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CFD STUDY OF MIXING PROCESS IN RUSHTON TURBINE STIRRED TANKS

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ABSTRACT

This paper reports on the CFD study of macro-mixing process of Rushton turbine in stirred tank. The code for mixing calculation is developed in the commercial CFD code CFX4.3. Mixing process simulation on different calculation method, different turbulent model and different tracer adding and detecting position are calculated. The simulation is three-dimensional and the impeller region is explicitly included using a sliding mesh method to account for the relative movement between impeller and baffles. Fluid flow is calculated with a turbulent *k-ε* and RNG *k-ε* model using a finite-volume method. The results show that the mixing time highly relies on the flow field, the feeding and detecting position. The improvements of macro-mixing simulation can be obtained by accurate flow prediction and modification to turbulence models applied to stirred tank.

NOMENCLATURE

C	off-bottom clearance, m
D	impeller diameter, m
H	liquid height, m
p	pressure
R	impeller radius, m
Re	Reynolds number
Sc	Schmitt number
T	tank diameter, m
t	time, s
u	axial velocity, m • s^{-1}
v	radial velocity, m • s^{-1}
w	tangential velocity, m • s^{-1}
ρ	density kg • m^{-3}
υ	dynamic viscosity m^2 • s^{-2}
θ_{95}	mixing time, s

INTRODUCTION

Stirred tanks are widely used in the chemical process industry to carry out many different operations. In the design of stirred tanks, detailed information on the flow and mixing phenomena is of great importance. Because of the complexity of fluid mechanics prevailing in stirred vessels, the present design procedures are still closer to an art than science. In order to understand the fluid dynamics and develop rational design procedures, there have been continuous attempts over the past century. Among the attempts, Computational fluid dynamics (CFD) may be the most important method.

Macro-mixing denotes the stage of a mixing process which refers to mixture concentration changes down to the scale of physical probes used for measuring local concentrations. It is different from the molecular scale mixing-micro-mixing. Macro-mixing in process equipment is of high importance in the analysis of other processes, such as crystallization or chemical reactions. The intensity of macro-mixing process in stirred tanks has been often characterized by mixing time, i.e. the time necessary to achieve a required degree of homogeneity measured by a mixing index applied.

The simulation of macro-mixing process is less popular than fluid field modelling. So there is only few papers reported concentrations obtained from CFD over the whole period of homogenisation process, and the results are often compared with experiments in order to validate the approach. Noorman (1993) compared the experiment and simulation results of a single Rushton turbine homogenisation. The tracer correspondence curve corresponded well with experiment results, but had some difference in detail. Schmalzriedt (1997) compared the results of a single Rushton turbine with literature data, and got the conclusion that the simulation results were highly relied on the turbulence model. Jaworski (2000) reported the simulation results of double Rushton turbine using CFD code FLUENT. The predicted mixing time θ_{95} was 2~3 times high than the experimental data. The discrepancy came from the under prediction of mass transfer between different circulation loops. Some researchers (Mao, 1997) also reported the process simulation with zonal mixing model.

This study is aimed at highlighting the effects of calculation method, turbulence model and different tracer adding and detecting position on the macro-mixing process and mixing time.

MODEL DESCRIPTION

Governing Equation

The predominant mechanism of momentum and mass transfer for macro-mixing is convection for the mean and eddy flows. Knowing the velocity and eddy diffusivity field within the stirred vessel, the mixing process can be modelled by solving the conservation equation for the tracer, that is,

$$\frac{\partial c}{\partial t}+\frac{\partial}{\partial z}(uc)+\frac{1}{r}\frac{\partial}{\partial r}(rvc)+\frac{1}{r}\frac{\partial}{\partial \theta}(wc)= \frac{\partial}{\partial z}(D_{eff}\frac{\partial c}{\partial z})+\frac{1}{r}\frac{\partial}{\partial r}(r\,D_{eff}\frac{\partial c}{\partial r})+\frac{1}{r}\frac{\partial}{\partial \theta}(\frac{D_{eff}}{r}\frac{\partial c}{\partial \theta}) \quad (1)$$

The turbulent diffusion coefficient is defined as

$$D_{eff}=\frac{\nu_{eff}}{Sc} \quad (2)$$

Tank Geometries

The stirred tank used for simulation was cylindrical with flat bottom. It had a diameter, T of 0.5m and a height of $H=T$. A six-bladed Rushton turbine impeller with a diameter of $D=T/3$ was placed in the tank. Both the impeller width, l and the impeller blade height, w were equal to $D/4$. The off-bottom clearance is $C=T/3$. Four baffles of $T/10$ in diameter were equally placed around the tank. The working material was water. The rotation speed of the impeller was 120 rpm. This corresponds to a Reynolds number, $Re=ND^2/\upsilon$ of 5.56×10^4.

