Numerical simulation on macro-instability of coupling flow field structure in jet-stirred tank

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Abstract. The velocity field macro-instability (MI) can help to improve the mixing efficiency. In this work, the MI features of flow field induced by jet-stirred coupling action is studied by using computational fluid dynamics (CFD) simulations. The numerical simulation method of jet-stirred model was established based on standard turbulent equations, and the impeller rotation was modeled by means of the Sliding Mesh (SM) technology. The numerical results of test fluid (water) power consumption were compared with the data obtained by power test experiments. The effects of jet flow velocity and impeller speed on MI frequency were analyzed thoroughly. The results show that the calculated values of power consumption agree well with the experiment measured data, which validates the turbulent model, and the flow structure and MI frequency distribution are affected by both impeller speed and jet flow rate. The amplitude of MI frequency increases obviously with the increasing rotation speed of impeller and the eccentric jet rate, and it can be enhanced observably by eccentric jet rate, in condition of comparatively high impeller speed. At this time, the MI phenomenon disappears with the overall chaotic mixing.

1. Introduction
The fluid turbulent flow is highly unstable circulation pattern in a stirred tank with the existence of large-scale low-frequency phenomenon termed as macro-instability (MI). The frequency of MI is represented as a distinct peak for frequency oscillations in power spectrum of the region close to the impeller which is usually located between 0.01 and 1 HZ frequency band. The studies have reported that the impeller stream region contains a large number of the symmetry flow field structure, so it is difficult to finish dissipating energy to outward effectively. As a result, near 70% of the mechanical energy will be dissipated in this region [1], which leads to the reducing of mixing efficiency. The energy dissipation concerned with turbulent flow and the large eddy pattern of the flow field may be described well with MI phenomenon [2]. The research on MI phenomenon is of significant value for the better understanding of the flow pattern and mixing mechanism since the existence of MI help to enhance the turbulent flow to an extent, improve the mixing efficiency, moreover, it has the distinct effect on mass and heat transfer and local gas content distribution in a stirred tank [3-4].

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In recent years, a number of studies have pointed to the likely effect of MI phenomenon in stirred tanks in different ways [5-9]. These results indicated that MI frequency is irrelevant to stirred tank size, impeller type and fluid property parameters, whereas MI frequency may produce a certain difference in condition of different Reynolds number and different ratio of kettle and impeller diameter. Up to now, there is few research on MI of coupling flow field in jet-stirred tank [10]. The studies concerned with the jet pattern found that the jet can form a kind of special flow structure different from that of agitation, and the nonlinear coupling flow field in jet-stirred tank inevitably induce the chaotic mixing of fluid. Therefore, it is necessary to analysis the flow field characteristic mixing of jet-stirred coupling flow pattern in more detail. The aim of this paper is to study MI characteristics of jet-stirred coupling flow field and explore the effective way of chaotic mixing induced by coupling flow field using numerical simulation method.

2. Stirred vessel configuration and meshing

The stirred vessel consists of a transparent cylindrical tank of diameter \((T)\) 0.3m. The flat-bottomed tank was fitted with four equally spaced flat baffles, each with a width \((w)\) equal to \(T/10\). The fluid height \((H)\) was maintained constant at a height equal to 1.25\(T\). The dual-impeller system was restricted to the Rushton turbine of impeller and 45° four pitch-blade turbine downflow as upper impeller. The dual-impeller with a diameter \((D)\) of 0.1m and thickness 2mm was mounted on a centrally positioned shaft of diameter 0.016m at an off-bottomed clearance\((C)\) and a layer clearance \((C1)\) of 0.1m. The jet nozzle of diameter 6mm was located at the bottom of the tank, the distance was 0.1m off the z axis. The tank was filled with tap water. The impeller speed was fixed at 2 r/s, corresponding to Reynolds number, \(Re\) equal to 19960. So the flow was in a turbulent state. The computational domain was separated into two zones: the rotor zone enclosing the impeller and the stator zone with the rest of the vessel. A pre-processor (Gambit 2.3) was used to discretize the flow domain with an unstructured tetrahedral mesh. The density of mesh cells in rotor zone was needed to be five enough to capture the flow details, as shown in Figure 1. Grid independence was verified by demonstrating the additional requirement on mesh cells that did not change the calculated power number and velocity magnitude in the region of high velocity gradients close to the impeller blade by more 3%. First, the original 3D mesh of the model had about 623100 cells for calculation, then the numbers were increased to about 851700 cells. It was found that this increase changed the velocity and power number in regions of high velocity gradients by more than 3%. When the number of the cells further were increased to about 1227400, the velocity and power number changed by less than 3% in the same regions. Therefore, about 1227400 cells were adopted to discretize the computational regions.

