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CFD Simulation of Power and Mixing Time for a Rushton Turbine in a Baffled-Tank Reactor

R. Zadghaffari[1], J.S. Mogaddas[1,*], M. Ahmadlouydarab[1], J. Revstedt[2]

[1] *Chemical Engineering Faculty, Sahand University of Technology, P.O. Box 51335/1996, Tabriz, Iran*
[2] *Faculty of Engineerig, Lund University Division of Fluid Mechanics, P.O. Box 118, SE-221 00 Lund, Sweden*

Abstract:

The flow field, power consumption and mixing time in a standard baffled stirred tank with 6-blade Rushton turbine over a range of Reynolds numbers was simulated using computational fluid dynamics (CFD). The flow field calculations were performed using a time dependent sliding mesh (SM) technique. Mixing time was simulated by injecting a tracer from top of the tank and recording concentration of species at a specific location in probe installation point. The Large Eddy Simulation (LES) as a turbulent model was used, and the effect of grid density was examined by repeating calculation with higher mesh density. Power number and velocity profile between these two grids were compared with reported results. Results of power number and flow field show very good agreement. There are in fairly reasonable agreements with the reported values of predicted mixing time in the literature at the similar conditions.

Keywords: CFD, Stirred Tank, Mixing Time, Power, LES

Introduction:

The mixing and agitation of liquids in stirred tanks being one of the oldest of unit operations are used by many industries such as chemical, biotechnological, pharmaceutical, and food processing for mixing of single or multiphase fluids. The optimum design and the efficiency of mixing operations are important parameters on product quality and productions costs. Mixing time, power consumption, tank and impeller geometry and flow field are the most crucial parameters. Mixing time considered as a time taken that variation reduced as a below ±5% of the fully mixed concentration. A large number of power and mixing time measurement and correlations are available in the literature for impellers of various geometries and for various fluids. These correlations have been obtained based on laboratory scale measurements and their scale up to industrial scale mixing devices has always been a matter of concern. In recent years, Computational Fluid Dynamics (CFD) techniques are being increasingly used as a substitute for experiments to obtain the detailed flow field for a given set of fluid, impeller and tank geometries [1,2,3,4,5,6]. One advantage with CFD based prediction methods is that these do not have scaling up or scaling down problems as these solves the fundamental equations governing fluid flow. Therefore, some approximation on the physical phenomena, such as phenomenological models for turbulence, is often required even in CFD simulations. Researchers have employed mainly Reynolds Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES) techniques in CFD simulations [3,7]. Results obtained through RANS agree well with the experimental measurements in terms of bulk mean flow in the agitated tank but they suffer from inaccurate turbulent kinetic energy distribution prediction especially in the regions close to the impeller due to isotropic nature of

* jafar.moghaddas@sut.ac.ir

the k-ε turbulence model [3,8]. Large eddy simulations (LES), first adopted in stirred tank by Eggels[9], have proved to be a good method of investigating unsteady behavior in turbulent flow. Revstedt et al [10], pointed out that LES could provide details of the flow field that can not be obtained with RANS and corresponding models. Derksen[11,12] used LES with Smagorinsky subgrid scale (SGC) model to simulate a baffled stirred tank driven by a Rushton impeller.

In CFD, fully predictive simulations of flow field and mixing time mainly use either the sliding mesh(SM) [13] or the multiple reference frame (MRF) [14] approaches for account impeller revolution. The SM approach is a fully transient approach, where the rotation of the impeller is explicitly taken into account. On the other hand, the MRF approach predicts relative to the baffles [8]. The SM approach is more accurate but it is also much more time consuming than the MRF approach. SM simulation of a stirred tank content homogenization was first published by Jawerski and Dudczak [15], they used the standard k-ε model and compared results with experimental data.

