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Volume 6 | Issue 5 Article 6

2022

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Vol. 6, No. 5, 2022 Journal of Engineering Research (ERJ)

Computational Treatment of Mixing Process in Stirred Tank

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***Abstract*- Stirred tanks are widely used in many industrial processes. The quality of mixing process generated by the impellers can be determined using either experimental and simulation methods by using computational fluid dynamics (CFD) or both methods. In this study computational fluid dynamics were performed to examine the flow characteristics of six flat blades Rushton turbine type in cases of one impeller only and two impellers in baffled tank, making an optimization design for mixing tank. The Multiple Reference Frame (MRF) approach was used to simulate the impeller rotation. ANSYS Fluent 15.07 solver and the RNG turbulence model were used.**

***Index terms:* Rushton turbine; Mixing; RNG Turbulence model; Optimization design; Flow visualization**

1- Introduction and Literature Review

The mixing processes include the chemical, petrochemical, oil and metallurgical industries. The details of the flow and the extent of mixing in a stirred tank are of interest in most industrial applications. CFD is being used as an engineering tool to aid in the understanding and design of process operations, while the motion of fluids in mixing is obvious applications of CFD.Middleton et al [1] the first researcher to present a fully three-dimensional numerical simulation of the flow in mixing tanks developed with Imperial College and based on the $k-\varepsilon$ turbulence model. The method in which empirical boundary conditions were imposed at the impeller boundary was not described in detail. Gosman et al [2] simulated two-phase (solid-liquid or gas-liquid) flow in tanks stirred by Rushton turbines using the k $-\varepsilon$ turbulence model and the two phases Implicit pressure-velocity coupling algorithm. The circumferential velocity and levels of k and ε were imposed throughout the volume swept by the impeller blades with reference to experimental data, while all other variables were solved for within that volume as in any other part of the flow.

Luo et al [3] observed that, the interface conditions between inner and outer domain are generally unsteady, there was a particular radial location at which, for all practical purposes, steady flow conditions can be assumed. This fact was exploited by the authors to compute the flow in the whole tank without paying the price of fully time dependent calculations; the steady-state governing equations were solved in each reference frame, with interface coupling performed by velocity transformation. This allowed a great reduction in computing time as compared to the previous transient simulations; results for the same reference geometry compared well with the experimental data of Yianneskis et al[4].Ranade [5] simulated turbulent flow generated by a Rushton turbine (six blades with disc) and a down flow pitched blade turbine (four blades, 45 inclined) using a computational snapshot approach. The approach was implemented using a commercial CFD code, FLUENT (Fluent Inc.,).Mean flow and turbulence characteristics were computed by solving the Reynolds averaged Navier-Stokes equations combined with the standard k-e turbulence model. The predicted results were compared with the comprehensive data set available in the literature. Simulated results show a pair of trailing vortex.

Aubin et al [6] simulated with CFD Single phase turbulent flow in a tank stirred by a down- and an up-pumping pitched blade turbine and investigated The effect of the modeling approach, discretization scheme and turbulence model on mean velocities, turbulent kinetic energy and global quantities, such as the power and circulation numbers. The results have been validated by LDV data. Alcamoa et al[7] computed the turbulent flow field generated in an un baffled stirred tank by a Rushton turbine using large-eddy simulation (LES). The computation was run with the help of a general purpose CFD ANSYS-CFX4.4 which was appropriately modified in order to allow the computation of the sub-grid viscosity and to perform statistics on the computed results. The numerical predictions were compared with the literature results for comparable configurations and with experimental data obtained using particle image velocimetry. Ghazi[8] numerically investigated the division of the tank into two or more compartments based on values of the dissipation rate of the kinetic energy of turbulence Ɛ, The results obtained include full field values of pressure, velocity, kinetic energy of turbulence, *k*, and its dissipation rate, Ɛ. The numerical results are validated against the results. Adams [9] studied the mixing inside of the cavern of a single phase non-Newtonian fluid by applying an adapted (Planar Laser Induced Fluorescence) PLIF technique and through the application of CFD. An adapted planar laser induced fluorescence technique showed that mixing inside of a shear thinning Herschel-Bulkley fluid is very slow a toroidal cavern model provided the best fit for single phase fluids but for the opaque fluids all models drastically over predicted the cavern size, with the cylindrical model only predicting cavern heights at high Reynolds numbers.

In the present work the simulation model to study the mixing in mechanically stirred tanks to predict the influence of different operating parameters such as the number of blades, diameter of impeller, length of impeller, the space between blades on the mixing process in baffled stirred tank, Making an optimization design for mixing tank. (GDO) is performed to allow generating a new sample set with 10000 sample points and sort its sample in order to satisfy the good mixing. There are three candidates chosen by the optimizer which are then verified using the CFD solver. It's clear that candidate C with (3-stars) would expect to satisfy the required design.

2- NUMERICAL MODEL OF THE PRESENT WORK

A. The Multiple Reference Frames (MRF) Model

A modification of the rotating frame model is the multiple reference frames (MRF) model Luo et al[3].The modification is that more than one rotating (or nonrotating) reference frame can be used simulation. This steady-state approach allows the modeling of baffled stirred tanks and tanks with other complex (rotating or stationary) internals. A rotating frame is used for the region containing the rotating components while a stationary frame is used for regions that are stationary (Fig.1).

