Stirred tank simulation using Partially-Averaged Navier-Stokes $k_u - \epsilon_u$ turbulence model

Srimanta Maji¹ · Akshaya K. Sahu¹Received: 25 August 2020 / Accepted: 9 March 2021 / Published online: 1 April 2021
© The Author(s) 2021 [OPEN](#)

Abstract

In the present study, simulation of a stirred tank using axial flow impeller has been studied numerically to see the behaviour of flow variables in the entire vessel. It is assumed that the flow is steady state, two dimensional, incompressible and axisymmetric. For simulation, Partially-Averaged Navier-Stokes (PANS) $k_u - \epsilon_u$ turbulence model has been taken into account. For discretization, control volume method along with upwind and power-law schemes have been taken. The solutions are obtained by using the SIMPLE algorithm. The boundary conditions for impeller are given by using the experimental data. The main objective is to investigate the influence of different filters width f_k of the PANS $k_u - \epsilon_u$ model parameter on the characteristic flow variables. The predicted results of the PANS $k_u - \epsilon_u$ model for different f_k have been compared with the experimental data at different axial levels of the stirred tank. It has been observed that the power-law scheme gives better agreement with the experimental data. Further, near the impeller region, PANS predicted results are better for smaller f_k . Also, Reynolds-Averaged Navier-Stokes Shear Stress Transport (SST) $k - \omega$ turbulence model has been tested for comparative study.

Keywords PANS $k_u - \epsilon_u$ turbulence model · SST $k - \omega$ turbulence model · Control volume method-stirred vessel · Axial flow impeller

1 Introduction

The simulation of flows generated by axial type impellers is still a challenging topic in many investigations since the last three decades. The flow fields generated by axial type impellers are of pumping down or pumping-up in nature. The impellers like, pitched blade turbines, marine propellers, hydrofoil impellers, etc., are of this category. Axial flow impellers are heavily used in pharmaceutical, chemical, food industries etc. for mixing/blending, solid suspension and also for the process of heat transfer. Due to the complexity of flow structures which are associated with turbulence by mechanical agitation, it is not an easy task to capture all the flow characteristics in the entire stirred tank. Therefore, an accurate modeling technique

is required to understand the phenomena for turbulent flow fields. There are various turbulence models available in the existing literature [1]. Among these turbulence models, the Large eddy simulation (LES) model predicted more accurately. However, the simulations using the LES model are very expensive [2]. Whereas RANS models are less expensive but the predictions of RANS models are not so much accurate. Therefore, a model is required which is computationally less expensive and also captures turbulent phenomena more accurately. The invention of the PANS $k_u - \epsilon_u$ model [3] may bridge the gaps. The model is based on the standard RANS $k - \epsilon$ model and it has two filter parameters f_k and f_ϵ which control the turbulent flow characteristics. The PANS model has been used for simulation of various problem in different fields [4], however,

✉ Srimanta Maji, maji.srimanta758@gmail.com | ¹Department of Mathematics, Institute of Chemical Technology, Mumbai, Maharashtra 400019, India.

the simulation of stirred vessel using PANS model has not been investigated till now.

Initially, Pericleous and Patel [5] tried to capture the action of a rotating impeller by providing momentum sources. The predicted radial and tangential velocities were well with the experimental data for radial flow impeller. In case of axial type impellers, the predicted axial velocity profiles gave better agreement, whereas the profiles for radial velocity were in poor agreement with the experimental data. However, the comparison for turbulent characteristics was absent in the study. Ranade et al. [6] were probably the first who attempted to simulate the stirred tank by using turbulence models for axial flow impeller. They used black box approach and for the simulation they had taken the standard $k - \epsilon$ model. They also studied the effect of model parameters, impeller boundary conditions (IBC) and grid size for simulation. They concluded that the prediction of axial velocity was fairly good. However, near the impeller region, the prediction for tangential velocity and turbulent kinetic energy (TKE) showed significantly good predictions. Further, Ranade et al. [7] studied the simulation for stirred tank for different axial flow impellers (PBD30, PBD60, curved PBD, three types of PBD45 with different blade width, convex type PBD, modified PBD, propeller and multiple type PBD). They observed that the pumping effects varied from 19% (for convex type PBD) to 89% (for propeller). Armenante and Chou [8] studied the stirred tank simulation by using standard $k - \epsilon$ model and algebraic stress model (ASM) model for three different IBCs. They observed that the prediction for axial and tangential velocities for the $k - \epsilon$ model were in poor agreement as compared to the ASM model. The prediction for radial velocities for both the models were not satisfied specially near the vessel center. Further, the predictions for TKE were severely underpredicted throughout the region of comparison for both the models. Sahu and Joshi [9] studied comprehensively the simulations of stirred tanks for axial flow impeller. For modeling purposes, they used black box approach and for simulation they had taken the standard $k - \epsilon$ model. Further, they studied the effect of initial condition, grid size, and sensitivity of model parameters. Prediction of axial velocities were in good agreement with the experimental data while predicted radial velocity profiles were well only below impeller region. The predictions for TKE profiles were also severely underpredicted. Bakker et al. [10] investigated the CFD simulation for stirred tanks to see the behaviour of flow fields. They made quantitative comparisons for radial and axial velocities profiles only in the turbulent regime. The predicted radial velocities were poor for each turbulence model near the bottom of the tank. The predicted axial velocities were also not so good with the experimental data near the bottom of the impeller. For CFD simulation in the stirred tank,