Osman and Varley [16] studied the mixing time in an unbaffled vessel with a Rushton turbine using the MRF approach. The predicted mixing time was found to be up to two times higher than the experimental one and the authors attributed the discrepancies to the under estimation of the mean velocity components near the Rushton turbine. Jaworski et al [17], studied homogenization in a baffled vessel stirred by a dual Rushton impeller using MRF approach. Converge solution of the flow field was then used as an input for the solution of the scalar transport equation using SM approach in order to simulate the time dependent mixing process, but not continuing the computation of the flow field. The predicted mixing time was found to be 2-3 times higher than the measured values, in agreement with [16], they attributed inaccuracies to under prediction of the mass exchange between the recirculation zones generated by the Rushton turbines and wrongly predicted tangential velocity field [17]. The same authors, Bujalski et al. [18], also predicted these simulations with denser grid in the regions of high velocity gradients and with more converged solution, while solving the transient scalar transport equation in a stationary reference frame, they obtained improved results but still the mixing time was over predicted by about two times. In contrast to these papers, Shekhar and Jayanti [19], successfully simulated flow field and mixing characteristics in an unbaffled vessel stirred by a paddle impeller using low Reynolds k-ε model for rather low Reynolds numbers.

There are very low number of CFD based computations of the power consumption and power curve simulation in literature. S.Jayanti et al [19] simulated power and mixing time of a Newtonian fluid by a paddle type impeller in an unbaffled vessel by using SM method and results compared with experimental data.

In most of CFD simulations the baffles, impeller disc, and impeller blades are treated as zero thickness walls that are unreal assumptions. In this work, actual dimensions of stirred tank reactor were modeled and thickness of baffles and impeller blades were not neglected. The mixing process was simulated numerically using LES with Smagorinsky-Lilly subgrid scale model and flow field, power consumption and mixing time were simulated in a standard baffled tank reactor stirred with flat 6-blade Rushton turbine. Results of simulation of power were compared with experimental data [19,20], and results of simulation mixing time were compared with empirical correlations [17]. Power number and velocity profile between these two grids were compared with reported results. Results of power number and flow field show very good agreement. There are in fairly reasonable agreements with the reported values of predicted mixing time in the literature at the similar conditions.

Mathematical Formulation

The basic equations solved in a mixing calculation are those describing the flow of fluids, namely, Conservation of mass, momentum and energy. In our case we can neglect the temperature rise due to viscous dissipation.

Continuity:

$$\frac{\partial r}{\partial t}+\nabla.(r\vec{u})=S_m$$

Momentum:

$$\frac{\partial}{\partial t}(r\vec{u})+\nabla.(r\vec{u}\vec{u})=-\nabla P+\nabla.(\bar{\bar{t}})+r\vec{g}+\vec{F}$$

In the above equations, the time dependent terms are retained as mixing time can be estimated directly from time-dependent simulations. For turbulent flow to obtain the true variation of the velocity field, the above set of equations solved with LES Turbulent model.

LES lies somewhere between the DNS (Direct Numerical simulation) and the RANS (Reynolds Average Navier-Stokes) approaches. Basically, large eddies are resolved directly in LES, while small eddies are modeled. The governing equations employed for LES are obtained by filtering the time-dependent Navier-Stokes equations in either Fourier (wave-number) space or configuration (physical) space. The filtering process effectively ignores the eddies whose scales are smaller than the filter width or computational grid spacing. The resulting equations thus govern the dynamics of large eddies.

A filtered variable is defined by:

$$\bar{f}(X)=\int_{\Omega} f(X')G(X,X')dX'$$

Where Ω is the fluid domain, and G is the filter function that determines the scale of the resolved eddies. The finite-volume discretization provides the filtering operation implicitly

$$\bar{f}(X)=\frac{1}{V}\int_{\Omega} f(X')dX',\ X'\in\Omega$$

Where V is the volume of a computational cell. Filtering the Navier-Stokes equations results in $\frac{\partial r}{\partial t}+\frac{\partial}{\partial x_i}(r\bar{u}_i)=0$ and $\frac{\partial}{\partial t}(r\bar{u}_i)+\frac{\partial}{\partial x_i}(r\bar{u}_i\bar{u}_j)=\frac{\partial}{\partial x_j}(m\frac{\partial\bar{u}_i}{\partial x_j})-\frac{\partial\bar{P}}{\partial x_i}-\frac{\partial t_{ij}}{\partial x_j}$

