Optimization for a centrifugal pump transporting brine using orthogonal design based on CFD-DEM simulation

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Abstract. To enhance the reliability of a centrifugal pump transporting brine solutions with crystallization, the effect of impeller geometrical configurations on crystal particle behaviors was investigated by an orthogonal design based on CFD-DEM coupled method. In this work, the main impeller geometrical configurations were set as the blade inlet angle $\beta_1$, blade outlet angle $\beta_2$, wrap angle $\phi$, and outlet width $b_2$. In the meanwhile, the $L_9(3^4)$ orthogonal design containing 4 factors with 3 levels was applied in this study. Given the crystal particle features, CFD-DEM coupling method was utilized to study inner flow in a pump with crystal particles. Current results indicated that the blade outlet angle $\beta_2$ could significantly affect the collisions between particles and blades. Moreover, a low-speed region at the blade pressure side in the optimal impeller has been reduced, declining the probability of the crystal particles adhering to the impeller.

1. Introduction

Crystallization is a common phenomenon during the transportation process of brine solutions in most of the major industries such as petrochemical, pharmaceutical and paper manufacture, where crystal particles continuously crystallize, grow, aggregate and break up. Due to factors such as temperature difference, surface roughness, and flow field, the crystal particles would crystallize from solution and absorb on the inner walls of pipelines or pumps, having negative effects on the related machinery and even causing serious economic losses. Early from the 1950s, studies of solid–liquid flow with a crystallization phenomenon have been reported and mainly concentrated in the petroleum, chemical industry and water conservation [1-3]. Although the numerical and experimental data have been obtained, research on the mechanism of crystallization, particle behaviors, and understanding of microscopic property is still inadequate. With lacking reliable research and numerical methods, it is hard to make enough in-depth study of mechanisms that allow the particles at a microscopic scale have an effect on the flow field at a macroscopic scale.

Currently, centrifugal pumps transporting a variety of brine solutions are widely applied in various industries, which leads to a common crystallization problem. So taking a common centrifugal pump as a research object, the study of inner flow in a centrifugal pump with crystal particles has universal significance. Some experiments have been made to investigate this flow in centrifugal pumps by several scholars [4-6]. In the early literature, research mainly focuses on the influence of the flow on the external characteristics of a pump. Forward [4] took a submersible pump as a research object and have studied the effect of accumulating salt deposition inside the impeller passage with the flow, and developed a
new method to improve pump performance. Lopez et al. [5] have studied the connection between crystallization and external characteristics of horizontal multistage centrifugal pump in saltwater disposal device. In subsequent research [6], the Particle Image Velocimetry (PIV) with a developed image processing method was applied to analyze the two-phase velocity fields and particle diameters. The results indicated that the particle number density near the shroud was smaller than that near the hub. Larger particles primarily distributed near the pressure side of the blade and evenly located at the blade outlet.

Studies of numerical methods have also been developed. Sakr [7] applied a finite element method and made a primary analysis of the impeller inlet and outlet flows when pumping seawater. Yang et al. [8] employ the commercial computational fluid dynamics (CFD) code Fluent containing the Euler model to simulate flows in a centrifugal pump. Results supported that crystal particles had a tendency to move towards the blade pressure side of the impeller. However, these results appeared considerable differences with experimental observations because the particle crystallization, growth, and other behaviors could not be reflected in the models. Therefore, the microscopic behaviors of particles have become a focus as research is going deep. From the literature above, it can be concluded that those previous multiphase flow models cannot meet further research requirements.

The DEM, which stands for Discrete Element Method, is an efficient numerical approach for dealing with discrete elements, and it has become an extensively-used tool in granular system simulation. DEM could accurately describe the particle’s nature and calculate the dynamic motion of the particle according to Newton’s second law. Therefore, in order to increase the calculation efficiency and numerical precision, Tsuji et al. [9] and Kafui et al. [10] proposed a method of CFD-DEM coupling methods. Compared with other CFD two-phase flow models, the CFD-DEM coupling method has unparalleled advantages, but this method was rarely utilized in the investigation of inner flow in centrifugal pumps. In a recent research [11], the transient solid-liquid two-phase flow was studied by a CFD-DEM coupling method in a centrifugal pump.

Notably, it could be observed that there are complicated connections between microscopic particle behaviors and macroscopic flow field in pumps. Given the fact that the geometric parameters of impeller significantly affect the flow field in pumps, it is necessary to optimize the pump design to obtain the optimal hydraulic model, whose performance can be least affected by the crystallization. So in this case, the optimization design method should be introduced. On account of a variety of factors and levels, the orthogonal design method, as a kind of optimization method based on orthogonality to reduce test times, has a unique advantage in this work.

In this paper, in consideration of crystal particle features and behaviors, CFD-DEM coupling method was utilized to predict the inner flows in a centrifugal pump with crystal particles. The simulation was performed by commercial CFD tool STAR-CCM+, with a DEM-code inside. Meanwhile, selecting the number of collisions between particles and the blade wall as the main optimization index, using the orthogonal experiment design, the centrifugal pump impeller geometric parameters were optimized. The research results have certain guiding significance for preventing crystal particles' bad behavior in the centrifugal pump.