they suggested using the sliding mesh technique. Bakker et al. [11] used sliding mesh (SM) technique for CFD simulation of both laminar and turbulent flow inside the stirred vessel by considering RNG $k - \epsilon$ model. No comparisons were made for the predicted velocities. Simulation of turbulent flow was only made for the comparison of flow numbers. For CFD simulation of turbulent flow in a flat bottomed stirred tank, Armenante et al. [12] used black box approach. For simulation they used the standard $k - \epsilon$ and the ASM turbulence models. The prediction of radial velocity was poor below the impeller, while the prediction for axial velocity was very good throughout the region of comparison. Further, the TKE predictions for ASM model were good above the impeller region whereas the TKE predictions below the impeller region were severely underpredicted. Ljungqvist and Rasmuson [13] carried out the simulation for stirred tank with open and close surfaces for axial flow simulation produced by pitched blade turbine with standard $k - \epsilon$ turbulence model using black box approach. They observed that no slip or free slip conditions do not effect on the impeller rotation. All the three components of the velocity were underpredicted near the bottom of the tank. Furthermore, the axial velocity profiles were larger as compared to other two velocity components. Naude et al. [14] used $k - \epsilon$ and RNG $k - \epsilon$ turbulence models to simulate the flow in the stirred tank produced by twin propeller with black box approach. The results were given in terms of power numbers and flow. However, the velocity comparisons were absent in their study. They observed that the predicted values of flow and power number gave good agreement for standard $k - \epsilon$ model whereas RNG $k - \epsilon$ model predicted power numbers were significantly lower. Further the predicted total energy dissipation rate was higher for $k - \epsilon$ model and for the RNG $k - \epsilon$ model, it was better in the near wall region. Brucato et al. [15] used sliding mesh method and inner-outer technique along with black box approach for modeling the action of rotating impeller. For the simulation they used the standard $k - \epsilon$ model. They observed that by using the sliding mesh technique some qualitative features for the rotating impeller were found. Further, they gave vector velocity plots generated by axial flow impellers for upstream and downstream flows in the plan. Sahu et al. [16] showed interest to study the mixing performance in the stirred tank using zonal modeling for different axial flow impellers. Also, they proposed a new method to estimate turbulent kinetic energy dissipation rate. They calculated mixing time for their simulation. They concluded that the predicted mixing times were in excellent agreement with the experimental data. Further, the predicted radial and axial velocities showed good agreement with the experimental findings. They also concluded that the zonal modeling approach improve the prediction of

the turbulent kinetic energy significantly. Nere et al. [17] studied the sensitivity analysis for the standard $k - \epsilon$ model constants like C_{μ} , C_1 , and C_2 for the simulation of stirred tank by using hydrofoil and pitched blade turbine with angle of 45° . Also, they attempted to develop a constitutive equation for C_{μ} which described eddy viscosity in the $k - \epsilon$ model. They observed that the modified model gave better prediction for axial, tangential and radial velocities. For simulation of stirred tank, Jaworski et al. [18] used six different turbulence models such as standard $k - \epsilon$, RNG $k - \epsilon$, realizable $k - \epsilon$, optimised Chen–Kim $k - \epsilon$, Chen–Kim $k - \epsilon$ and Reynolds stress model (RSM). They compared the predicted results for flow characteristics with their own experimental data. They observed that TKE was underpredicted by all the turbulence models while the standard $k - \epsilon$ model was better with the experimental data. Aubin et al. [19] studied the effect of various turbulence models, standard $k - \epsilon$ and RNG $k - \epsilon$ models along with upwind schemes of different orders for discretisation. Also, they studied the effect of discretisation schemes and the effect of different turbulence models on the predictions of mean velocities and TKE profiles. They also used a sliding mesh technique for simulation and concluded that the sliding mesh technique is superior to others method. Further, they observed that higher order schemes gave better predictions and there was not so much variation in the predicted results with the changing of turbulence models. Murthy and Joshi [20] made a comprehensive study for the flow characteristics for stirred tank simulation by using standard $k - \epsilon$, RSM, and LES models. They compared the predicted results in the impeller region as well as in the bulk region. They concluded that LES followed by RSM predicted well with the experimental findings. All the model predicted axial velocities gave satisfactory results. The deviation in the radial velocities for all models were observed. Further, for pitched blade impellers, they observed that the standard $k - \epsilon$ model underpredicted the TKE. Wang et al. [21] simulated the stirred tank by using Multiple Reference Frame (MRF) and standard $k - \epsilon$ model to analyze the mixing process in the tank and compared the predicted results with their own experimental PIV data. They observed that the increasing trends in the predicted axial velocity fields from the numerical simulation matched well with that of the experimental observation, while the points of highest speed were different. At the bottom area of the tank, the results are consistent, whereas the highest speed of simulation on impeller discharge and impeller inflow region are little lower than the experiment data respectively. Ge et al. [22] carried out the study for modified pitched blade turbine (m-PBT) by using the $k - \epsilon$ turbulence model for axial flow impeller. The simulation showed a good agreement with the PIV experimental data for the mean velocity. It

underestimated the TKE prediction near the blade. They also shown that the change of the blade shape helped to increase the magnitude of velocities near the impeller. However, the axial velocity mixed poorly in the central region of the tank. Mule et al. [23] studied the effect of the number of different branches of fractal impellers in the simulation of stirred vessels. They found similar observations for all the branches of the fractal impeller in the prediction of axial and radial velocities. However, they found the highest magnitude in velocity for the tangential components for all the configurations. Recently, Lane [2] studied the axial flow simulation of a tank stirred by a Lightning A310 hydrofoil to improve CFD modeling for more accurate predictions. He found that a high resolution mesh along with an appropriate choice of turbulence model was needed to get a more appropriate design. However, this improvement was very expensive. Therefore, a model has been required with less computational cost and able to capture all the turbulence characteristics well. The invention of Partially- Averaged Navier-Stokes (PANS) model approach [3] might fulfill the said requirements as this model is an filtering approach. Also, it is a bridging model between RANS and DNS (Direct Numerical Simulation) and less expensive in term of computational cost. Thus, with the changes in the values of the filter parameters how the model will predict the flow characteristics, we want to look for it.

Thus, in the present study, we investigated numerically the simulation of stirred tank for axial flow impeller using the PANS $k_u - \epsilon_u$ model approach to see how the model predicts the flow characteristics. None of the researchers have studied the simulation of stirred tank using the PANS model till now as per the authors concerns. Further, RANS SST $k - \omega$ models have also been included for the simulation. In the next section, we discuss briefly about the mathematical formulation and about the proposed models for the present study. Section 3 includes the boundary conditions for the model variables. Numerical method for the simulation of turbulent flow has been considered in the Sect. 4. Results and discussion has been taken in Sect. 5. Lastly, the conclusions are outlined in Sect. 6.

