# Impeller Layer Spacing of Stirring Reactor Impact Study of the Internal Flow Characteristics

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## Abstract

Based on the method of computational fluid dynamics (CFD), a combination of double paddle stirred reactor internal flow characteristics is simulated by the standard k- $\epsilon$  model. Respectively, under the same impeller within the different layers spacing, the flow field, turbulent kinetic energy distribution and mixing power are simulated in the kettle. And torque and stirring power are measured by the torque sensor power in the different conditions, the simulation analysis for verification. The results shows that: impeller in the middle of the installation works best; impeller power consumption is minimum, the impeller in high-mounted. CFD simulation and experimental test torque's maximum relative error is 6.4%; Numerical simulation and experimental results are in good agreement, CFD simulation analysis for the practical engineering application.

### **Keywords**

### CFD, Double Combination Paddle, Impeller Layer Spacing, Torque Sensor.

### **1.** Introduction

Stirred tank reactors are widely used in the chemical, pharmaceutical, wastewater treatment and other industrial fields. With the continuous expansion of the industrial scale, the diameter ratio of stirring shaft is also growing. It is difficult to meet gas dispersion and mixed better, the long-time of bubble residence, the high requirements of mass transfer coefficient for single impeller, so the multi-impeller has been widely used [1-4]. There are many kinds of combination forms in the multi-impeller, in which the combination of axial flow and radial flow patterns is widely used [5-6]. The combined-impeller has better gas - liquid dispersion effect and higher mixing efficiency than single-impeller. However, the complexity of the flow field is much greater than that of the singleimpeller [7-8]. Many researchers have done a lot of work on the internal flow field characteristics of the combined propeller. Szymon Wojewodzki had established the conventional model in which without baffles for reactor, so the results of mixing time and power were inaccurate [9]. Pan Chenmei only used three different size impellers but didn't provide the boundary conditions, which would increase the difficulty to analyze the flow field characteristics of double-impeller with different spacing for stirred reactor [10]. Tong Ming has analyzed the flow field characteristics of the stirred reactor, but only changed the position of middle impeller, so that the analysis results didn't have reference value [11].

With the popularization of computer technology and the new development of computational methods, computational fluid dynamics (CFD) has been more and more applied. Through the numerical simulation of the internal flow field for the stirred reactor, the flow characteristics under different operating conditions can be simulated by CFD, so the method of CFD numerical simulation is used to discuss the effect of changing the spacing of double-impellers on the internal flow characteristics. The numerical simulation results are compared with the experimental results, which provide the basis for the agitated reactor from the selection of the design to the structural optimization and the optimization of the input production.

### 2. The Structure of Stirred Reactor

## 2.1 The Model of Experiment





Fig.1 Physical diagram of experimental device

Fig.2 Installation drawing of mixing tank

The test bench of stirred tank reactor is shown in Fig. 1, in which the cylindrical vessel and normal ellipsoidal head were selected. The stirring impeller is a double-impeller combination (new three-leaf and six-inclined). According to the experimental requirement, the process that the stirring impeller has been mounted on the stirring shaft, and the layer spacing between the two impellers has been adjusted. Through the host computer control system, the desired speed has been achieved to simulate the internal flow field simulation in stirred reactor. The stirred reactor is made of transparent organic glass, in which the diameter of the cylinder is380mm, 1000mm in height, liquid level is 845mm, the diameter of the stirring shaft is 30mm, stirrers with outer diameter of 200mm, the distances of the lower stirrer from bottom of reactor is 95mm, the spacing of double-layer combined-impeller for lower, middle, upper is 200mm, 400mm, 600mm, respectively, the speed of stirring impeller is 100r/min.

### 2.2 The Three-Dimensional Model of Stirred Reactor

The three-dimensional model was modeled as 1: 1, in which the moving region stirring impeller and static region (reactor) have been modeled separately, and then assembled together. As the spacing of double-layer stirring impeller is studied, it is necessary to move the regional spacing C by lower, median, higher to make adjustments, as shown in Fig. 3.