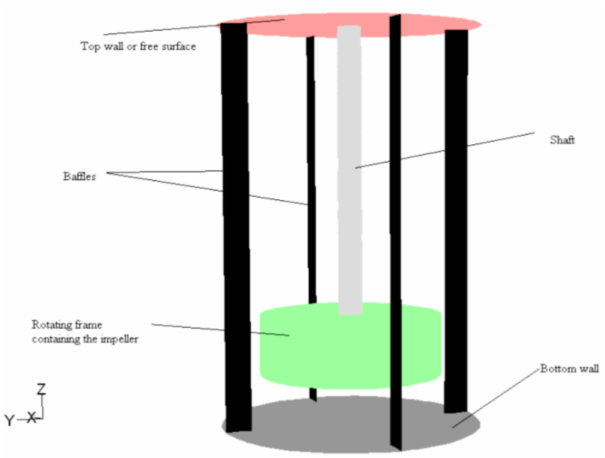

Fig. 1. Outline of rotating reference frame region in a mixing tank

In the rotating frame containing an impeller. In the stationary frame containing the tank walls and baffles, the walls and baffles are at rest. The fact that multiple reference frames can be used means that multiple impeller shafts in a rectangular tank can each be modeled with separate rotating frames (with separate rotation frequencies) while the remaining space can be modeled with a stationary frame. The grid used for an MRF solution must have a perfect surface of revolution surrounding each rotating frame. The momentum equations inside the rotating frame are solved in the frame of the enclosed impeller while those outside the rotating frame are solved in the stationary frame. A steady transfer of information is made at the MRF interface as the solution progresses. While the solution of the flow field in the rotating frame in the region surrounding the impeller imparts the impeller rotation to the region outside this frame, the impeller itself does not move during this type of calculation. Its position is static. If the impeller is mounted on a central shaft in a baffled tank, this means that the orientation of the impeller blades relative to the baffles does not change during the solution.

B. Boundary Conditions

On the walls, no-slip conditions have been imposed, the flow in the stirred tanks is fully turbulent, at fully turbulent flow, the inertial forces due to the fluctuating velocity overwhelm the viscous forces, so the flow field becomes independent of the fluid viscosity (the viscous heating is negligible), the surface of the liquid is always considered as flat plane, that is to say that the vortex phenomenon is considered absent and the liquid surface is free.

C. Equations

Momentum equation:

$$\frac{\partial(\rho U_i)}{\partial t}+\frac{\partial}{\partial x_j}(\rho U_i U_j)=-\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}-\frac{2}{3}\frac{\partial U_k}{\partial x_k}\delta_{ij}\right)\right]+\rho g_i+F_i \quad (1)$$

In equation (1). the convection terms are on the left. The terms on the right-hand side are the pressure gradient, a source term; the divergence of the stress tensor, which is responsible for the diffusion of momentum; the gravitational force, another source term; and other generalized forces (source terms), respectively.

D. The Standard k-ε Model

The k-ε model is one of a family of two-equation models for which two additional transport equations must be solved to compute the Reynolds stresses. It is a robust model, meaning that it is computationally stable. It is applicable to a wide variety of turbulent flows and has served the fluid modeling. It is semi empirical, based in large part on observations of high Reynolds-number flows. The two transport equations that need to be solved for this model are for the kinetic energy of turbulence, k, and the rate of dissipation of turbulence, ε:

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial}{\partial x_i}(\rho U_i k)=\frac{\partial}{\partial x_i}\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_i}+G_k-\rho\varepsilon \quad (2)$$

$$\frac{\partial(\rho\varepsilon)}{\partial t}+\frac{\partial}{\partial x_i}(\rho U_i\varepsilon)=\frac{\partial}{\partial x_i}\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial k}{\partial x_i}+C_1\frac{\varepsilon}{k}G_k+C_2\rho\frac{\varepsilon^2}{k} \quad (3)$$

The quantities C1, C2, σk, and σε are empirical constants. The quantity Gk appearing in both equations is a generation term for turbulence. It contains products of velocity gradients and also depends on the turbulent viscosity:

$$G_k=\mu_t\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}\right)\frac{\partial U_j}{\partial x_i} \qquad (4)$$

$$\mu_t=\rho C_\mu\frac{k^2}{\varepsilon} \qquad (5)$$

To summarize the solution process for the k–ε model, transport equations are solved for the turbulent kinetic energy and dissipation rate. The solutions for k and ε are used to compute the turbulent viscosity, μt. Using the results for μt and k, the Reynolds stresses can be computed from the Boussinesq hypothesis for substitution into the momentum equations. Once the momentum equations have been solved, the new velocity components are used to update the turbulence generation term, Gk, and the process is repeated.

3- DESIGN EXPLORATION AND OPTIMIZATION

The optimization process is performed using the Design Exploration algorithm described in Fig. (2). The optimization is the process to choose the optimal input parameters that achieve the desired performance of the system in an automated manner. This performance is evaluated by means of output parameters. There are several choices to examine the system performance using a certain output parameter such as maximize its value, minimize its value, or seeking target value. The complete analysis of an initial design has to be held including drawing, meshing, solving the governing equations, defining the input and output parameters.

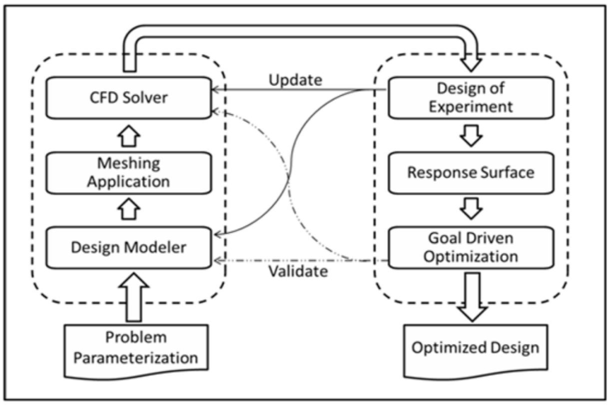

Fig. 2: Design of Exploration flowchart

A. *Mesh Generation*

The domain is meshed using an unstructured grid with an average skewness factor of 0.227 and average orthogonality of 0.857. The inflation layers are near the stirred-tank reactor wall and on the impeller surface with mesh size growth rate of 1.2. We have tried coarse, medium, fine and refinement grids. Table 1 shows grid size in each case for one impeller. Fig. 3 shows grid Figures in each case for one impeller.

