CFD-based fluid calculation model selection and field analysis for small reactors

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Abstract. To improve the accuracy of reactor design, this article uses k-ε, DES, LES, and SST four methods to compare the simulation results of the velocity field in the blade area, turbulence intensity, and velocity distribution of the fluid in the reactor, and predict the appropriate field model of the reactor calculation. Therefore, the calculation process is more suitable for the SST model of small reactors.

1. Introduction
The reactor is a reaction mixing device widely used in chemical processes. In the design of the reactor, to achieve its mixing function, the design of the reactor usually includes a stirring blade. Usually, single-layer four-leaf blades are used in small reactors. The process from laboratory small testing to pilot scale will inevitably lead to a lot of time and economic consumption. To effectively study the fluid flow in the reactor, CFD technology has been widely used in recent years. By using the CFD method, the economic cost can be greatly reduced. In the design of CFD, this algorithm plays a very important role as the basis of calculation. Therefore, this paper compares the four methods of k-ε, DES, LES, and SST to analyze the field changes of blade area. A clear and reasonable response model can guide reactor design and optimization.

2. Materials and Methods
This article focus on the Analysis of the Reactor Fluid Calculation Model Based on CFD, 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.

This article uses four calculation models: k-ε, DES, LES, and SST. The core calculation formulas of the four models are as follows:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = S_m
\]  
(1)

\[
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_j u_i) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ji}}{\partial x_j} + \rho g_i + F_i
\]  
(2)
The k-ε model has high stability, economy, and calculation accuracy, so it has been widely used. It is suitable for high Reynolds number turbulence. It is a semi-empirical formula, mainly based on turbulent kinetic energy k and Diffusion rate ε; DES and LES are the most accurate turbulence models, but they require a lot of grids, a lot of calculation, and memory requirements, and a long calculation time. Currently, there are few engineering applications. The SST equation has been appropriately modified and is usually suitable for simulating the flow field with pressure gradient changes.

The size of the reactor is shown in figure 1 (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 the turbine blade is installed in variable value as follows Figure 1.

![Figure 1. size and structure of the stirred reactor and grid schematic](image)

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

![Figure 2. contours of velocity Section with y = 50 mm of reaction kettle](image)
It can be seen from the velocity vector diagram that these four models all simulate the process of Under the action of the rotation of the impeller, the fluid is discharged at high speed along the tip of the blade to form a larger vortex. The fluid velocity gradually decreases from the end of the blade to the wall surface. The back part of the blade rotation is the fluid high-speed area, and the simulation speed obtained by the LES model is the largest. SST, LES model simulation results, the relative two-blade velocity vortices present axisymmetric characteristics, while the k-ε model simulation results are opposite.

| Form 1. results report | k-ε | DES | LES | SST |
|------------------------|-----|-----|-----|-----|
| Mass Imbalance(residuals) kg/s | -1.164×10^{-12} | -5.401×10^{-13} | -2.524×10^{-13} | -1.715×10^{-13} |
| Mass Flow Rate | -1.586×10^{-5} | -1.513×10^{-5} | -1.598×10^{-5} | -1.571×10^{-5} |
| Subgrid Turbulent Viscosity kg/m/s | 2.312×10^{-5} | 9.554×10^{-6} | 1.126×10^{-7} | 3.914×10^{-3} |

From the form, it can be seen that the turbulent intensity between the blades of the k-ε model is fully exhibited and the simulation results are more consistent with the turbulent viscosity.
The comparison of the velocity intensity of the four models in the linear region of $Y = 65$ mm and $Y = 35$ mm $z = 0$ mm shows that the k-ε and LES models are located at $x = 0.09$ m, $x = 0.38$ m, and $x = 0.49$ m, respectively. There is a peak near this point. The maximum value obtained by the SST model is close to 0.081 m·s⁻¹, and the speed value simulated by the LES model is approximately 0.083 m·s⁻¹.

The comparison of the velocity intensity of the four models in the linear region of $x = 40$ mm and $z = 0$ mm shows that the DES, SST, k-ε and LES models have extremely large peaks before $y = 49$mm-52mm.

4. Conclusions
1. All four models simulate that when the impeller rotates, the fluid velocity decreases sequentially from the end of the blade to the wall. The back part of the blade rotation is the high-speed area of the fluid, and the fluid is discharged at a high speed along the end of the blade, forming a larger vortex.
2. For the simulation process of stirring in a small reactor, the SST model is slightly better than the other three models.

   The results of the fluent field are different from the actual situation. This may be because the two models themselves require higher grid accuracy, and there are more model parameters. This model needs to be further adjusted.

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References
[1] Zhang, L., (2019) Research on mixing characteristics of stirred reactor based on CFD simulation analysis. Salt&Chemical Industry, 048:16-18.
[2] Deng, Q.Q., Wan, B.F., He, H., Liu, H.J., (2020) Numerical simulation study on the influence of reactor baffle length on its flow field characteristics. Chemical Engineering & Equipment, 12:189-192.
[3] Chen, Q.Y., Zhou, H.C., Li, H.Y., Xia, Q., Ren, J.Y., (2020) Applicability analysis of SST, LES, and DES to tire flow field. Proceedings of the Annual Meeting of the Society of Automotive Engineers of China, 2020, 056:453-459.
[4] Li, Q.Y., (2020) Comparison of SST and LES simulation results of the flow field in the small reactor. Guangdong Chemical Industry, 47:22-24+29.
[5] Li, W.J., Zhou, Y.J., Yuan, M.Y., He, H., Sun, J.P., (2021) Comparative study on the flow characteristics of several frame-type impellers stirred tanks. CIESC Journal, 72:1998-2005.