Where t_{ij} is the subgrid-scale stress defined by $t_{ij}\equiv r\overline{u_iu_j}-r\bar{u}_i\bar{u}_j$. The subgrid-scale stresses resulting from the filtering operation are unknown, and require modeling. A common subgrid-scale model is Smagorinsky-Lilly model. In this, the eddy viscosity is modeled by $m_t=rL_s^2|\bar{S}|$. L_s is the mixing length for subgrid scales. In the Fluent program used, L_s is computed using $L_s=\min(Kd,C_sV^{1/3})$. K is the Von Karman constant, d is the distance to the closest wall, V is the volume of the computational cell. In this paper C_s is set to 0.1 [12]. And $|\bar{S}|\equiv\sqrt{2\bar{S}_{ij}\bar{S}_{ij}}$, where $\bar{S}_{ij}$ is the rate-of-strain tensor for the resolved scale.

A number of strategies can be used to deal with the movement of the impeller blades as mentioned before. In this study, MRF approach is used. Converged solution of the flow field was then used as an input for the solution of the scalar transport equation using the SM approach in order to simulate the time-dependent mixing process [8].

Estimation of Mixing Time:

For measurement of mixing time, a species injected from top of the tank and its concentration is simulated at a specific point with a conductivity probe. As shown in (Fig. 1) a Species is injected just below the free surface, at a horizontal distance of T/4 from the vessel wall, opposite the probe (Concentration reported point in simulation).
Mixing time considered as a time taken that variation reported as a below ±5٪ of the fully mixed concentration.
The concentration of species is governed by the following transport equation:

$$\frac{\partial}{\partial t}(rY_i) + \nabla.(r\vec{u}Y_i) = -\nabla.\vec{J}_i + R_i + S_i$$

Where Y_i is local mass fraction of each species R_i is the net rate of production by chemical reaction, as there is no chemical reaction, R_i is zero in the present case. r is the density of the carrier fluid, $\vec{u}$ is its velocity and S_i is the rate of creation by addition from the dispersed phase. In the turbulent flows, mass diffusion, $\vec{J}_i$ can be written as: $\vec{J}_i = -(rD_{i,m} + \frac{m_t}{Sc_t})\nabla Y_i$

Where Sc_t is the turbulent Schmidt number, $\frac{m_t}{rD_t}$ and $D_{i,m}$ are the diffusion coefficient for species i in the mixture.

Power Consumption:

The flow field around the impeller and also the shear stress and the pressure distribution on the impeller blade are resolved after simulation. Then power can directly can be estimated from a calculation of the total torque require to rotate the impeller. The torque on each blade can be calculated as:

$$T = \sum_i (\Delta P)_i A_i r_i$$

When the summation is over the control cells i corresponding to each blade, ΔP ,is the pressure difference between the front and the back side of the blade at the surface element i and r_i is the radial distance from the axis of the shaft on which the impeller is mounted. The power required for rotation of the impeller at a steady rotational speed of N revolution per second for an impeller having m blades is given by: $P = 2pNmT$

The power number is then computed as: $N_p = \frac{P}{rN^3d^5}$

Where d is the outer diameter of the impeller.[19]

CFD Method:

Three-dimensional CFD code fluent, version 6.1, a finite volume based fluid dynamic analysis program is used for solving a set of nonlinear equations formed by discretization of the continuity, the tracer mass balance, and momentum equations.
For simulation of mixing the computational mesh consisted of two parts: inner rotating cylindrical volume enclosed the impeller and part of the shaft and outer stationary volume filling the rest of the vessel.
A unstructured grid composed of hexahedral cells was made in gambit 2.1 pre-processor.

The system (Fig. 1), consist of cylindrical standard stirred tank reactor with dimensions that shown in table 1. The grid has 370997 nodes in the axial, radial and tangential directions. The calculations were repeated with a grid consist 612324 cells and solution is not changing with higher number of cells.