A-1 Mesh independency

Figure 4 shows the mean radial velocity profiles at radial positions of 20 cm from the centre line of tank using all meshes. It can be seen that the solution is independent of the grid size so in this section, Fine grid (412226 cells) was used as the base grid for all cases in order to reduce the computational time.

B. *Problem Parameterization*

The goal is to optimize the cross section of the impeller geometry in order to make the circulation and homogenization. The objective function is circulation flow rate is defined as:

$$Q_z = Q_c = \int_{r^*}^{R} 2\pi r \,|(v_z)_{z=z^*}|dr$$

C. *Design of Experiment (DOE)*

In this step a test sample of the input parameters is generated to cover the whole range of these parameters with minimum number of design points, keeping this sample efficiently represents the effects of the input parameters on the output parameters. The ranges of input design parameters are given in table 2. DOE technique tries to locate the sampling points in the design space such that the space for random input parameters is explored in most efficient way, or to obtain the required information with a minimum of sampling points. After generation of the test sample in the DOE table using one of DOE methods, the update process is performed in which the optimizer repeats all the steps have been done in the initial design (Drawing /meshing /solving /generating output parameters) for all the design points in the DOE table. Fig.(6) show the parameters parallel chart for 28 sample points with input parameters.

Table 1. Grid size of one impeller mixing tank

no	Grid type	Cells
1	Coarse	287313
2	Medium	302165
3	Fine	412226
4	refinement	1743093

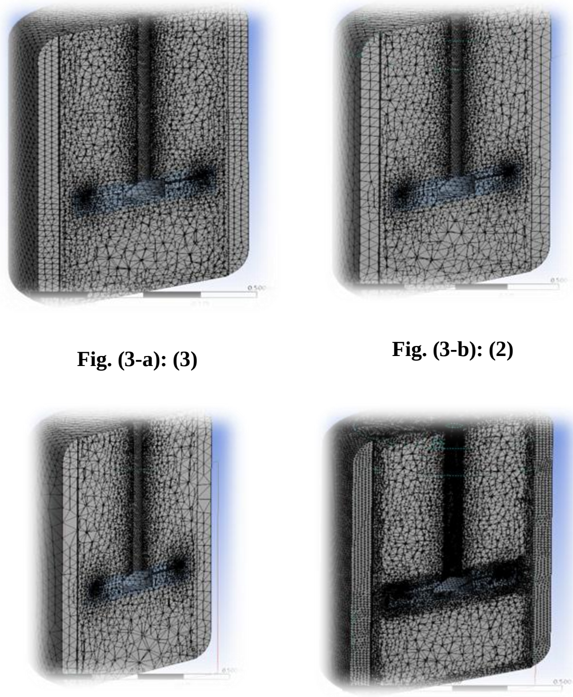

Fig. (3-a): (3) **Fig. (3-b): (2)**

Fig.(3-c): (1) **Fig.(3-d): (4)**

Fig. 3: Fine grid, Medium grid, Coarse grid and refinement grid of one impeller mixing tank