2 Mathematical formulation

The physical system which has been incorporated for the present study, consists of a cylindrical tank along with four baffles (of width $T/10$) which are spaced equally around the perimeter, T being the diameter of the tank ($T = 500$ mm) and the pitch bladed downflow turbine (PTD) with impeller diameter as 167 mm have considered for simulation. The impeller location is at the height $H/3$ from the bottom of the tank, H being the height of the liquid ($H = T$). In this study,

a two-dimensional, steady-state, axisymmetric turbulent flow in a baffled cylindrical tank has been considered. The origin of the tank is taken at the center of the impeller plane (Fig. 1). With these assumptions, the dimensionless form of the governing equations can be written in generalized compact form:

$$\frac{1}{r} \frac{\partial}{\partial r}(ur\Theta) + \frac{\partial}{\partial z}(v\Theta) = \frac{1}{r} \frac{\partial}{\partial r} \left[r \Gamma_{eff} \frac{\partial \Theta}{\partial r} \right] + \frac{\partial}{\partial z} \left[\Gamma_{eff} \frac{\partial \Theta}{\partial z} \right] + S^\Theta \quad (1)$$

where, Θ indicates for general representation of the flow characteristics (u, v, k, ω, k_u and ϵ_u) and S^Θ for source terms. In Tables 1 and 2, the values of Θ , Γ_{eff} and S^Θ are given. The non-dimensional quantities u, v, p, k, ϵ, r and z have been defined as follows: $u = \frac{\bar{u}}{U_{tip}}$, $v = \frac{\bar{v}}{U_{tip}}$, $p = \frac{\bar{p}}{\rho U_{tip}^2}$, $k = \frac{\bar{k}}{U_{tip}^2}$, $\epsilon_u = \frac{\bar{\epsilon} R}{U_{tip}^3}$, $r = \frac{\bar{r}}{R}$ and $z = \frac{\bar{z}}{R}$, where $\bar{u}, \bar{v}, \bar{p}, \bar{k}, \bar{\epsilon}, \bar{r}, \bar{z}, U_{tip}$ and R are the dimensional mean radial velocity, mean axial velocity, pressure, total TKE, total turbulent energy dissipation rate, radial and axial co-ordinate, impeller tip velocity and radius of the vessel respectively. The non dimensional unresolved TKE, k_u and turbulent energy dissipation rate, ϵ_u for PANS $k_u - \epsilon_u$ model are obtained from the relations $k = k_u/f_k$ and $\epsilon = \epsilon_u/f_\epsilon$. Then, by using these relation in the k and ϵ equations for $\Theta = k, \epsilon$ in Eq. (1), the equation for k_u and ϵ_u for PANS $k_u - \epsilon_u$ model can be obtained.

Fig. 1 Solution domain for mathematical model

Table 1 The source terms (S^Θ) for generalized Eq. (1) for PANS $k_u - \epsilon_u$ model

Θ	Γ_{eff}	S^Θ
1	0	0
u	$\mu + \mu_t$	$C_\mu \left[\frac{1}{r} \frac{\partial}{\partial r} (r \Gamma_{eff}) \frac{\partial u}{\partial r} + \frac{\partial}{\partial z} (\Gamma_{eff}) \frac{\partial v}{\partial r} \right] - \left(\frac{\partial p}{\partial r} + \frac{2}{3} \frac{\partial k_u}{\partial r} \right)$
v	$\mu + \mu_t$	$C_\mu \left[\frac{1}{r} \frac{\partial}{\partial r} (r \Gamma_{eff}) \frac{\partial u}{\partial z} + \frac{\partial}{\partial z} (\Gamma_{eff}) \frac{\partial v}{\partial z} \right] - \left(\frac{\partial p}{\partial z} + \frac{2}{3} \frac{\partial k_u}{\partial z} \right)$
k_u	$\mu + \frac{\mu_t}{\sigma_{k_u}}$	$G - \epsilon_u$
ϵ_u	$\mu + \frac{\mu_t}{\sigma_{\epsilon_u}}$	$\frac{\epsilon_u}{k_u} (C_{1\epsilon}^* G - C_{2\epsilon}^* \epsilon_u)$

where $G = C_\mu \mu_t [2(\frac{\partial u}{\partial r})^2 + (\frac{u}{r})^2 + (\frac{\partial v}{\partial z})^2] + (\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r})^2$, $\mu = \frac{\bar{\mu}}{C_\mu Re}$
 $Re = \frac{\rho U_{tip} R}{\mu}$, $\mu_t = \frac{k_u}{\epsilon_u}$

3 Boundary conditions

Due to the presence of baffle in the stirred vessel the flow can be considered as asymmetric and the boundary conditions for the non-dimensional flow variables $u, v, k, k_u, \epsilon_u, \omega$ for the two dimensional axisymmetric problem are defined as follows:

On the axis of symmetry: $r = 0; u = 0, \frac{\partial v}{\partial r} = \frac{\partial k_u}{\partial r} = \frac{\partial \epsilon_u}{\partial r} = \frac{\partial \omega}{\partial r} = 0$.

On the vertical wall: $r = 1; u = v = k_u = \epsilon_u = \omega = 0$.

On the bottom of the vessel: $z = 0; u = v = k_u = \epsilon_u = \omega = 0$.

On the top surface of the liquid: $z = 2; v = 0, \frac{\partial u}{\partial z} = \frac{\partial k_u}{\partial z} = \frac{\partial \epsilon_u}{\partial z} = \frac{\partial \omega}{\partial z} = 0$.