3. CFD model and simulation methods

The CFD simulation method of flow field in a stirred tank is based on the calculation of the scalar transport equations, considering the stirred tank with the characteristics of the flat bottomed cylindrical vessel, the cylindrical coordinate was used to solve the transport equation in this work as follows:

\[
\frac{\partial}{\partial t}(\rho \phi) + \nabla \cdot (\rho u_{\phi} \phi) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho_{\phi} \phi) = \frac{\partial}{\partial r} \left( \Gamma \frac{\partial \phi}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( r \Gamma \frac{\partial \phi}{\partial \theta} \right) + \frac{1}{r} \frac{\partial}{\partial z} \left( r \Gamma \frac{\partial \phi}{\partial z} \right) + S
\]

The initial condition for CFD simulation was that of still liquid. A flat liquid surface was assumed.
at the top surface by setting all the shear stress equal to zero. No-slip boundary conditions were adopted at the impeller blades, the shaft and tank walls, and the speed boundary condition was set to the nozzle entrance. The interface between the rotor and stator zone was set as the interior. For modeling the impeller rotation, the sliding mesh (SM) method was used for the $k-\varepsilon$ model computation.

The pressure-based Navier-stoke algorithm was used for the solution of the CFD model with implicit solver formulation. The momentum conservation equation was discretized using the second upwind scheme to obtain a high-precision result. The standard wall function was adopted in near-wall region and the SIMPLE algorithm was performed to couple velocities and pressure terms. Furthermore, the time step of CFD computation is 0.005s. Within each time step, a maximum of 20 iteration was conducted to ensure the accuracy of convergence when the normalized residuals of all variables were less than $1\times10^{-4}$. All the simulation were carried out using commercial CFD software Fluent v6.3 (Fluent Inc.) on a HPXW6200 workstation with 8GB RAM.

The spectrum analysis is a time series method by making Fourier transform for the time series of velocity fluctuation signal. This method may exhibit the periodic time series pulse information based on the analysis of the powers spectral density distribution at the different frequency band. The frequency of MI can be determined using spectrum analysis method according to the CFD simulation results of the time series of velocity signal [11]. In this paper, spectrum analysis is realized by programming with the help of Matlab software, and using the Welch average overlap method and Hanning window function method to improve the resolution of the spectrum map. This may be suitable for the time series spectrum analysis of the flow field in a stirred tank [12]. The literature have reported that the location of the velocity monitoring point has few effect on the MI characteristics of flow field [13]. As a result, the sample point was selected at $r=T/3$, and $Z=0$ in the $\theta=0$ plane, which located at the center height of the impeller. The monitoring frequency at the different windows was 20 HZ, and the monitoring time is 30s.

4. Result and discussions

4.1. Validation of CFD model

The power consumption of the impeller may be conducted based on the shaft torque obtained through numerical simulation. The results of the simulations are compared with the original experimental data and good agreement is obtained in all case, as shown in Figure 2. It can be seen that the power consumption increases as the increasing impeller speed and the same tendency is exhibited between the simulations and the experimental measurement. The maximum deviation is less than 10%, which verifies the turbulent model for simulations in this work.