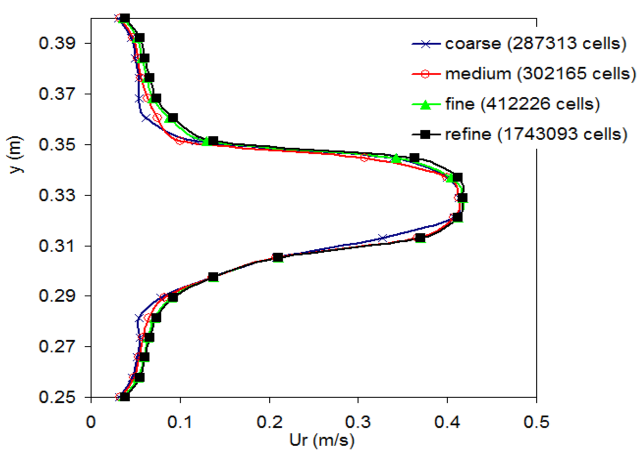

Fig. 4: velocity distribution with grid in each case

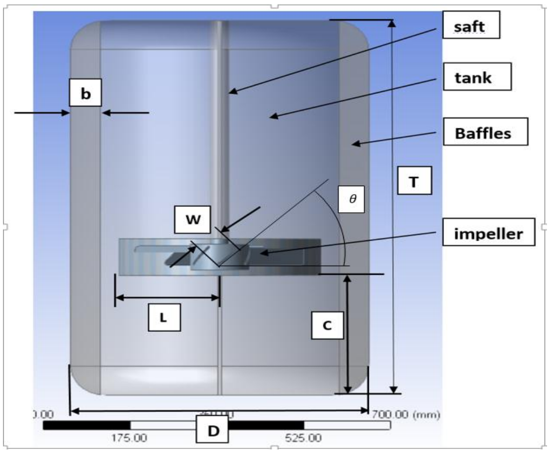

Fig. (5-a): Parametric geometry of mixing tank

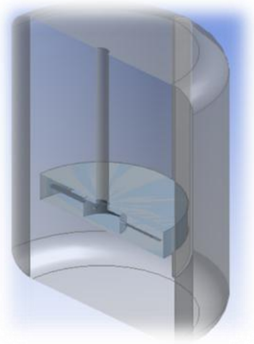

Fig. (5-b): One impeller geometry

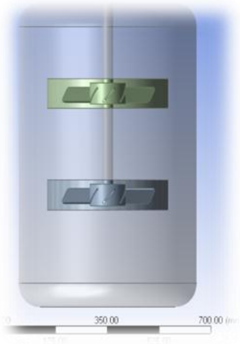

Fig.(5-c): Two impeller geometry

Table 2: The ranges of input design parameter

Input design parameter	Lower value	Higher value
Height(T)	810	990
Blade length (L-blade)	153	187
Blade width (W-blade)	54	66
blade thickness (t-blade)	4.5	5.5
blade angle(θ) (°)	30	50

4- RESULTS AND DISCUSSION

CFD simulation is performed using ANSYS FLUENT 15 to handle the axi-symmetric steady incompressible turbulent flow. RNG turbulence model with enhanced wall treatments implemented. Figures (8-a) and (9-a) show the velocity magnitude contours through the mixing tank for one and two impellers. It can be observed that the maximum velocity at blades tips and flow is homogenous Fig (8-b and 9-b) show the velocity magnitude contours on horizontal plan through blades. Fig (9-c) shows the wake area characterized by the maximum of the turbulent kinetic energy which is localized around the mechanics source and at baffles. Fig (9-d) 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.

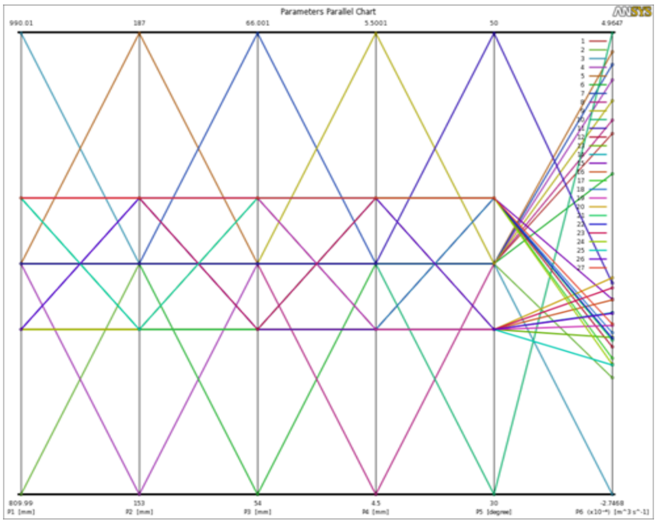

Fig. 6. The parameters parallel chart,(for one impeller)

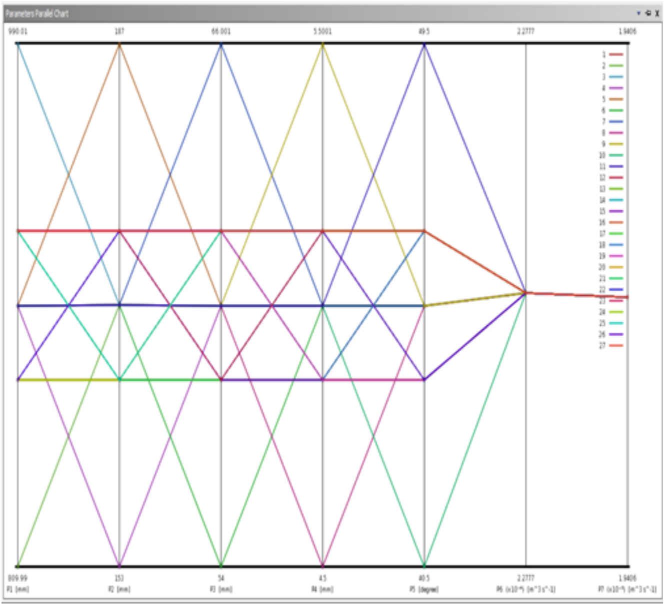

Fig. 7. The parameters parallel chart, (for two impeller)