In case of PANS $k_u - \epsilon_u$ model, for numerical computation wall function and logarithmic velocity profile for turbulent region are used to replace no slip boundary condition and the turbulent dissipation rate has been calculated by the formula $\epsilon_u = C_v^4 k_u^2 / \kappa y_p$. (y_p being the shortest distance from the wall to first node point). The

Table 2 The source terms (S^Θ) for generalized Eq. (1) for SST $k - \omega$ model

Θ	Γ_{eff}	S^Θ
1	0	0
u	$\mu + \mu_t$	$C_\mu \left[\frac{1}{r} \frac{\partial}{\partial r} (r \Gamma_{eff}) \frac{\partial u}{\partial r} + \frac{\partial}{\partial z} (\Gamma_{eff}) \frac{\partial v}{\partial r} \right] - \left(\frac{\partial p}{\partial r} + \frac{2}{3} \frac{\partial k}{\partial r} \right)$
v	$\mu + \mu_t$	$C_\mu \left[\frac{1}{r} \frac{\partial}{\partial r} (r \Gamma_{eff}) \frac{\partial u}{\partial z} + \frac{\partial}{\partial z} (\Gamma_{eff}) \frac{\partial v}{\partial z} \right] - \left(\frac{\partial p}{\partial z} + \frac{2}{3} \frac{\partial k}{\partial z} \right)$
k	$\mu + \frac{\mu_t}{\sigma_k}$	$G - \beta^* k \omega$
ω	$\mu + \frac{\mu_t}{\sigma_\omega}$	$\alpha \frac{\omega}{k} G - \beta \omega^2 + 2 \sigma_d (1 - F_1) \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}$

$G = C_\mu \mu_t [2(\frac{\partial u}{\partial r})^2 + (\frac{u}{r})^2 + (\frac{\partial v}{\partial z})^2] + (\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r})^2$, $\mu = \frac{\bar{\mu}}{C_\mu Re}$

$Re = \frac{\rho U_{tip} R}{\mu}$ and $\mu_t = \frac{k}{\omega}$

boundary conditions for u , v and k_u are given (30mm below the impeller position) from the experimental data in the impeller region and the data for local dissipation rate in the impeller region has been given by the formula $\epsilon_u = C_v^4 k_u^2 / 0.07l$ (l being the length of the tank diameter). For SST $k - \omega$ model, ω have been calculated by the formula $60/0.075 Re(\Delta y_n)^2$ and ω have been calculated in the near wall node by the formula, $60/0.075 Re(\Delta y_n)^2$.

4 Numerical method

For numerical simulation the governing equations for flow variables from Eq. (1) are discretized by using control volume method with stable upwind and power law schemes for convective part and second order central difference scheme for diffusive term. After discretization we obtain the algebraic equations for all the flow variables. They can be written in compact form as follows:

$$a_p \theta_p = a_E \theta_E + a_W \theta_W + a_N \theta_N + a_S \theta_S + \bar{S}^\theta \quad (2)$$

where

$$a_p = a_E + a_W + a_S + a_N + (F_e - F_w) + (F_n - F_s) \quad (3)$$

and

$$\bar{S}^\theta = (S^\theta)_p r_p \Delta r \Delta z \quad (4)$$

The source term S^θ is different for different flow variables which have been obtained from Tables 1 and 2. After discretizing the term S^θ we have got the discretized source term $\bar{S}^\theta$ from Eq. (4) for each variable. Further, to obtain

diagonally dominant matrix the Expression (4) can be written as

$$\bar{S}^\theta = (S_C + S_p \theta_p) r_p \Delta r \Delta z \quad (5)$$

where the term S_p is negative and S_C is positive. Since the variables k_u , ϵ_u , ω , etc. are positive quantities, thus the term $\bar{S}^\theta$ should be positive for those quantities. Then, we apply the SIMPLE algorithm [24] to solve the pressure and mean velocity equations simultaneously. After correcting the velocity fields, the variables k_u , ϵ_u , k and ω are calculated. Then by applying Gauss-Seidel iterative method, the set of algebraic equations are solved iteratively for different flow characteristics. The computations are carried out by using in-house code. Iterative process terminates when the mass residue term is less than 10^{-6} at each control volume.

5 Results and discussion

The simulation of cylindrical baffled stirred tank agitated by axial flow impeller has been investigated numerically by using various turbulence models. The flow domain for the simulation has been given in Fig. 1. A non-uniform grid of size 61×85 which gives grid independent solution has been taken for numerical computation as shown in the Fig. 2a,b. Firstly, the results are simulated numerically for upwind and power-law schemes for different turbulence models. The predicted radial, axial and turbulent kinetic energy (TKE) at two different locations at $z = 0.18$ and $z = 0.907$ are plotted in the Figs. 3, 4 and 5 respectively. It has been observed that power law

Fig. 2 Results for radial and axial velocity profiles with different grid sizes

Fig. 3 Comparison between upwind and power-law scheme for PANS $k_u - \epsilon_u$ and SST $k - \omega$ model. PANS $k_u - \epsilon_u$ power-law —, PANS $k_u - \epsilon_u$ upwind —, SST $k - \omega$ power-law - - - and SST $k - \omega$ upwind —

(a) $z=0.18$

(b) $z=0.907$

Fig. 4 Comparison between upwind and power-law scheme for PANS $k_u - \epsilon_u$ and SST $k - \omega$ model. PANS $k_u - \epsilon_u$ power-law —, PANS $k_u - \epsilon_u$ upwind —, SST $k - \omega$ power-law - - - and SST $k - \omega$ upwind —

(a) $z=0.18$

(b) $z=0.907$

scheme has shown better predictions with the experimental data as compared to the predicted results of upwind scheme for different turbulence models. Thus, the power-law scheme has been taken for numerical computation throughout the study. The model predicted profiles for mean radial velocity, mean axial velocity, TKE and turbulent kinetic energy dissipation rate have been plotted to analyse the flow characteristics and are also compared with the experimental data [25].

5.1 Radial velocity

Figure 6a represents the radial velocity profiles predicted by different turbulence models at the axial location $z = 0.18$, just above the bottom wall. At this location, the radial flow is feeble near the axis as the axial flow is more dominant at this region. Then gradually, it increases along the radial axis and attains its maximum and then it

Fig. 5 Comparison between upwind and power-law scheme for PANS $k_u - \epsilon_u$ and SST $k - \omega$ model. PANS $k_u - \epsilon_u$ power-law —, PANS $k_u - \epsilon_u$ upwind —, SST $k - \omega$ power-law — and SST $k - \omega$ upwind —

(a) $z=0.18$

(b) $z=0.907$

Fig. 6 Radial velocity profiles below the impeller at different z -location for $f_k = 0.2$ (---), $f_k = 0.5$ (---), $f_k = 0.8$ (---), $f_k = 1.0$ (---) of PANS $k_u - \epsilon_u$ model, SST $k - \omega$ model (---) and experimental data (■)