Fig.3 The three-dimensional model

# 3. Mathematical Model

### 3.1 VOF Model

According to the volume function F that the fluid in the grid unit, VOF modal has been established to construct and trace the free surface. If F = 1, it means that the unit is occupied by the specified fluid. If F = 0, it means that the unit is a fluid unit without specified phase. If 0 < F < 1, the unit is called interface unit[12].

The continuous equation, volume fraction continuity equation, momentum equation of VOF model are respectively:

$$\frac{\partial \rho}{\partial t} + \nabla \left( \rho V \right) = 0 \tag{1}$$

$$\frac{\partial \alpha_i}{\partial t} + V \bullet \nabla(\alpha_i) = 0 \tag{2}$$

$$\frac{\partial}{\partial t} \left( \rho v \right) + \nabla \left( \rho v v \right) = -\nabla \rho + \nabla \left[ \mu \left( \nabla v + \nabla v^{T} \right) \right] + \rho g + F$$
(3)

Here:  $\alpha_1 + \alpha_2 = 1$ ;  $\rho = \alpha_2 \rho_2 + (1 - \alpha_2) \rho_1$ ;  $\mu = \alpha_2 \rho_2 + (1 - \alpha_2) \mu_1$ 

The momentum equation Source that caused by surface tension and wall adhesion is:

$$\vec{\mathbf{F}} = 2\sigma_{ij}\rho K_i \nabla \alpha_{i'} (\rho_i + \rho_j) \tag{4}$$

Wherein,  $\rho$  is density; v is speed;  $\mu$  is fluid dynamic viscosity; k is surface curvature; 1,2 respectively is air and liquid;  $\alpha$  is the i-th phase I volume fraction.

### 3.2 Turbulence Model

The k- $\varepsilon$  turbulence model with swirl correction (realizable k- $\varepsilon$  model) is used to simulate the flow field in the stirred tank. Compared with the standard k- $\varepsilon$  model, the swirl correction k- $\varepsilon$  model not only increases a formula for the turbulence viscosity, but also increases a new transport equation for the dissipation rate. What's more, for a rotating flow, the strong counter-pressure gradient of the boundary layer flows, flow separation and secondary flow have a good performance.

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_{i}}(\rho k \mu_{j}) = \frac{\partial}{\partial x_{j}}\left[\left(\mu + \frac{\mu_{t}}{\sigma_{k}}\right)\frac{\partial k}{\partial x_{j}}\right] + G_{k} + G_{b} - \rho\varepsilon - Y_{M} + S_{k}$$
(5)

$$\frac{\partial}{\partial t} \left( \rho \varepsilon \right) + \frac{\partial}{\partial x_j} \left( \rho \varepsilon \mu_j \right) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_{\varepsilon}} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \rho C_1 S \varepsilon$$

$$-\rho C_2 \frac{\varepsilon^2}{k + \sqrt{v\varepsilon}} + C_{1\varepsilon} \frac{\varepsilon}{k} C_{3\varepsilon} C_b + S_{\varepsilon}$$
(6)

Here: C1=max[0.43,  $\eta/(\eta+5)$ ],  $\eta=S\cdot k/\epsilon$ ;  $G_k$  and  $G_b$  is the turbulent kinetic energy respectively generated by the laminar velocity gradient and buoyancy; the transitive diffusion in the compressible turbulence creates a ripple  $Y_M$ ;  $C_1$ ,  $C_2$ ,  $C_3$  are constants;  $\sigma_k$ ,  $\sigma_e$  is the turbulence Prandtl number of the k-equation and e-equation;  $S_k$ ,  $S_e$  is the user-defined.