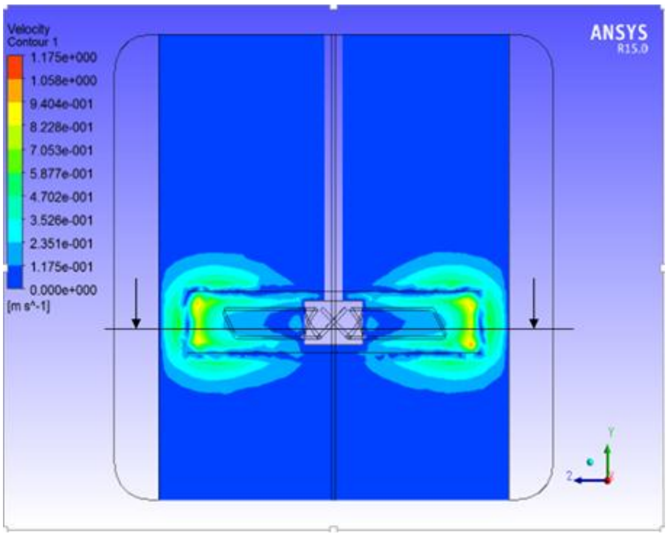

Fig. (8-a). Velocity distribution on vertical plan

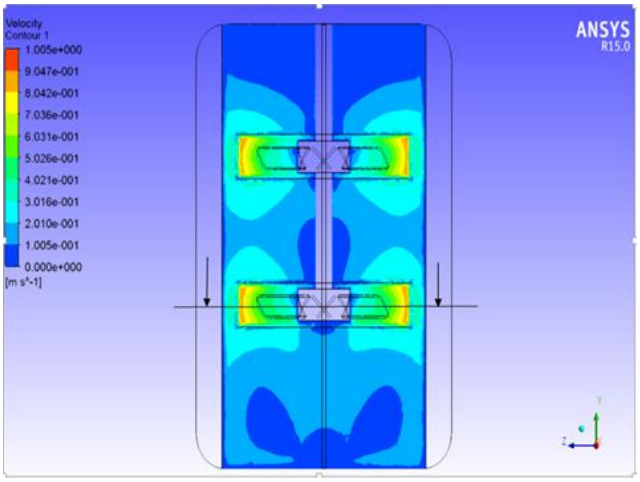

Fig. (8-b). Velocity distribution on horizontal plan

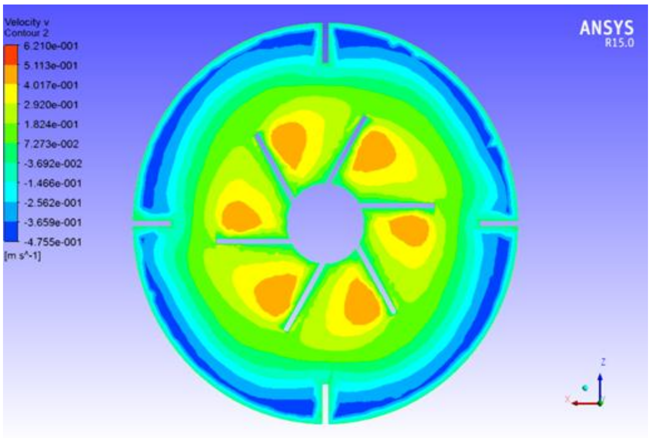

Fig. (9-a). Velocity distribution on vertical plan

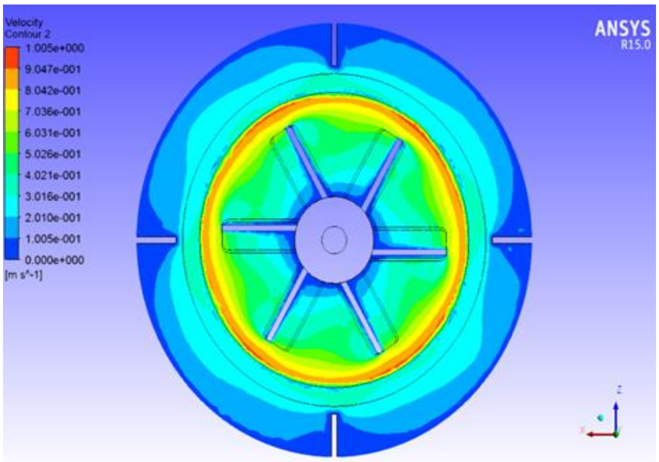

Fig. (9-b). Velocity distribution on horizontal plan

Figures (10 and 11) show the velocity vectors through the mixing tank for one and two impeller. It can be observed that the two circulation loops (lower and upper from impeller) and the flow is homogenous for predicted results. The results generated in DOE table is utilized to build a multidimensional correlation. This correlation will be used to predict the response or the behaviour of the system to any change of the input parameters.