The computational grid is shown in Fig.1. The grids are structural hexahedrons. Only one half of the tank is modelled because of symmetry, which includes two baffles and three impeller blades. The grid consists of 39 $\times36\times60$ grid cells in radial, circumferential and axial directions, respectively. The grid is compressed in the impeller region in order to resolve the flow details. At the blade surface, the grid consists of 10×9 grid cells.

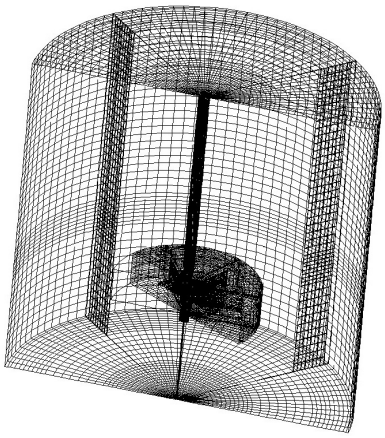


Figure.1: Computational grid

Modelling methodology

The simulation used the commercial CFD package CFX4.3. In order to model the impeller and baffle interaction, the Sliding Grid (SG) technique is adopted in the simulation. In the SG technique, the inner part of the grid is rotating with the impeller, whereas the outer part, containing the walls and baffles, is fixed. The simulation using SG is a time consuming task. So, the time step is chosen in such a way that the inner part of the grids slides several grid cells per time-step at the initial period and exactly one grid cell per time-step at the last revolutions.

Experimentally, the mixing time is estimated by giving an input of the tracer at a certain location in the vessel, and monitoring the change of concentration with time at some other location in the equipment. The mixing time is considered as the time in which the measured concentration of the tracer reaches within 95~99% of the final concentration. In this study, 95% is adopted and the mixing time is labelled as θ_{95}. Fig.2 showed the tracer adding position (I1,I2,I3) and detecting position (P1,P2,P3) in the tank. The detecting and tracer adding position are all located at the mid-baffle plane and at the same height.

In the CFD package, an USER SCALAR is added through user-defined function as the tracer. At time t=0, the USER SCALAR value of grid cell at adding position is set to 1.0, while the value of other grid cells are all set to 0. As time gone, different detecting position has different tracer concentration. The mixing time, θ_{95} is taken as the time at which the concentration of detecting position reached 95% of the final concentration (completely mixed). In the simulation, two dealing methods are adopted. In the first method, all the equations are solved at the same time. In the other method, only the tracer conservation equation is solved, and other equations (the continuity equation and the momentum equations) are all locked. This method could save lots of computing time. It should note that all the simulations are all started from a stable flow field. In the calculation, two different flow fields from k- ε and RNG k- ε turbulence model are adopted.

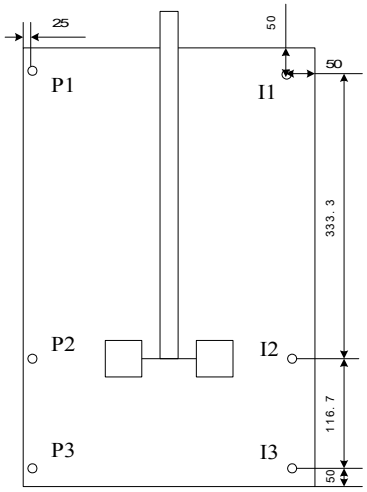
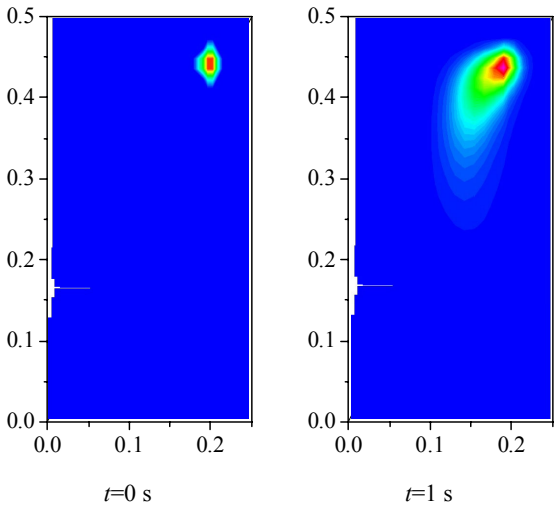


Figure.2: Tracer adding and detecting position

RESULTS

Tracer dispersion

Figure.3 showed the tracer distribution at different time. The plane was selected at the mid-way of two baffles. From these figures we could see how the tracer was diffused in the vessel.