#### 4. Numerical Calculation

#### 4.1 Meshing of modal

The meshing process is simulated in GAMBIT which is pre-processing software of CFD. The impeller has been set as the moving area and the rest of the modal was the static area, where the moving area and the static area boundary layer were coupled through the interface. According to double-layer stirring impeller set up in the stirred reactor, the combination of different sizes of unstructured meshes is used. In other words, the finer tetrahedron mesh is used in the impeller area, and the hexahedral mesh is used in other areas. Because hexahedral meshes have higher quality, faster convergence and lower computational cost than tetrahedral meshes, the advantages of tetrahedral meshes are that they are adaptable and can adapt to complex geometrical shapes. In principle, hexahedral Mesh has been given priority to choose, and the tetrahedral mesh has good using in an irregularly shaped area. In this way, not only ensure the accuracy of calculation but also ensure to shorten the calculation time and reduce the calculation cost in the calculation process. The spacing of double-layer stirring impeller is studied, so the model is divided into three types according to the low, medium and high pitch of the stirring impeller. The total number of grids obtained from the three paddling models are: 526142, 639482, 607065. As shown in Fig. 4 for the grid quality inspection section.



(a)low level (b)medium level (c)high level Fig.4 The sectional view of mesh

### 4.2 Boundary Conditions and Solution

According to the simulation theory, the two mixing regions as the moving region, and the rest as the static region. The interface between the moving and static regions is defined as the sliding surface, the boundary condition is set to interface, which coupled with the static area. The face of and stirring shaft have been set as moving wall, which is defined as a non-slip solid wall in GAMBIT.

Based on the fluid volume (VOF) model, the multiphase model was used to simulate the stirred reactor by means of the software of FLUNT. And meanwhile the agitator rotation is adjusted as 100r/min and Mesh Motion is set for the model. The coupling of velocity and pressure is based on the phase coupled SIMPLE algorithm. The residual monitor convergence accuracy is set to  $10^{-3}$ .

# 5. The Discussion and Analysis for Calculation Results

The simulation results are based on the transient method, the agitator rotating a week to be 0.6 s, recorded as the cycle T = 0.6s. The simulation results show that the flow field characteristics of the reactor are almost stable after 50T. According to the low, medium and high level of the pitch of the stirring impeller, the results of 50T have been compared and analyzed. The simulation results are mainly velocity diagram, flow field and gas-liquid two-phase diagram.

### 5.1 The Change of Velocity Distribution in Different Layer Spacing for Flow Field

Fig. 5 indicates the velocity field distribution in the three different layers for the upper mixing impeller in the low, medium and high levels. By compared the velocity of the flow field at different layer spacing, the upper layer of stirring blades forms an axial flow, and the bottom layer of the stirring blades forms a radial flow. In each case, the speed-effect area is mainly concentrated around the impeller. The speed is far from the agitator area, and the bottom of the stirred tank is lower, which forming a low velocity area. Over time the speed-effect area gradually expands outwards from the stirring paddle. The axial flow generated by the upper impeller and the radial flow generated by the lower impeller form a circular flow in the stirred reactor. It can been seen from Fig. 5, due to the relative spacing of the layer is too small or too large, stirring reactor speed distribution is not uniform, can not be a better form of circulation when installed in the low level and high level for the upper-impeller. In comparison, the medium installation is better.



(a)low level (b)medium level (c)high level Fig.5 The velocity diagram of flow field under different layer-spacing

### 5.2 The Vector Distribution of Flow Field with Different Spacing

As shown in Fig. 6, the liquid has circulation rising motion in area of the double-impeller, which also includes less circulation drop motion, and the motion of the blade area is relatively strong. According to the fact that area of the lower impeller has not been affected by the circulation rising motion, making where the circulation drop motion be more intense, as shown in Fig. 6. The liquid in the upper impeller area flows up to the surface through the circulation and then flows back down to the impeller area along the agitation axis, which causes the phenomenon of center concave and rising around other area in the gas-liquid two-phase interface, in which the high-mounted impeller when the most obvious.