2. Methodology

2.1. Pump configuration and mesh

For demonstrating the simulation correctness, this paper chooses a single-stage centrifugal pump composed of the inlet pipe, impeller and volute, which has the same configuration as the experimental one [6]. The centrifugal pump’s basic parameters are discharge $Q=20\text{m}^3/\text{h}$, head $H=10\text{m}$, rotational speed $n=1450\text{rpm}$, inlet diameter $D_i=75\text{mm}$. And the main structural parameters of the impeller are blade number $Z=5$, impeller inlet diameter $D_1=75\text{mm}$, impeller outlet diameter $D_2=185\text{mm}$, blade inlet angle $\beta_1=29^\circ$, blade outlet angle $\beta_2=40^\circ$, wrap angle of blade $\varphi=120^\circ$, and outlet width $b_2=10\text{mm}$. The three-dimensional model of the original impeller was generated, as shown in Fig. 1. The full computational domain was discretized by polyhedron mesh. Also, to obtain an appropriate
resolution of the near-wall area, five prism layers are required to create all nearby walls to enhance the flow solution's accuracy. A necessary mesh dependency test of the pump head was done, as shown in Table 1. Considering a large amount of calculation of the CFD-DEM coupling method, a relatively small number of grids is essential for computational efficiency during the consequent simulations. Therefore, the grid number was finally 534,664.

2.2. CFD-DEM coupling
The particle modeling by DEM is based on each particle. The liquid flow by CFD is based on every cell [12]. The two-way coupling is adopted in this study. Firstly, the CFD simulation method is used to analyze the transient flow, and then the flow solving process is repeated during an assumed time step until convergence. Subsequently, the DEM solving process begins from a grid cells' transient flow conditions containing specific particles and calculates the instantaneous drag force on each DEM particle. DEM continuously determine the particles' instantaneous position, velocity, and forces, then update and transfer them to the CFD solver. For this reason, considering the volume fraction of solid particles in CFD grid cells, a momentum source is introduced into each grid cell to represent the energy transfer of every single DEM particle [11].

2.3. Particle model
The density of crystal particles (sodium sulfate) is 2680kg/m³. According to Liu’s research [9], the number of medium-sized particles accounted for the most during the process of crystallization in the centrifugal pump. So the particles were selected in diameter of 82.5μm, referring to the result of the Phase-Doppler Particle Analyzer (PDPA). The particle volume fraction at the pump inlet was 4.5×10⁻⁴. During particles collide with each other or the walls, their momentum and energy will exchange. So this particle-particle and particle-wall interaction require a DEM interaction model to describe. This model uses the Hertz-Mindlin contact model [13] and the linear cohesion model [14] to solve the particle
Contact force characterized by the soft-sphere model [15]. To be specific, the Hertz-Mindlin contact model is a standard model describing particle interactions with neighbor elements. The linear cohesion model facilitates the simulation of inter-molecular attraction forces between particle surfaces, which are proportional to adhesion energy density and contribute to the progress of smaller crystal particles aggregating into bigger ones or bigger particles breaking into smaller ones. Remarkably, all the pump walls used in the experiments were made of unique material and possessed high surface accuracy, causing the crystal particles to not be absorbed on the inner walls. Given this, the simulation of behavior between particle and wall would not take the linear cohesion model. The collision configurations are concluded in Table 2.

2.4. Fluid model
Depended on the transient Reynolds number average Navier-Stokes (RANS) equation, the transient fluid phase flow was studied by a CFD tool. Moreover, for modeling the turbulence, a realized two-layer k-ε model with ‘high-y+ wall treatment’ were used. The ‘high-y+ wall treatment’ makes an assumption that the near-wall cells are located inside a boundary layer region. The flow is an isothermal incompressible sodium sulfate solution, $\mu=3.096\times10^{-3}$ Pa·s, $\rho=1356$ kg/m$^3$. The pump wall and particle surface are described as the non-slip wall, and the pump outlet is described as a p=1.0 bar pressure outlet. Besides, a constant profile is defined at the velocity-inlet. The pressure variations are monitored during the calculation at the pump inlet, as demonstrated in Fig 2.

| Collision                         | Particle-particle | Particle-wall |
|-----------------------------------|-------------------|---------------|
| Restitution coefficient           | 0.5               | 0.5           |
| Static friction coefficient       | 0.61              | 0.8           |
| Rolling friction coefficient      | 0.01              | 0.01          |
| Adhesion energy density/ (J/m$^3$)| $5\times10^4$     |               |

Figure 2. Variations of average pressure at the pump inlet.
3. Orthogonal design

The orthogonal test is an optimal method that uses orthogonal tables to organize and evaluate the multi-factor test. According to the impact of impeller geometrical configurations on the pump head and particle-blade collision, the blade outlet angle $\beta_2$ (A), blade inlet angle $\beta_1$ (B), wrap angle $\phi$ (C), and outlet width $b_2$ (D) were chosen as test factors, with three levels for each factor, as shown in Table 3. Based on the $L_9(3^4)$ table, nine schemes are formed with the corresponding results achieved by the CFD-DEM coupling method, as shown in Table 4.