4.2. Micro structure of the flow field

Figure 3 shows the velocity vector plots within the axial lengthwise section of the stirred tank at impeller speed $N=2r/s$. It can be seen that the flow between the two impeller can be considered as connected flow without the layer compartment existing. The flow field is almost similar to that of single impeller. However, in condition of no jet, the structure of flow field exhibits the obvious symmetry with double vertex ring shape, which will necessarily result in low mixing efficient because of mixing isolation region existing, as shown in Figure 3 (a). When the jet velocity ($v$) equals to 2 m/s, the symmetrical structure of flow field is destroyed, accompanied by the asymmetrical flow pattern emergence, and this trend of asymmetrical pattern will increase as the jet velocity increases, as shown in Figure 3 (b) and (c). So the fluid in stirred tank is alternatively stretched and folded under the couple action of agitation and jet, which will induce the chaotic mixing, and furthermore, improve the mixing efficiency.
4.3. Action of impeller velocity
MI frequency plots of different impeller speed are shown in Figure 4. It can be seen that MI frequency mainly concentrated on the band of 0–2 Hz, which means the low turbulent intensity at the speed $N=2$ r/s. The single frequency peak value is found to be 0.040 Hz, corresponding to the dimensionless frequency $f^* = f/N = 0.02$. When the speed reaches to 3.5 r/s, the amplitude of MI frequency increases in the whole frequency band. At this time, the fluctuation strength of fluid is enhanced obviously, and two MI frequency peak values are observed, i.e., 0.231 Hz and 0.315 Hz, corresponding to the dimensionless frequency 0.066 and 0.09, respectively, which indicates that the flow is in unstable state obviously. As a result, the distribution of MI frequency may be controlled by the different stirring speed.

4.4. Action of jet velocity
Figure 5 reports the MI frequency plots of different jet velocity at the impeller speed $N=2$ r/s. It can be found that the fluctuation strength increases and the frequency band of high amplitude becomes a wider distribution as the jet velocity increases. The MI frequency peak value is 0.068 Hz as the jet velocity ($v$) equals to 2 m/s. When the jet velocity reaches to 2.5 m/s, 3 m/s and 4 m/s, corresponding peak value is 0.097 Hz, 0.113 Hz and 0.187 Hz, respectively. It is seem that the MI frequency diverts to the high frequency band and the MI intensity is improved. This indicates that the jet action can make a big effect on the coherent structure of flow field and MI frequency increases as the jet velocity increases. Therefore, it is concluded that MI intensity of flow field may be improved by adding jet action.
Under the high impeller speed $N=3.5 \text{ r/s}$, the effect of jet velocity on MI frequency is shown in Figure 6. It is found that the characteristics of MI frequency disappear due to the jet action. This means that the coherent structure of flow field is thoroughly destroyed and the multi-scale structure
characteristics appear, which makes the flow field into whole chaos.

Figure 5. MI frequency under different jet speeds at \( N = 2 \) r/s.

Through the study on the MI frequency variation in the different working condition, it is known that, with the impeller speed increased, the frequency amplitude distribution on the whole band would increase and the fluctuation intensity is also improved corresponding. At this time, the spectrum plot exhibits the characteristics of multiple peak frequency with the high peak values. This indicates that the flow field is of a more apparent random fluctuation character associated with the turbulence intensity of the fluid in stirred tank. Owing to the fact that intensity of MI frequency on the whole band increases as the impeller speed increases, the MI phenomenon can be taken as the weakened signature, which would lead to the rapid mixing. Similarly, Fan Jianhua et al.[7] also obtained such
conclusion from the average sequence spectrum plot for the turbine impeller. Moreover, at low impeller speed \( (N=2 \text{ r/s}) \), MI frequency and intensity of flow field have been proved to make a better improvement through the eccentrical jet action. When the speed reaches to high \( (N=3.5 \text{ r/s}) \), a more dominant effect of jet action on MI may be observed that is a broader distribution band of frequency peak value appears in the spectrum plot, which means that MI frequency disappears and the flow field leads to the chaotic state accompanied by the multi-scale coherent structure feather.