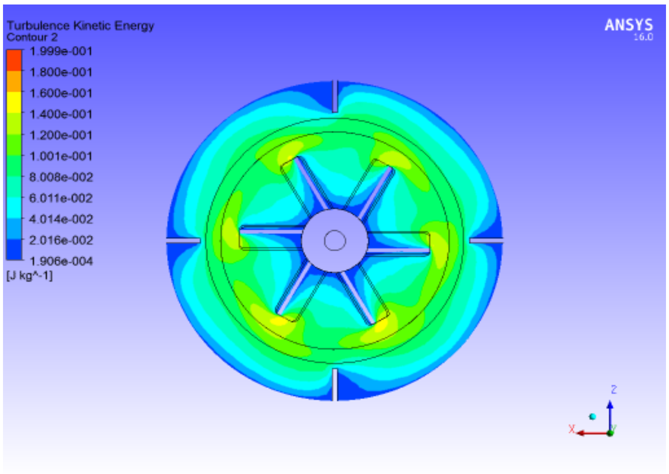

Fig. (9-c). Turbulent kinetic energy distribution on horizontal plan

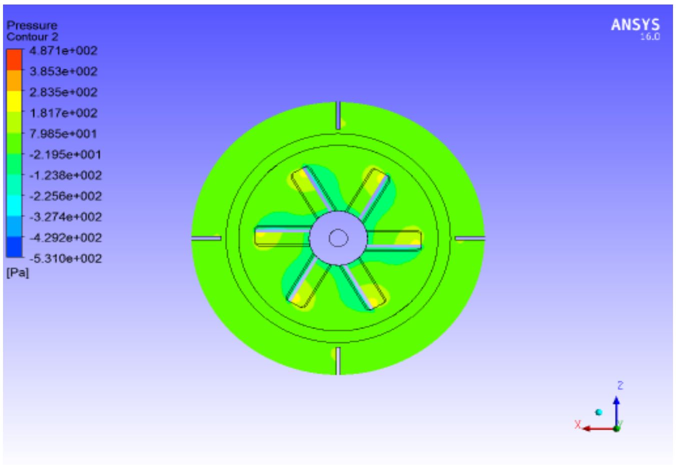

Fig. (9-d). Pressure distribution on horizontal plan

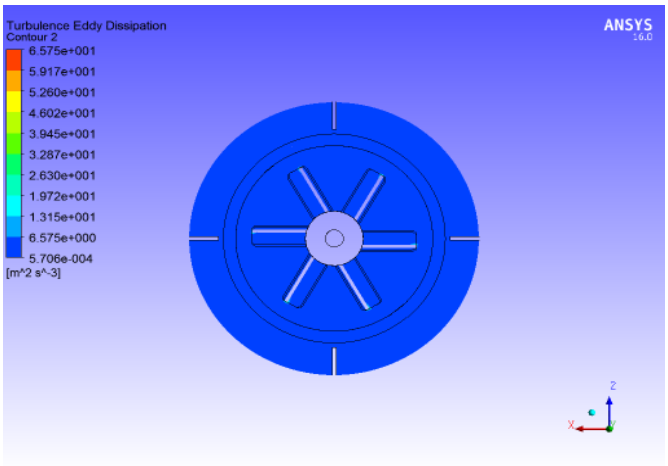

Fig. (9-e). Turbulence eddy dissipation on horizontal plan

The predicted response surface is used to get the value of the output variables to any combination of the input parameters without the need to perform a complete simulation. Figs. (12-a and 12-b) shows the 3-D response surface of output parameter variation as a result of variation of two input design parameters for one impeller. Figs. (12-c and 12-d) shows the 3-D response surface of output parameter variation as a result of variation of two input design parameters for two impellers.

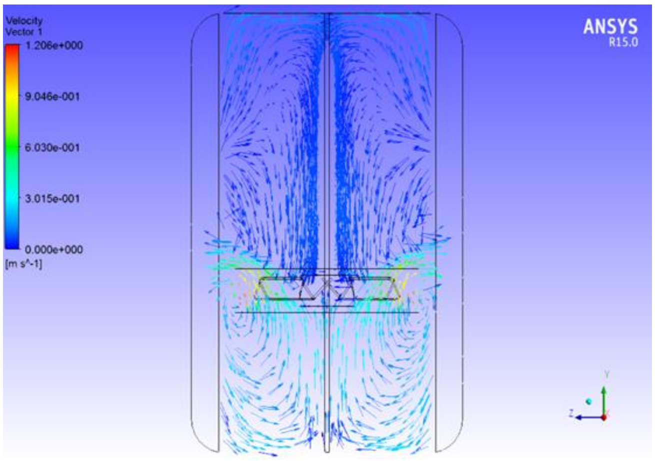

Fig. 10. Velocity distribution by vectors (One impeller)

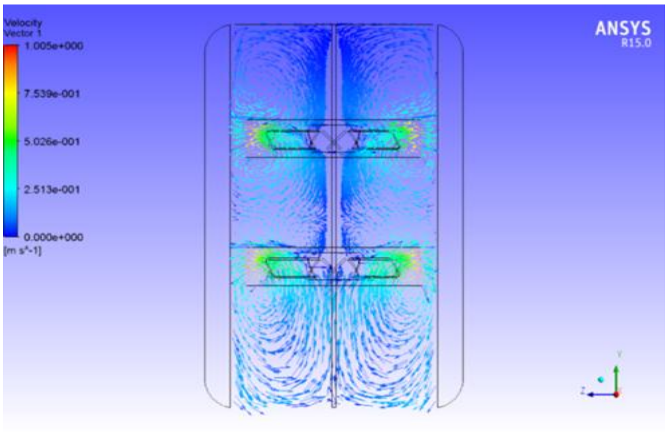

Fig. 11. Velocity distribution by vectors (Two impeller)

The predicted response surface is utilized to choose the optimal input parameters that achieve the desired performance or characteristics of the tested system using a comparative study by checking the output parameters to be maximized, minimized, seeking target value. The initial design is setup. The Design of Experiments (DOE) technique is used for sampling. The Enhanced-Rotatable Central Composite Design (CCD) is chosen for DOE that is a five-level sampling design as the other three level sampling methods is insufficient to describe the problem. DOE sample points have sent to the CFD solver to update the value of the output parameter. These values are used to generate the response surface by fitting it using multidimensional regression techniques.

In the current study, the Non-Parametric Regression (NPR) has been chosen as meta-modelling (surrogate) technique to create the response surface to meet the highly nonlinear behaviour of the relation between the output parameter and input parameters. Once the response surface has been created the so-called Goal Driven Optimization (GDO) is performed based on screening method. The screening method allows generating a new sample set with 10000 sample points and sort its sample based on the objective that is set to seek the impeller and tank geometries to satisfy the good mixing.

The design candidates chosen by the optimizer are then verified using the CFD solver. Table (3-a) shows that there are three candidates. It's clear that candidate C with (3-stars) would expect to satisfy the required design while candidate B is far from the expected answer. However, Candidate A achieves the required design answer, but it has significant error corresponding to candidate C. Note that Fig. (9) shows candidates with blue colour. Table (3-b): The goals with weights of parameters and the best three candidates with their verifications, (one impeller). Candidates with their verifications, (two impeller). Table (3-c) shows that there shows that there are three candidates if we take in consideration minimize the power consumption as output parameter. It's clear that candidate Point 3 is the lowest power consumption, Fig.(13) show the samples chart of all input parameters and output parameters .all input parameters have a history chart shoes the number of iteration used in CFD solver through the rang e between Lower value and higher value.