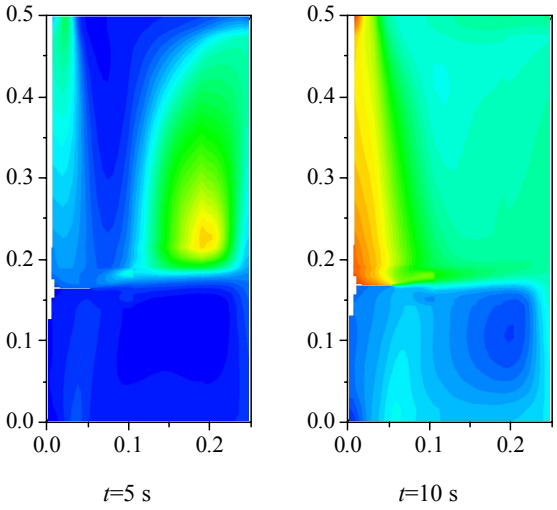
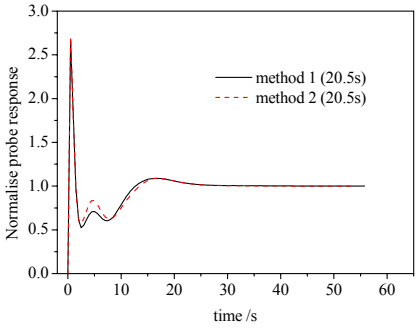


Figure.3: Tracer concentration at different time

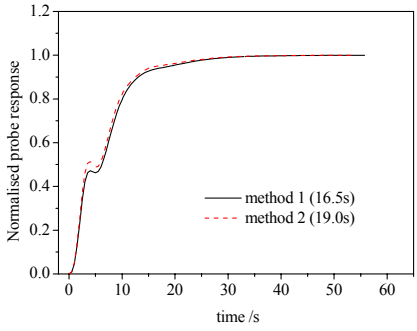
Calculation method

Figure.4 showed the results of response curve at different detecting position using the two dealing methods described above. The tracer response curves from the two methods were consistent in trend, with little variance at the middle of the curve. Table 1 showed the mixing time, θ_{95} calculated using the two methods. At the top detecting position, the two methods predicted the same value. While at detecting position P2 and P3, method 1 predicted lower value compared with method 2. This difference might come from the change of the flow field. As we know, the flow field in the stirred tank is three-dimensional, unsteady and periodic. Especially at regions near the impeller, this transitional effect is stronger. This unsteady-state fluid movement can accelerate mass transfer. So, method 1 predicted lower value at position P2 and P3.

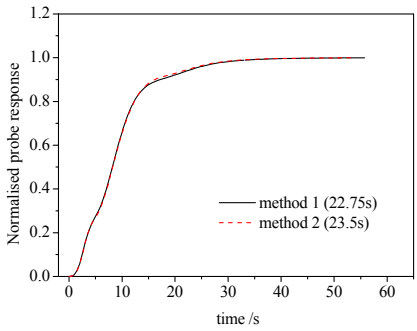
Theoretically, method 1 could give more accurate results. But this method had its shortcoming, i.e. the intensive calculation. At the same set-up, method 1 needed about 2.2 times more CPU time than method 2. If the step-time was reduced further and iteration number was increased, the calculation time would increase about 1~2 order of magnitude. The second method could predict the same rule of mixing time as method 1, but it needed less calculation time and had more flexibility. So lots of researchers used the second method described above in their study, such as Schmalzriedt(1997), Jaworski(2000), etc. This paper also adopted the second method in the later simulation.



(a) P1



(b) P2



(c) P3

Figure.4: Response curve from different calculation methods (Tracer adding position I1).

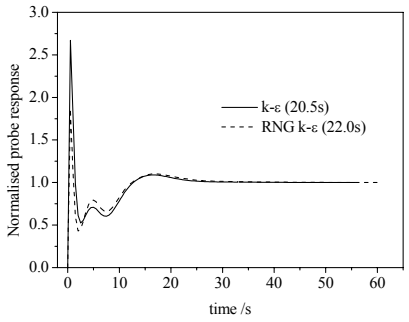
	Mixing time, θ_{95} (s)		
	P1	P2	P3
Method 1	20.5	16.5	22.75
Method 2	20.5	19.0	23.5

Table 1: Mixing time from different calculation methods. (Tracer adding position I1)

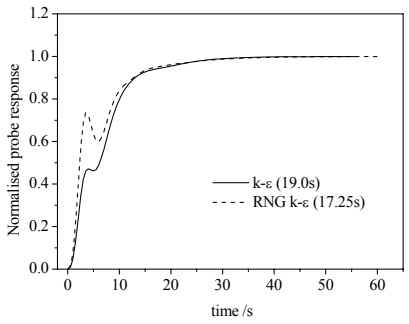
Turbulence model

Figure.5 showed the results of response curve at different detecting position using different flow field predicted from standard k- ε model and RNG k- ε model. At detecting position P1 and P3, the results were in consistent. While at position P2, the response curves had large variance at the initial period. From table.2, the mixing time detected at P2 also showed difference compared with P1 and P3. At detecting position P1 and P3, mixing time from RNG k- ε model was little larger than that from k- ε model. While at position P2, mixing time from RNG k- ε model was smaller than that from k- ε model. Zhou (2002) had found that the RNG k- ε model predicted larger velocity and turbulent kinetic energy than k- ε model at impeller region in flow field simulation. This may be the reason for the smaller mixing time of RNG k- ε model.

