Study on velocity field analysis and back-mixing of fluid in reactor based by simulation

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Abstract. During the operation of the reactor, the degree of back mixing directly reflects the concentration distribution, temperature distribution, reaction process of the fluid in the reactor, and so on, thereby affecting the practical value of the reactor. Therefore, this article uses computer simulation to analyze the influence of inlet flow rate on the degree of back mixing. It can provide data support for the preparation of organic semiconductor materials under different reaction conditions. The research results show that when the inlet flow velocity reaches 0.3 m/s, the stirring effect of the fluid weakens, the jetting effect of the inlet pipe is dominant, and the model parameters are the largest.

1. Introduction
The Tank reactor is a reaction mixing device widely used in the process of chemical experiments[1]. In the reactor equipment, various stirring paddle devices are used to ensure the complete mixing of materials and liquids. Small reactors commonly used in laboratories usually use single-layer four-blade propellers and place them in the center of the reactor, while this type of reactor is rarely equipped with baffles. When the viscosity of the liquid in the reactor is small, vortexing is likely to occur around the stirring blade, resulting in insufficient mixing.[2-3] To study the fluid flow in the reactor, CFD technology has a wide range of applications. Using the CFD method for simulation can reduce the amount of experimentation[4]. When the turbulence model is selected appropriately, the flow field of the reactor can be simulated more accurately.

This article combines standard k-ε, RNGk-ε, SSTk-ε, RSM, and other four common turbulence model calculation methods to simulate the flow field results of the tank reactor and conduct different simulations such as velocity field, velocity vector, turbulent kinetic energy, and so on. What’s more, it will find out the turbulence model suitable for small reactor flow field simulation, and guide stirring and optimizing reactor-type equipment[5]. To solve the problem of the interaction between the area of the stirring blade and the surrounding quiet zone, this article adopts a multi-reference system method in the flow field simulation of the tank reactor[6]. This method is mainly used to stabilize the flow field and simulate the unsteady state fitting calculation method.

2. Materials and Methods
This article focus on how the inside structure affects the stirred reactor, use the SIMPLE calculation based on the speed-filed pressure-filed combination (Doormal & Raithby, 1984). This article considered the speed-filed and pressure-filed were two separated processes, according to the law of Conservation of mass we can calculate pressure-filed by speed-filed which is know If it didn’t meet the need of the law of Conservation the correction to pressure where needed. at the same time speed was also corrected.
when the speed was corrected considered each correction to speed value doesn’t affect each other. Then calculate though iteration repeated to get each value for each grid.

2.1. standard k-epsilon model

This article used the standard k-epsilon model to simulate the fluid inside the reactor, though out the mass conservation and momentum conservation we were able to know equations during the stable calculation. The Continuity equation, momentum equation, energy equation of each phase will be as follow:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = S_m
\]  

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial \rho}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + F_i
\]

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial \rho}{\partial x_i} \sigma_{ij}
\]

\[
\frac{\partial (\rho E)}{\partial t} + \frac{\partial (\rho u_i (\rho E + p))}{\partial x_j} = -\frac{\partial}{\partial x_i} \left( k_{\text{eff}} \frac{\partial T}{\partial x_i} - \sum J_{l,j} \tau_{ij} \right) + S_h
\]

standard k-epsilon (2 eqn)

\[
k = \frac{3}{2} \left( u_{\text{ave}} \right)^2
\]

\[
\varepsilon = C_{\mu}^\frac{3}{2} \frac{k^2}{l}
\]

2.2. CDF modeling

The size of the reactor is shown in the figure1 (Ignore the space occupied by the turbine blade to establish a model). we choose the disc turbine blade as the inside agitator, the height of turbine blade is installed in variable value as follows Figure 1.

Measuring point positions and naming are shown in tab.2. Split schematics how as follow in figure 2. Since the volume was very small and the structure of the blade was complex, so using an unstructured grid to divide the whole structure, scale factor valued 0.1, stirred blade and some moving parts were divided as 0.05 grid.
3. Results & Discussion

The inlet flow rate has little effect on the interrupted interface of the reactor. It can be seen from the comparison in Figure 3 that when the inlet flow rate is low, the flow rate in the middle of the reactor is more uniform. The reason is that the smaller inlet jet velocity affects the overall flow trend in the reactor. As a result, the inlet jet velocity is too large to reduce the uniformity of the target flow.
Figure 4. Change of residence time distribution curve of fluid during different liquid flow rate

By comparing the degree of back mixing, it can be found that as the inlet flow rate increases, the degree of back mixing in the reactor first increases and then decreases, between 0.3 m/s and 0.4 m/s. Inlet flow rates reach the lowest value.

Figure 5. Velocity vector diagram of reaction kettle (y=0 mm, x=0 mm)

a: Dead area b: Active area

It can be seen from the vector diagram analysis that the velocity distribution of the fluid is unbalanced under the action of the stirring blade, and there will appear a dead area and an active area. The uneven distribution of the fluid in the two zones leads to insufficient mixing of the materials in the reactor.

4. Conclusions
1. The low inlet flow rate is conducive to the uniform stirring of the reactor.
2. It is believed that in the flow of a small reactor, the degree of back mixing in the reactor reaches the lowest value, which is between 0.3 m/s and 0.4 m/s.
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