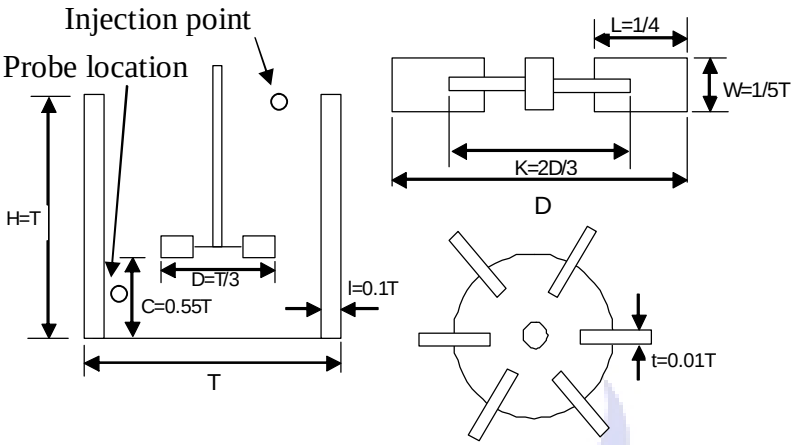

Fig.1- main dimentions of the Rushton impeller and tank that used for simulation

The fluid was water with a density of 1000 kg/m^3 and viscosity of 10^{-3} cp. The simulation was run as a transient problem in several impeller rotational speeds with an initial condition of zero velocity at all grid nodes and used the second-order upwind discretization scheme for discretization.

The simulation was run until the developed flow pattern became periodically repeatable, indicating that a statistical steady-state was reached. The power number was then calculated from the pressure distribution on the impeller. Mixing time calculations were then initiated with this velocity field as the starting point. The evolution of the concentration field with the introduction of tracer was then calculated by marching forward in time. Mixing time was obtained when the tracer mass fraction lay within a specified interval (95%) throughout the vessel.

Result and Discussion:

The typical velocity field produced for a turbulent flow case is shown in (fig.2). Along a cross-section of the tank, through the middle of the tank the flow field exhibits the characteristic pattern of a Rushton turbine, with radial discharge from the impeller, which splits into upper and lower circulation zones, with liquid returning axially to the top and bottom of the impeller. A stronger circulation pattern extending over a larger volume of the vessel is created. A low velocity region persists away from the shaft at the top of the vessel. This region decrease with increasing the Reynolds number.

Figure 3 shows the pressure distribution in a horizontal plane through the impeller, showing the region of high pressure in front and low pressure behind each blade.

Figure 4 shows the results obtained for power consumption under turbulent flow conditions that compared in table 2 with experimental data reported by walas [21].

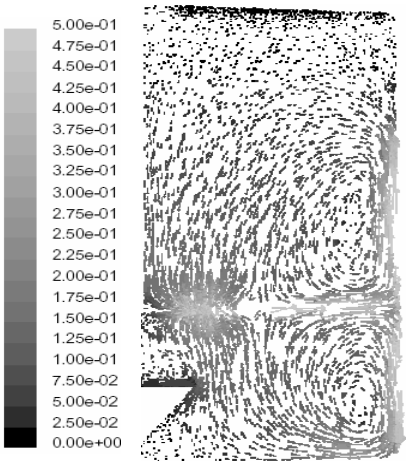

Fig.2- velocity field (m/s) along a cross-section Of the tank, through the middle of the tank in N_{Re}=250

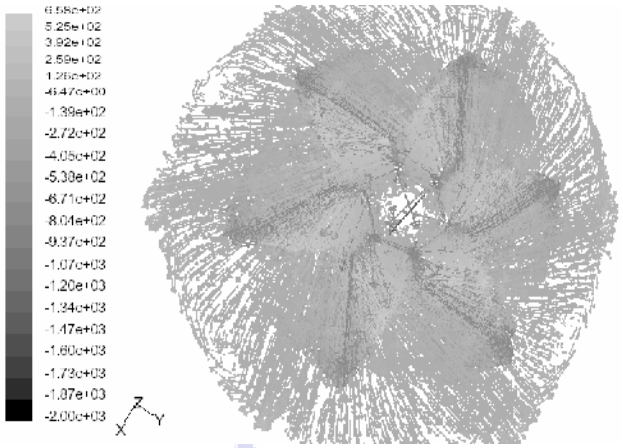

Fig.3- pressure distribution (pascal) in a horizontal plane through the impeller in N_{Re}=250

According to the experimental data N_p is independent from Reynolds number in turbulent region and is about 4.8 [21]. Predicted N_p values are in good agreement with experimental value with maximum deviation of 3٪.