(a) $z=0.18$

(b) $z=0.306$

decreases gradually towards the wall. For the PANS $k_u - \epsilon_u$ model, the predicted radial profiles for all f_k are almost the same upto $r = 0.8$. However, towards the wall for $f_k = 0.2$, PANS $k_u - \epsilon_u$ model deviates more from others f_k . Further, for SST $k - \omega$ model, the radial profile attains a maximum at $r = 0.37$ and then gradually decreases towards the wall. Thus, at this axial level, throughout the radial location except $0.6 < r < 0.78$, SST $k - \omega$ model gives better prediction with the experimental data as compared to PANS

$k_u - \epsilon_u$ model. Further, amongst all the filter width f_k , for $f_k = 1$, PANS $k_u - \epsilon_u$ (i.e., standard $k - \epsilon$ model) gives better agreement with the experimental data. Just below the impeller location at $z = 0.36$, the axial flow is much more dominant. Thus, near the axis of symmetry the prediction of radial profiles is very weak. In this axial location (Fig. 6b) initially upto $r = 0.4$, the predictions of the PANS $k_u - \epsilon_u$ model are very good. In the range $0.2 < r < 0.4$, $k - \epsilon$ (i.e., for $f_k = 1$) model predicts better agreement with the

experimental data. However, PANS $k_u - \epsilon_u$ underpredicts the experimental data for all its f_k upto $r = 0.9$ and beyond $r > 0.9$, it overpredicts the experimental data. Moreover, in the range $0.4 < r < 0.85$, SST $k - \omega$ model predicts better agreement with the experimental data as compared to PANS $k_u - \epsilon_u$ model. Just above the impeller at $z = 0.787$ (Fig. 7a), the prediction for radial velocities for various turbulence models have been shown. Near the axis and

towards the wall, predictions of all the models are feeble. Near the axis PANS $k_u - \epsilon_u$ gives better prediction for all f_k except $f_k = 0.2$. However, towards the wall $k - \epsilon$ gives excellent agreement. Further, in the region $0.2 < r < 0.8$ predicted radial velocities are much stronger for all models and maximum occurs at the point $r = 0.4$ for SST $k - \omega$ model. Therefore, in the region $0.2 < r < 0.35$, SST $k - \omega$ and $r > 0.4$ for $f_k = 0.2$, PANS $k_u - \epsilon_u$ gives better prediction

Fig. 7 Radial velocity profiles above the impeller at different z -location for $f_k = 0.2$ (---), $f_k = 0.5$ (---), $f_k = 0.8$ (---), $f_k = 1.0$ (---) of PANS $k_u - \epsilon_u$ model, SST $k - \omega$ model (---) and experimental data (■)

(a) $z=0.787$

(b) $z=0.907$

(c) $z=1.147$

(d) $z=1.38$

amongst all the models. At this axial level $z = 0.907$, all the model predictions are good with the experimental data (Fig. 7b). In this range $0.2 < r < 0.25$, SST $k - \omega$ model and in the range $0.35 < r < 0.4$ and $0.4 < r < 0.5$ for $f_k = 0.5$ and $f_k = 0.2$ respectively, PANS $k_u - \epsilon_u$ give better agreements. Near the wall all the model predictions are poor with the experimental data. Thus at this axial level, $f_k = 0.2$ give better agreement amongst all the model predictions. Away from the impeller, at $z = 1.147$ (Fig. 7c), PANS $k_u - \epsilon_u$ model gives better estimate with the experimental data for $f_k = 0.2$ in the region $0 < r < 0.6$. In this region the predictions for others f_k for PANS $k_u - \epsilon_u$ model are very poor. However, for $r > 0.7$, $k - \epsilon$ and PANS $k_u - \epsilon_u$ model for $f_k = 0.8$ give good agreement with the experimental data. The predicted results for SST $k - \omega$ model are in good agreement in the region $0 < r < 0.5$ and beyond $r > 0.5$, it underpredicts the experimental data. Thus, in this axial level, PANS $k_u - \epsilon_u$ model predictions are superior to SST $k - \omega$ model predictions for some f_k . Far away from the impeller location, at the level $z = 1.38$ (Fig. 7d), the prediction for radial velocity is very good for SST $k - \omega$ model in the region $0.05 < r < 0.4$. Moreover, PANS $k_u - \epsilon_u$ gives good prediction in the region $0 < r < 0.2$. Beyond $r > 0.45$, PANS $k_u - \epsilon_u$ gives better prediction for all its f_k and towards the wall $f_k = 0.2$ gives better agreement whereas SST $k - \omega$ model underpredicts the experimental data.

Thus, for the prediction of radial velocity profiles for different turbulence models, it has been observed that below the impeller region, radial velocity predictions for SST $k - \omega$ model are better than PANS $k_u - \epsilon_u$ model. Above and away from the impeller, the SST $k - \omega$ model gives

good agreement in some regions near the axis. Otherwise PANS $k_u - \epsilon_u$ model gives better prediction in the region $r > 0.5$ for $f_k = 0.2$. Also, the prediction for the PANS $k_u - \epsilon_u$ model is better below the impeller. Further, away from the impeller $k - \epsilon$ give good agreement for $r > 0.6$.

5.2 Axial velocity

As the simulation of stirred tank has been taken for axial down flow type impeller, the flow field will be much stronger near the axis at all axial levels. The model predicted data for axial velocity profiles are also following the same trends for different turbulence models as shown in the Figs. 8 and 9. Axial velocity at the level $z = 0.18$ (Fig. 8a) increases rapidly near the axis and attends maximum at $r = 0.21$ and then it decreases slowly. The gradient is sharp from $r = 0.21$ to $r = 0.33$. From $r = 0.33$ onwards the velocity decreases gradually and becomes very small at $r = 0.78$ and beyond this point axial flow changes direction to upwards and increases upto near the wall. The same flow patterns have been observed for all models at these axial locations. Initially in the range $0 < r < 0.28$, SST $k - \omega$ model prediction is better with the experimental data. Then, in the region $0.28 < r < 0.83$, all the models underpredict the experimental data. Beyond this region, all the models give good agreement. Thus, at this axial level, throughout the radial direction, SST $k - \omega$ gives good prediction, whereas, near the wall $k - \epsilon$ model gives good prediction with the experimental data. At the axial location $z = 0.306$, the prediction for axial velocity profiles (Fig. 8b) for different turbulence models have followed