5. CONCLUSIONS

Using CFD along with optimization tools can shorten the design optimization cycle time. The use of CFD has increased the flexibility of shape considered and allowed the use of design exploration algorithm to optimize the mixing flow through mixing tank in an automated manner. The different design points were rated based on a goal-driven optimization to choose the best design set and verified by the CFD solver to define the profile. The predicted results based on RNG turbulence model is in good agreement for one and two impellers. Using two impellers gives more division to the flow that double circulation achieving more homogeneity, in the other hand it requires much more power.

Table (3-a). The three candidates chosen by the optimizer

Name	P1-T(mm)	P2:L-Blade(mm)	P3:W-Blade (mm)	P4:t- Blade (mm)	P5:Angle(degree)	P6:Qc (m3/sec)	
						Parameter value	Variation from reference
Candidate point 1	900	154.76	56.43	5.273	49.692	★★0.00033157	0.003%
Candidate point 2	899.91 36.316	180.58	59.81	5.4973		★★0.00033156	0.000%
Candidate point 2(verified)						×2.985E-05	-91.268%
Candidate point 3	900 39.173	159.33	63.817	4.5069		★★0.00033156	0.000%
Candidate point 3(verified)						★★★0.00049326	48.77%

Table (3-b). The goals with weights of parameters and the best three

Table of Schematic B4: Optimization , Candidate Points

	A	B	C	D	E	F	G	H	I	J	K
1	Reference	Name	P1 - T (mm)	P2 - L_Blade (mm)	P3 - W_Blade (mm)	P4 - t_Blade (mm)	P5 - Angle (degree)	P6 - Qc lower (m^3 s^-1)		P7 - Qc upper (m^3 s^-1)	
2								Parameter Value	Variation from Reference	Parameter Value	Variation from Reference
3	◉	Candidate Point 1 (DP 5)	810.09	153.02	54.006	4.5005	40.505	0.00022777	0.000 %	1.9406E-05	0.000 %
4	○	Candidate Point 2	810.63	178.52	55.339	5.1005	44.362	0.00022777	0.000 %	1.9406E-05	0.000 %
5	○	Candidate Point 3	838.71	186.09	57.907	5.3501	47.195	0.00022777	0.000 %	1.9406E-05	0.000 %
*											

Table (3-c). The three candidates chosen by the optimizer when power consumption is a gaol driven optimization

	Candidate Point 1	Candidate Point 2	Candidate Point 3
P1 - T (mm)	810	850.41	830.25
P2 - L_Blade (mm)	153	153.95	154.88
P3 - W_Blade (mm)	66	65.068	59.537
P4 - t_Blade (mm)	4.505	5.4861	5.0125
P5 - Angle (degree)	40.5	41.344	40.9243250728863
P6 - Qc lower (m^3 s^-1)	0.00022776962	0.00022776962	0.00022776962
P7 - Qc upper (m^3 s^-1)	1.9405754E-05	1.9405754E-05	1.9405754E-05
P8 - power consumption (kg m^2 s^-3)	★★★0.056532	★★★0.040665	★★★0.035507

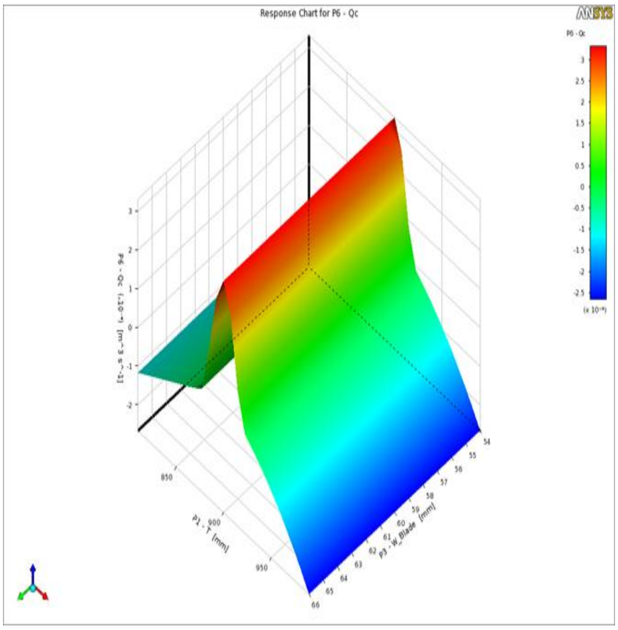

Fig. (12-a). The 3-D response surface for T, W-blade and Q (one impeller).

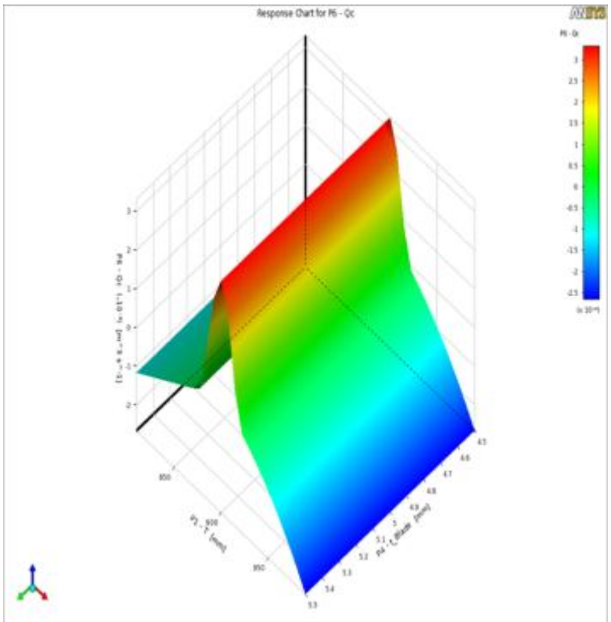

Fig. (12-b). The 3-D response surface for T, t-blade and Q (one impeller).