![Frequency/Hz](a) V=4 m/s ![Frequency/Hz](d) V=6 m/s

**Figure 6.** MI frequency under different jet speeds at \( N = 2 \text{ r/s} \).

5. **Conclusions**

The eccentric jet-stirring may make an asymmetric flow field structure, therefore, lead to an extensive chaos in the tank and improve the flow and mixing efficiency.

Increasing the impeller speed may improve MI frequency intensity of the flow field, and then the MI phenomenon is weakened. So the random fluctuation level is enhanced in the whole tank, which will finish a rapid mixing progress.

The effect of the eccentric jet action on MI frequency intensity may be observed, and a more dominant improvement can be obtained specially at high impeller speed with MI frequency disappearance. This indicates that the flow field is into the chaotic mixing.

**NOMENCLATURE**

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\begin{align*}
C & \quad \text{off-bottom clearance, m} \\
D & \quad \text{impeller diameter, m} \\
T & \quad \text{tank diameter, m} \\
Re & \quad \text{apparent Reynolds number} \\
t & \quad \text{time, s} \\
\Gamma & \quad \text{generalized diffusion coefficient} \\
\phi & \quad \text{field variable} \\
u_\theta & \quad \text{tangential velocity, m/s} \\
C_1 & \quad \text{layer clearance} \\
H & \quad \text{fluid height, m} \\
N & \quad \text{impeller speed, r/s} \\
\rho & \quad \text{density, kg/m}^3 \\
r & \quad \text{radial position, m} \\
S & \quad \text{Generalized source term} \\
u_r & \quad \text{radial velocity, m/s} \\
u_z & \quad \text{axial velocity, m/s}
\end{align*}
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References
[1] Wang K and Feng L F [M] 2001 The designation of mixed equipment (Beijing: China Machine Press)
[2] Hartmann H, Derksen J and Van Den Akker H E A [J] 2004 Macro-instability uncovered in a Rushton turbine stirred tank by means of LES American Institute of Chem Eng 50 2383
[3] Hasal P, Montes J L and Boisson H C [J] 2000 Macro-instabilities of velocity field in stirred vessel: detection and analysis Chem Eng Sci 55 391
[4] Ducci A, Doulgerakis Z and Yianneskis M [J] 2008 Decomposition of flow structures in stirred reactors and implications for mixing enhancement Ind Eng Chem Res 47 3664
[5] Paglianti A, Liu Z and Montante G [J] 2008 Effect of macro-instabilities in single-and multiple-impeller stirred tanks Ind Eng Chem Res 47 4944
[6] Fan J, Rao Q and Wang Y [J] 2004 Spatio-temporal stirred vessel via digital particle image velocimetry macro-instability analysis of DPIV Chem Eng Sci 59 1863
[7] Fan J H, Rao Q and Wang Y D [J] 2004 Spectral analysis of the velocity fluctuations in a mechanically stirred tank J Chem Eng of Chinese Univ 18 287
[8] Galletti C, Paglianti A and Yianneskis M [J] 2005 Observations on the significance of instabilities turbulence and intermittent motions on fluid mixing processes in stirred reactors Chem Eng Sci 60 2317
[9] Galletti C, Lee K C and Paglianti A [J] 2004 Reynolds number and impeller diameter effects on instabilities in stirred vessels Chem Eng Sci 50 2050
[10] Liu Z H, Ning W Z and Sun R X [J] 2010 Comparative study on macro-instability of liquid / gas-liquid in stirred tank J Chem Eng of Chinese Univ 29 100
[11] Yang F L, Zhou S J and Wang G C [J] 2012 Detached eddy simulation of the Macro-Instability in eccentrically stirred tanks J Chem Eng of Chinese Univ 26 228
[12] Yin L B [D] 2005 Experimental study of Macro-Instabilities in a stirred tank (Beijing: Beijing University of Chemical Technology)
[13] Nikiforaki L, Yu J and Baldi S [J] 2004 On the variation of processional flow instabilities with operational parameters in stirred vessels Chem Eng J 102 217