Fig. 8 Axial velocity profiles below the impeller at different z-location for $f_k = 0.2$ (---), $f_k = 0.5$ (---), $f_k = 0.8$ (---), $f_k = 1.0$ (---) of PANS $k_u - \epsilon_u$ model, SST $k - \omega$ model (---) and experimental data (■)

(a) $z=0.18$

(b) $z=0.306$

Fig. 9 Axial velocity profiles above the impeller at different z -location for $f_k = 0.2$ (---), $f_k = 0.5$ (---), $f_k = 0.8$ (---), $f_k = 1.0$ (---) of PANS $k_u - \epsilon_u$ model, SST $k - \omega$ model (---) and experimental data (■)

similar trends as shown in Fig. 8a and the predictions are much better with the experimental data at this axial level $z = 0.306$. Near the axis of symmetry, SST $k - \omega$ model predicts better result and in the range $0.25 < r < 0.43$, the prediction for PANS $k_u - \epsilon_u$ are well with the experimental data for $f_k = 0.5$, $f_k = 0.8$. Beyond $r > 0.43$, all the model gives better predictions upto near the wall. At the near wall $k - \epsilon$ model and PANS $k_u - \epsilon_u$ for $f_k = 0.5$ give better prediction. However, at this axial location, SST $k - \omega$ model overpredicts the experimental data. Just above the

impeller at $z = 0.787$ and $z = 0.907$, the predictions for axial velocities have been shown in the Fig. 9a,b. In both the locations the model predicted values are with good agreement with the experimental data. Near the axis of symmetry, PANS $k_u - \epsilon_u$ model prediction are better for all its f_k as compared to SST $k - \omega$ model. $f_k = 0.2$ gives better predictions amongst all f_k throughout the region. Near the wall, $k - \epsilon$ predictions are also better as compared to others f_k for PANS $k_u - \epsilon_u$ model. Much away from the impeller location at $z = 1.147$ (Fig. 9c), SST $k - \omega$ model predicted

results are in better agreement with the experimental data in the range $0 < r < 0.65$. Beyond $r > 0.65$, it overpredicts the data. Whereas in the range $0 < r < 0.65$, PANS $k_u - \epsilon_u$ model overpredicts the experimental data. Further, for $f_k = 0.2, 0.8, 1.0$, PANS $k_u - \epsilon_u$ model gives better agreement beyond $r > 0.65$. At the location $z = 1.38$ (Fig. 9d), SST $k - \omega$ model gives better agreement in the range $0 < r < 0.6$ with the experimental data. Beyond $r > 0.6$, PANS $k_u - \epsilon_u$ predictions are given better results. However, $k - \epsilon$ model predicts more accurately upto $r < 0.83$. Beyond the location for $f_k = 0.2$, PANS $k_u - \epsilon_u$ model predictions are much closer with the experimental data.

Thus, it can be concluded for the prediction of axial flow in the stirred tank that below the impeller, for the range $r > 0.5$ and much away from the impeller for the region $0 < r < 0.6$ SST $k - \omega$ model yields better prediction with the experimental data. Whereas, just above the impeller PANS $k_u - \epsilon_u$ model predictions are superior to SST $k - \omega$ model. Further, throughout the domain near the vertical wall $k - \epsilon$ model predicts good agreements with the experimental data.

5.3 Turbulent kinetic energy

The predictions for turbulent kinetic energy (TKE) in the solution domain at different axial levels have been plotted in Figs. 10 and 11. At $z = 0.18$ (Fig. 10a), TKE increases sharply upto $r = 0.2$ from near the axis and then decreases beyond the point. Then from $r = 0.65$ onwards predictions for TKE are very small and approximately constant upto near the wall. At this axial level, most of the predictions for

TKE have occurred in the range $0.1 < r < 0.4$. In the case of PANS $k_u - \epsilon_u$ model for $f_k = 0.2$, it gives better prediction with the experimental data amongst all f_k throughout the radial direction. Whereas the prediction for the $k - \epsilon$ model gives poor prediction at this axial location. In the PANS model, when f_k is less, it implies that the unresolved TKE is also less. Therefore the prediction is also less. Thus, the predicted results follow the physical phenomena. Further, in the case of SST $k - \omega$ model, in the range $0.08 < r < 0.34$, it underpredicted and from $r = 0.42$ upto $r = 0.6$, it overpredicts the experimental data. Beyond this, it gives excellent predictions with the experimental data. In case of PANS prediction, for all its f_k from $r = 0.6$ upto near the wall are overpredicted from the experimental data expect $f_k = 0.2$ which gives excellent agreement near the wall. Thus, at this axial level in the range $0.1 < r < 0.4$, PANS $k_u - \epsilon_u$ for $f_k = 0.2$ and in the range $0.65 < r < 0.9$, SST $k - \omega$ model and near wall again for $f_k = 0.2$, PANS $k_u - \epsilon_u$ model gives better predictions, whereas $k - \epsilon$ model give poor prediction at this location. At $z = 0.306$ (Fig. 10b), the prediction of TKE profiles for different turbulence models predictions have followed the same trends as the axial location $z = 0.18$. But at this axial level, the value of the TKE attends its maximum for all the models. These predictions are more as compared to the TKE prediction at the location $z = 0.18$. PANS $k_u - \epsilon_u$ model for $f_k = 0.2$, gives better prediction in the range $0 < r < 0.45$ and then in the range $0.45 < r < 0.9$, SST $k - \omega$ model and near wall $f_k = 0.2$ and $f_k = 0.8$ give better prediction. However, at this location $k - \epsilon$ model overpredict from the experimental data. Just above the impeller at $z = 0.787$ (Fig. 11a),

Fig. 10 Turbulent kinetic energy profiles below the impeller at different z -location for $f_k = 0.2$ (—), $f_k = 0.5$ (---), $f_k = 0.8$ (—), $f_k = 1.0$ (—) of PANS $k_u - \epsilon_u$ model, SST $k - \omega$ model (—) and experimental data (■)