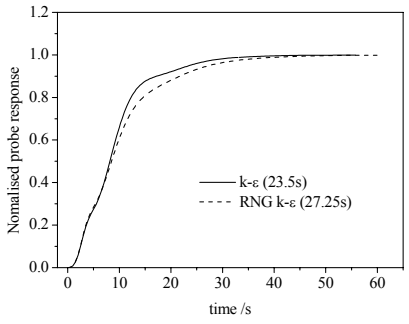
These results showed that the mixing simulation highly relied on the flow field. Accurate flow prediction can provide sound base for mixing simulation.



(a) P1



(b) P2



(c) P3

Figure.5: Response curve from different turbulence model (Tracer adding position I1).

	Mixing time, θ_{95} (s)		
	P1	P2	P3
k- ε	20.5	19.0	23.5
RNG *k- ε*	22.0	17.25	27.25

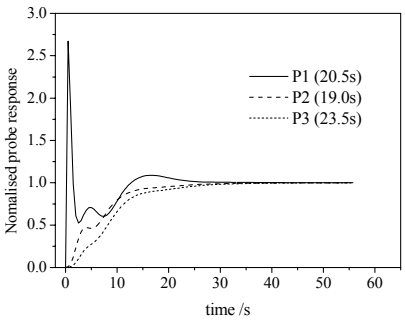
Table 2: Mixing time from different turbulence model. (Tracer adding position I1)

Tracer adding position

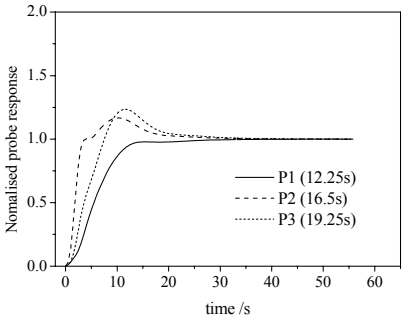
Figure.6 and table 3 showed the results of response curve and mixing time from different tracer adding position. At different tracer adding position, the same detecting position got different response curve and mixing time. For the three adding position, the mixing process from I3 need more time than other positions; while mixing time from position I2 was the smallest. At position I1, the time needed for homogenisation laid between the other two positions. This result is very useful for fast reaction systems. Lots of other literature also got the conclusion that feeding position near the impeller could get faster homogenisation. This is from the reason that the velocity and turbulence intensity are higher than other areas, and feeding material can be dispersed quickly.

The mixing time did not only relied on adding position, but also relied on detecting position. At the same adding position, different detecting position got different response curve and mixing time. At position I1, the concentration of P1 fluctuated greater than other positions. Because at the top of the tank, there is large tangential velocity, while the turbulence intensity is small. So lots of the tracer could be transported through the large eddy movement, but could not be dispersed in time. Mixing time detected from the top of the tank was smaller than that from the bottom of the tank. This result showed that the flow and turbulence condition at the top was better than that at the bottom of the tank.

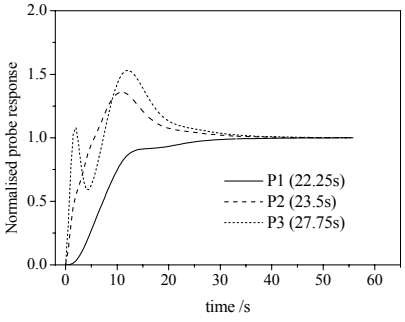
All these results correspond well with literature data and conclusions from other researchers.



(a) I1



(b) I2



(c) I3

Figure.6: Response curve from different tracer adding position.

	Mixing time, θ_{95} (s)		
	P1	P2	P3
I1	20.5	12.25	22.25
I2	19	16.5	23.5
I3	23.5	19.25	27.75

Table 3: Mixing time from different tracer adding position.

CONCLUSION

Based on the CFD code CFX4.3, numerical mixing calculation was studied on the single Rushton turbine stirred tank. The following general conclusions can be drawn on the basis of the results obtained so far:

CFD methods are efficient in the modelling of macro-mixing.

The two calculation methods predict the same rule of mixing time, but the method of single calculation of tracer concentration equation has more advantages.

Mixing simulation highly rely on the flow field predicted from different turbulence model.

Different tracer adding position and detecting position can get different mixing time.

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