. [11], [12] to include scalar transport equations based on the work of Ponoth el al. [14]. The implementation is simple and the species solver couples with LBM naturally (unlike the traditional NSE solver which is known to have mass conservation problems for generalized boundaries). The basic idea is to use markers to simulate the scalar (the number density of the markers would be the scalar concentration). The markers are advected according to the following equations:

$$\boldsymbol{r}_{\left\{n+\frac{1}{2}\right\}} = \boldsymbol{r}_n + \Delta t\, \boldsymbol{v}_{\left\{\frac{1}{2}\right\}},$$

$$\boldsymbol{r}_{\{n+1\}} = \boldsymbol{r}_{\left\{n+\frac{1}{2}\right\}} + \boldsymbol{s}_n.$$

Here **r** is the position vector of the marker, **v** is the velocity at the marker position and $\mathbf{s_n}$ is chosen from a Gaussian random distribution designed to produce correct rate of diffusion. Marker particles would be introduced as necessary to mimic the source for the scalar and would be removed to mimic the sinks.

Medium sized reactors (~100 to 500L) will be simulated and detailed flow characteristics will be provided. Mixing time, gas holdup, detailed velocity field and shear rates, DOT, temperature field (where applicable) and scaling of these parameters with reactor volume will be presented. Indeed this would be a step towards simulating and designing a full scale industrial reactor using CFD with all of the complex physical phenomena acting together.

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