(a) $z=0.18$

(b) $z=0.306$

Fig. 11 Turbulent kinetic energy profiles above the impeller at different z-location for $f_k = 0.2$ (---), $f_k = 0.5$ (---), $f_k = 0.8$ (---), $f_k = 1.0$ (---) of PANS $k_u - \epsilon_u$ model, SST $k - \omega$ model (---) and experimental data (■)

from the axis of symmetry upto $r = 0.4$, the PANS $k_u - \epsilon_u$ model prediction for $f_k = 0.2$ and SST $k - \omega$ give better agreement with the experimental data. Beyond this point $k - \epsilon$ model and PANS $k_u - \epsilon_u$ model for $f_k = 0.8$ give good agreement in the region $0.6 < r < 0.8$. In this range PANS prediction for $f_k = 0.2$ and SST $k - \omega$ models underpredict the TKE predictions from the experimental data. Beyond $r > 0.8$, SST $k - \omega$ and PANS $k_u - \epsilon_u$ for $f_k = 0.2$ give good prediction whereas $k - \epsilon$ and PANS $k_u - \epsilon_u$ for $f_k = 0.8$ are strictly decreased. At the location $z = 0.907$ (Fig. 11 b) in

the range $0 < r < 0.44$, PANS $k_u - \epsilon_u$ model gives good prediction with the experimental data whereas the SST $k - \omega$ model gives good prediction initially upto $r = 0.1$ and after that it underpredicts from the experimental data throughout the region. Whereas, in the same region, PANS $k_u - \epsilon_u$ model for $f_k = 0.5$ overpredicts and for $f_k = 1$ (i.e. for $k - \epsilon$ model) underpredicts from the experimental data. Further, for $f_k = 0.8$, PANS $k_u - \epsilon_u$ gives a good prediction upto $r = 0.25$. After that it underpredicts from the experimental data. Beyond $r > 0.44$, $k - \epsilon$ model and $f_k = 0.8$,

PANS $k_u - \epsilon_u$ gives good predictions with the experimental data. Rest all the models overpredict the experimental data at this axial level. Away from the impeller location at the axial location $z = 1.147$ the prediction for TKE profiles for different turbulence models are predicted in the Fig. 11c. At the axial level all the model predicted TKE are overpredicted from the experimental data except in the region $0 < r < 0.18$ where SST $k - \omega$ model gives better prediction. Again, in the region $0.6 < r < 0.8$, $k - \epsilon$ model gives better agreement amongst all other models. At the location $z = 1.38$ (Fig. 11d), the prediction for SST $k - \omega$ is good in the range $0 < r < 0.18$ with the experimental data. Beyond the point $r > 0.18$ upto the near wall, all the models overpredict the experimental data. Thus, much away and above the impeller the predictions for TKE of turbulence models are not satisfactory for the simulation of stirred tank.

5.4 Turbulent kinetic energy dissipation rate

Figures 12 and 13 present the PANS $k_u - \epsilon_u$ model predicted turbulent kinetic energy dissipation rate for different f_k . As the experimental data are not available for energy dissipation rate, therefore, only model predicted results are plotted for the rate of dissipation. When the prediction of TKE is higher, the predicted energy dissipation rate is also more. Therefore, from the Fig 12a at $z = 0.18$, it has been observed that the prediction of energy dissipation rate is more for the $k - \epsilon$ model and less for $f_k = 0.2$ and $f_k = 0.5$. Just below the impeller at $z = 0.306$ (Fig 12b), the predictions for energy dissipation rate follow the similar patterns as the axial location at $z = 0.18$. However, after

$r > 0.4$, PANS $k_u - \epsilon_u$ model predicts the highest dissipation rate for $f_k = 0.8$. Moreover, at this level predictions of TKE for all f_k are higher as compared to the predictions of the axial level $z = 0.18$. This happens because this location is near to the impeller and also the impeller is of axial flow type. Close and just above the impeller location at the axial level $z = 0.787$ and $z = 0.907$, the predictions for turbulent energy dissipation rate are smaller throughout the radial location. Except the region $0.32 < r < 0.42$, in Fig. 13a and the region $0.41 < r < 0.45$, in Fig. 13b, PANS $k_u - \epsilon_u$ predictions are more for $f_k = 0.8$. However, throughout the radial location for $f_k = 0.2$, PANS model prediction is lesser amongst all f_k . Away from the impeller at $z = 1.147$ (Fig. 13c), near the axis of symmetry, the predicted values are very small for all the models and then gradually they increase. But towards the wall, predictions are much lesser for the $k - \epsilon$ model. At the axial level $z = 1.38$, the predicted turbulent energy dissipation rate follows the similar patterns as in Fig. 13d. At this level predictions are lesser as compared to the level $z = 1.147$ and towards the wall, $f_k = 0.8$ gives the lesser prediction.

To see the visualisation of the flow field inside the flow domain, Fig. 14 has been plotted for different f_k of PANS $k_u - \epsilon_u$ model. From the Fig. 14a–d it is noted that after interaction with the impeller, the flow field has been directed towards downwards. After the contact with the bottom wall, the direction of flow moves towards the vertical wall. Then with the interaction with the vertical wall, it directed upwards. Due to less energy, near the surface, it changes its direction to downwards. In this way the velocity fields rotate inside the stirred tank using axial flow impeller. As the simulation is studied for axial flow

Fig. 12 Profiles for turbulent energy dissipation rate below the impeller at different z -location for $f_k = 0.2$ (---), $f_k = 0.5$ (---), $f_k = 0.8$ (---), $f_k = 1.0$ (---) of PANS $k_u - \epsilon_u$ model

Fig. 13 Profiles for turbulent energy dissipation rate above the impeller at different z -location for $f_k = 0.2$ (---), $f_k = 0.5$ (---), $f_k = 0.8$ (---), $f_k = 1.0$ (---) of PANS $k_u - \epsilon_u$ model

impeller, there is no such impact of radial velocity in the impeller region.