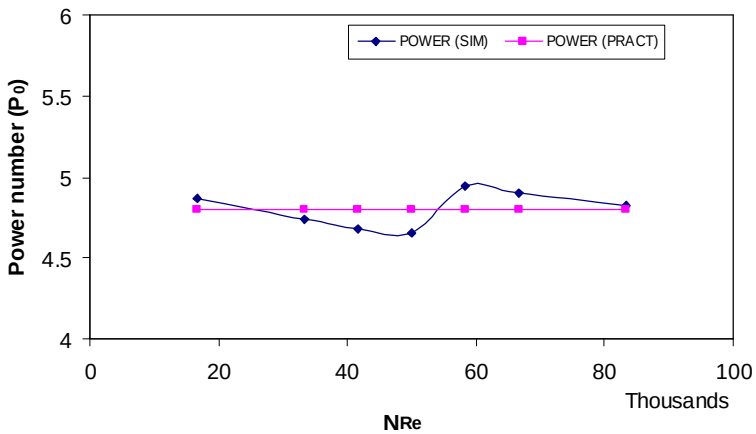

Fig. 4- comparison result of simulated power number (P_0) with experimental data [21].

Mixing Time:

The progress of mixing is specific to the flow field which is characterized by a circulation pattern and an effective diffusivity. For turbulent flows, the molecular diffusivity is augmented by turbulent fluctuations and the effective diffusivity being a strong function of local velocity gradients. There are several empirical relations in literatures that have been proposed for prediction of mixing time. Results of simulation of mixing time are illustrated in figure 5 and compared with empirical correlation [21-25].

As shown in fig. 5, by increasing the Reynolds number the stronger radial out flow pushes the species rapidly into the lower and the upper recirculation loops and reduced mixing time. There are in fairly reasonable agreement with the values of calculated mixing time by using equation 2 that consider the detail characteristic of tank and impeller.

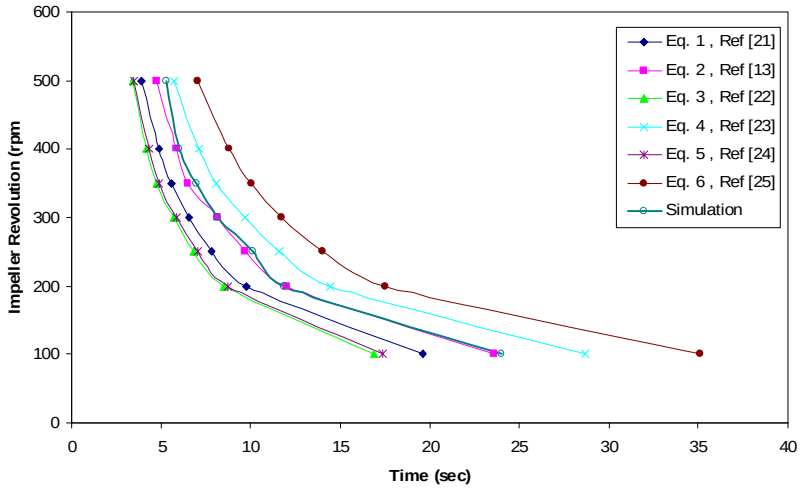

fig. 5- comparison result of simulated mixing time with experimental data

Conclusion:

In the present paper, the flow field, power consumption and mixing time in a baffled tank stirred by a flat 6-blade Rushton turbine were predicted using the CFD code, fluent 6.1, over a range of impeller Reynolds numbers in turbulent regime by using LES. The tank and impeller geometry had standard dimensions so that we can compare simulated data with experimental data that are available in literatures [21] for flow field and power calculation. Predicted mixing times are compared with empirical correlations. The computations reported in the present paper show that reasonable predictions of the velocity field, power consumption and mixing time in turbulent Reynolds numbers. Therefore we could be readily used CFD simulation for industrial application and to investigate scale-up effects in mixing.

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