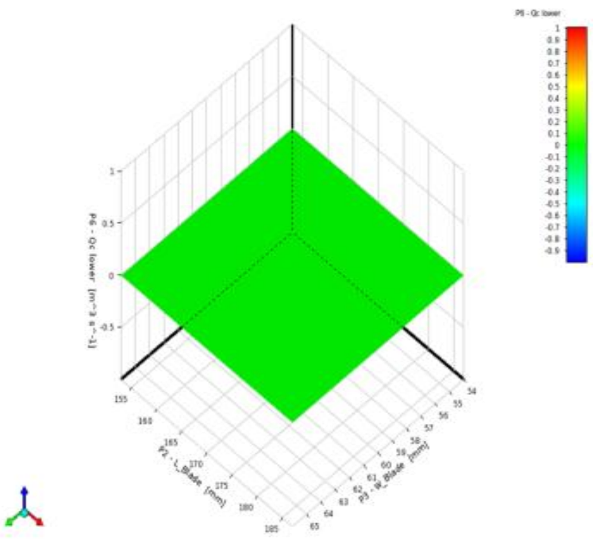

Fig. (12-c): The 3-D response surface for L-blade, W-blade and Q (two impeller).

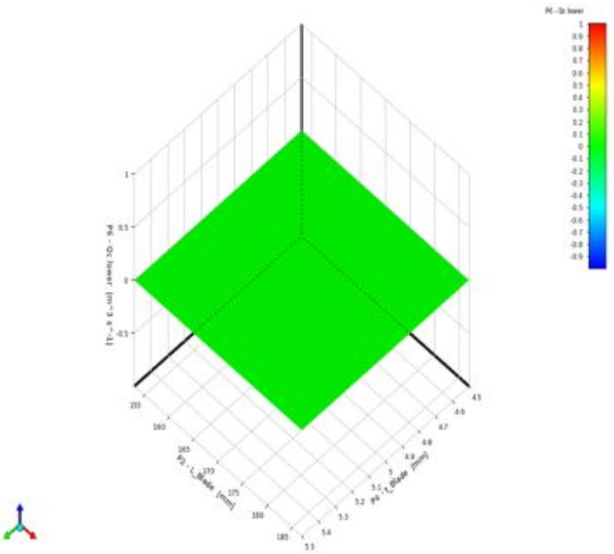

Fig. (12-d): the 3-D response surface for L-blade, t- blade and Q (two impeller)

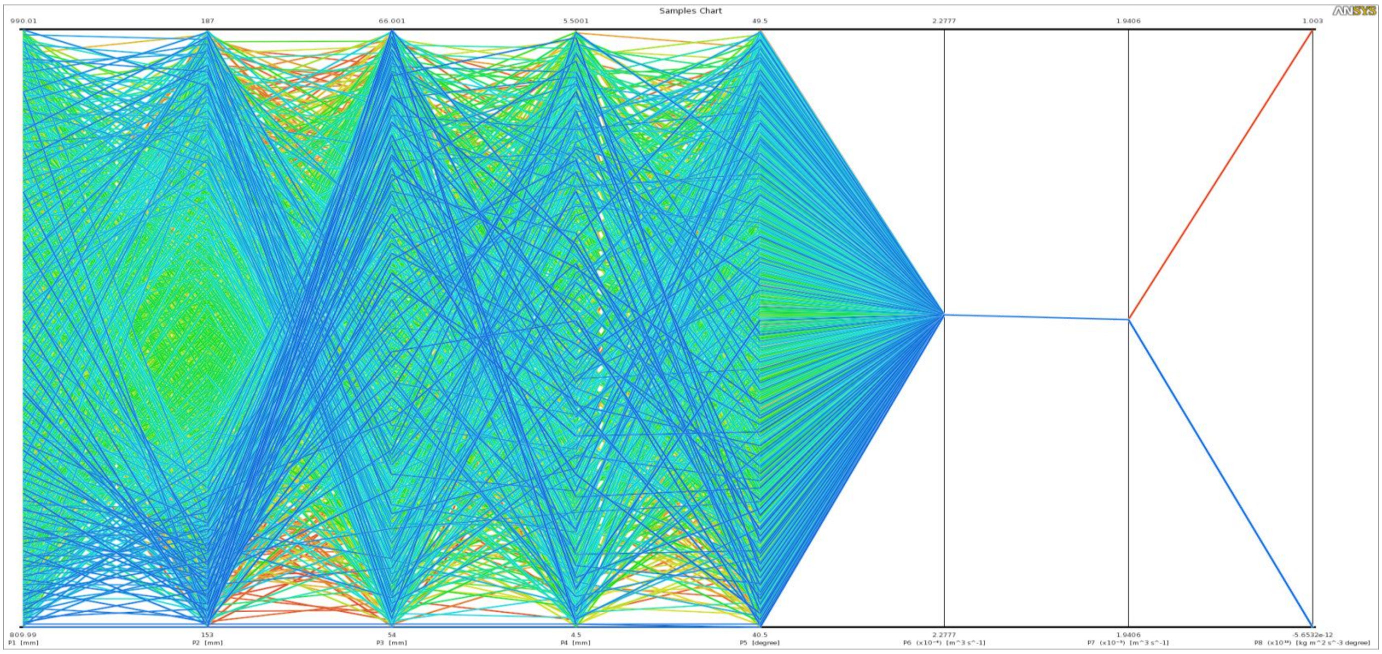

Fig. 13. The samples chart, (for two impeller) when power consumption is a gaol driven optimization

Funding:

This study was not funded by any organization.

Conflicts of Interest:

The authors do not have any conflict of interest.

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