6 Conclusions

In this study, the numerical simulation of a stirred vessel for axial flow impeller using PANS $k_u - \epsilon_u$ model has been studied to see the behaviour of flow variables throughout the domain. Also, RANS SST $k - \omega$ model have been

included for comparative study. It is noted that the power-law scheme gives better agreements with the experimental data as compared to the upwind scheme. PANS $k_u - \epsilon_u$ predicted results for non-dimensional radial and axial velocities are good for all its f_k below the impeller region. Above the impeller at $f_k = 0.2$, the PANS $k_u - \epsilon_u$ model predicts better than other f_k . For turbulent kinetic energy, the PANS $k_u - \epsilon_u$ model gives a good prediction for $f_k = 0.2$ below and above the impeller region. Away from the impeller, it overpredicts the experimental data

Fig. 14 Flow visualisation of the domain after computation for different f_k by using PANS $k_u - \epsilon_u$ model

for all its f_k . PANS $k_u - \epsilon_u$ model predicts more dissipation rate for $f_k = 0.2$ below and away from the impeller and the prediction of dissipation rate is higher for $f_k = 0.5$ and $f_k = 0.2$ just above the impeller. The prediction of all the

flow characteristics for SST $k - \omega$ model are better near the bottom wall. However, just below the impeller the predictions are not as good as PANS $k_u - \epsilon_u$ model prediction for some of its filter width f_k .

Acknowledgements Srimanta Maji was funded partially by a research fellowship from Technical Education Quality Improvement Programme (TEQIP), Government of India. Also, authors are grateful to the anonymous reviewers and editor for suggestions that improved significantly the manuscript from its earlier version.

Funding Partial financial support was received from Technical Education Quality Improvement Programme (TEQIP), Government of India.

Declarations

Conflict of interest The author declare that they have no Conflict of interest

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

References

1. Joshi JB, Nere NK, Rane CV, Murthy B, Mathpati CS, Patwardhan AW, Ranade VV (2011) CFD simulation of stirred tanks: comparison of turbulence models (Part II: axial flow impellers, multiple impellers and multiphase dispersions). *Can J Chem Eng* 89:754–816
2. Lane GL (2017) Improving the accuracy of cfd predictions of turbulence in a tank stirred by a hydrofoil impeller. *Chem Eng Sci* 169:188–211
3. Girimaji SS (2006) Partially-averaged navier-stokes model for turbulence: a reynolds-averaged navier-stokes to direct numerical simulation bridging method. *J Appl Mech* 73:413–421
4. Srinivasan R, Girimaji SS (2014) Partially-Averaged Navier-Stokes Simulations of High-Speed Mixing Environment. *J Fluids Eng*, 136
5. Pericleous KA, Patel MK (1987) The modelling of tangential and axial agitators in chemical reactors. *Phys Chem Hydrodyn* 8:105–123
6. Ranade VV, Joshi JB, Marathe AG (1989) Flow generated by pitched bladed turbine part ii: mathematical modelling and comparison with experimental data. *Chem Eng Commun* 81:225–248
7. Ranade VV, Mishra VP, Saraph VS, Deshpande GB, Joshi JB (1992) Comparison of axial flow impellers using a laser doppler anemometer. *Ind Eng Chem Res* 31:2370–2379
8. Armenante PM, Chou C (1996) Velocity profiles in a baffled vessel with single or double pitched blade turbines. *AIChE J* 42:42–54
9. Sahu AK, Joshi JB (1995) Simulation of flow in stirred vessels with axial flow impellers: effects of various numerical schemes and turbulence model parameters. *Ind Eng Chem Res* 34:626–639
10. Bakker A, Myers KJ, Ward RW, Lee CK (1996) The laminar and turbulent flow pattern of a pitched blade turbine. *Chem Eng Res Des* 74:485–491
11. Bakker A, Laroche RD, Wang MH, Calabris RV (1997) Sliding mesh simulation of laminar flow in stirred reactors. *Chem Eng Res Des* 75:42–44
12. Armenante PM, Chou C, Fort I, Medek J (1997) Velocity profiles in a closed, unbaffled vessel: comparison between experimental LDV Data and numerical CFD predictions. *Chem Eng Sci* 52:3483–3492
13. Ljungqvist M, Rasmuson A (1997) Hydrodynamics of open and closed stirred vessels. *Proc 9th Euro Conf Mix* 11:97–104
14. Naude I, Xuereb C, Trifu M, Bertrand J (1997) Numerical simulation of industrial propellers in a multi-stage agitated vessel. *Proc 9th Euro Conf Mix* 11:211–218
15. Brucato A, Ciofalo M, Grisa F, Micale G (1996) Numerical prediction of flow fields in baffled stirred vessels: a comparison of alternative modelling approaches. *Chem Eng Sci* 53:3653–3684
16. Sahu AK, Kumar P, Patwardhan AW, Joshi JB (1999) CFD modelling and mixing in stirred tanks. *Chem Eng Sci* 54:2285–2293
17. Nere N, Patwardhan A, Joshi JB (2001) Prediction of flow pattern in stirred tanks: new constitutive equation for eddy viscosity. *Ind Eng Chem Res* 40:1755–1772
18. Jaworski Z, Dyster K, Nienow A (2001) The effect of size, location and pumping direction of pitched blade turbine impellers on flow patterns: LDA measurements and CFD predictions. *Chem Eng Res Des* 79:887–894
19. Aubin J, Fletcher DF, Xuereb C (2004) Modeling turbulent flow in stirred tanks with CFD: The influence of the modeling approach, turbulence model and numerical scheme. *Exp Therm Fluid Sci* 28:431–445
20. Murthy BN, Joshi JB (2008) Assessment of standard $k - \epsilon$, RSM and LES turbulence models in a baffled stirred vessel agitated by various impeller designs. *Chem Eng Sci* 63:5468–5495
21. Chunlin W, Yayun L, Yating S, Jian D, Changjun L (2010) Numerical simulation and piv test of internal flow field in paddle stirred tank. *J Drain Irrig Mach Eng*, 4
22. Ge CY, Wang JJ, Gu XP, Feng LF (2014) Cfd simulation and piv measurement of the flow field generated by modified pitched blade turbine impellers. *Chem Eng Res Des* 92:1027–1036
23. Mule GM, Lohia R, Kulkarni AA (2016) Effect of number of branches on the performance of fractal impeller in a stirred tank: mixing and hydrodynamics. *Chem Eng Res Des* 108:164–175
24. Patankar S (1980) Numerical heat transfer and fluid flow. CRC Press, USA
25. Kumar P (1997) Design of Bioreactor. PhD thesis, University of Mumbai

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.