(a)low level (b)medium level

dium level (c)high level

Fig.6 The velocity vector diagram for cross-section of flow field under different layer-spacing

From the vector diagram can be saw the fluid movement in reactor: the axial flow of the reactor caused by the upper impeller, the radial flow caused by the lower impeller. The radial flow generated by the lower impeller which collided with the inner wall of the reaction vessel and then divided into two strands. A part of the fluid flows upward along the inner wall and involved in the axial flow by the disturbance of the upper two impellers. Another part of the fluid flowed down along the inner wall, when it reached the bottom of the reactor, it will return to the upward flow after the second collision. When it reached the disturbing area of the lower impeller, it will continue to participate in the radial flow, which was consistent with the simulation result of velocity cloud.

### 5.3 The Change of Turbulent Kinetic Energy with Different Layers in Flow Fields

It can be seen from Fig. 7 that the maximum value of k appeared in the peripheral region of the blade, decreased gradually outward along the blade region, and the minimum value at the liquid level and the bottom of the reactor. It's indicated that the turbulence kinetic energy has been mainly generated in the blade peripheral region, in which the turbulence is relatively high, making better of the mixing effect. In addition, the turbulent kinetic energy of the upper impeller is relatively large, which will aggravate the internal liquid sloshing. When the upper impeller was at a low and high position, the turbulent kinetic energy distribution is obviously inhomogeneous, When the stirring blade is in the middle position, the turbulent kinetic energy distribution in the reactor is relatively uniform, which indicates that the mixing effect is the best.



(a)low level (b)medium level (c)high level Fig.7 The cloud of turbulence kinetic energy cloud under different layer in flow field

## 5.4 The Change of Power Value under Different Layers

The stirring power in the low, medium and high positions has been simulated and experimentally verified for the stirring paddle.

According to the formula (7), the speed and torque value acquired by the experimental device have been converted into the power value.

$$P = T * n * 2\pi / 60 \tag{7}$$

Where T is the torque value (Nm); n is the speed value (r / min).

The simulation result has been based on the transient simulation method. The liquid level is 845mm and the mixing speed is 100r / min, the results were viewed by post-processing software CFD-POST when the mixing has been stability. Table 1 shows the variation of the torque value and the power value and the error between the numerical simulation and the experimental test under different layers.

spacing	Simulation Torque (r/min)	Experimental torque (r/min)	Simulation power (W)	Experimental power (W)	Error (%)
low	0.21	0.20	1.67	1.57	6.4
medium	0.20	0.20	2.09	2.09	0
high	0.16	0.15	2.20	2.09	5.3

Table 1 The results of CFD simulation and experimental test

From Table 1 we can see that the maximum error of the experiment was 6.4%, indicating that the result of numerical simulation and experimental test are basically consistent. In the process of experiment, the precision of machining and installation have not been considered. What's more, as the structure of bolts and nuts that have less influence on the simulation and modeling process were neglected, which is the reason for the deviation between simulation and experiment. Therefore, the method of numerical simulation can be used to provide the basis for the selection of the driving power for the stirred reactor.

## 6. Conclusion

The VOF multiphase flow model and the k- $\epsilon$  model with swirl correction are used to simulate the flow field in the stirred reactor. The results are compared with the experimental results to obtain the following conclusions:

(1)The axial flow generated by the upper impeller and the radial flow generated by the lower impeller are merged and formed a circulating flow field in the stirred reactor. The middle position of the upper impeller can better form the circulating flow field, and the liquid phase is stable for inside reactor and has better mixing effect.

(2)By studying the influence of different-layer spacing on the driving power, it was found that the driving power of the stirring blade was the least when the stirring blade was installed at the high position. And the maximum error of the agitator driving power obtained by the experimental method and the numerical simulation method is 6.4%

The experimental results show that the CFD simulation results are in good agreement with the experimental results, which proves the feasibility for CFD numerical simulation, and provides technical support and theoretical basis for the design, and structural optimization to improve production efficiency.

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