Table 3. Level of orthogonal test factors.

| Level | A     | B     | C     | D     |
|-------|-------|-------|-------|-------|
| 1     | 25°   | 26°   | 110°  | 8     |
| 2     | 30°   | 29°   | 120°  | 10    |
| 3     | 40°   | 32°   | 130°  | 12    |

Table 4. Orthogonal test results.

| No. | A | B | C | D | Collision times | Pump head [m] |
|-----|---|---|---|---|-----------------|--------------|
| 1   | 1 | 1 | 1 | 1 | 148             | 10.03        |
| 2   | 1 | 2 | 2 | 2 | 162             | 9.16         |
| 3   | 1 | 3 | 3 | 3 | 170             | 11.31        |
| 4   | 2 | 1 | 2 | 3 | 187             | 11.30        |
| 5   | 2 | 2 | 3 | 1 | 174             | 10.21        |
| 6   | 2 | 3 | 1 | 2 | 200             | 10.93        |
| 7   | 3 | 1 | 3 | 2 | 344             | 11.24        |
| 8   | 3 | 2 | 1 | 3 | 310             | 11.94        |
| 9   | 3 | 3 | 2 | 1 | 305             | 10.41        |

Figure 3. Comparison between experimental head and simulation.
4. CFD-DEM simulation results and verification

4.1. Performance curves
The centrifugal pump's head and efficiency as a function of flow rate are shown in Fig. 3. Also, the pump test curves are added for comparison purposes. The curves obtained from numerical simulation follow the tendency of those corresponding to the experimental result with acceptable accuracy. However, the heads predicted by CFD-DEM simulation was greater for all conditions. This discrepancy could be due to the neglect of mechanical and volume losses caused by bearings and seals in the numerical simulation. Moreover, the head of the centrifugal pump was calculated through the flow simulation of single-phase without crystal particles. From this comparison between CFD-DEM coupling and CFD simulation, the liquid has little influence on the solid phase, as the pump head calculated by single-phase simulation was slightly higher than that by CFD-DEM simulation.

4.2. Particle-fluid interaction
Figure 4 (a) presents liquid relative velocity distribution in an impeller. It can be obtained that along the radial direction, the flow speed increases near the blade's pressure side and gradually decreases in the vicinity of the suction side. The liquid phase's relative velocity near the pressure side is smaller than the suction side due to the impeller's rotation. These conclusions of the fluid velocity field in this kind of two-phase flow are highly consistent with those in single-phase flow calculated by Yang et al. [8]. The preliminary analysis shows that the particle size is micron, which lightly affects the flow field.

Figure 4(b) presents the particle relative velocity distribution in the impeller. By Comparing Fig. 4(a) with Fig. 4(b), the observation that the velocity magnitude and distribution of solids at the middle region of the impeller are similar to that of liquid reveals the dominant influence on the crystal particles exerted by the liquid. However, at the impeller inlet and outlet, especially near the pressure side, there is a certain difference between liquid and particles. The liquid flows relatively faster than particles in the vicinity of the impeller inlet. In comparison, the solid phase moves more rapidly at the impeller outlet than the liquid. The analysis supports that particles' inertia impedes their acceleration from the fluid drag forces, causing their velocities to be smaller. However, due to the rise in an impeller passage, liquid velocity has a large drop. In contrast, due to the solid particles' inertia, particles maintain a higher speed. This result of interaction between the two phases is similar to the experimental one [6].

Figure 4. Relative velocity fields of liquid and particles in pump impeller.
Table 5. Range analysis of parameters on collision times.

|     | $\beta_2(A)$ | $\beta_1(B)$ | $\phi(C)$ | $b_2(D)$ |
|-----|--------------|--------------|------------|----------|
| $K_1$ | 480          | 679          | 658        | 627      |
| $K_2$ | 561          | 646          | 654        | 706      |
| $K_3$ | 959          | 675          | 688        | 667      |
| $k_1$ | 160          | 226.333      | 219.333    | 209      |
| $k_2$ | 187          | 215.333      | 218        | 235.333  |
| $k_3$ | 319.667      | 225          | 229.333    | 222.333  |
| $R$   | 159.667      | 11           | 11.333     | 26.333   |

Table 6. Range analysis of parameters on pump head.

|     | $\beta_2(A)$ | $\beta_1(B)$ | $\phi(C)$ | $b_2(D)$ |
|-----|--------------|--------------|------------|----------|
| $K_1$ | 30.5         | 32.57        | 32.90      | 30.65    |
| $K_2$ | 32.44        | 31.31        | 30.87      | 31.33    |
| $K_3$ | 33.59        | 32.65        | 32.76      | 34.55    |
| $k_1$ | 10.167       | 10.857       | 10.967     | 10.217   |
| $k_2$ | 10.813       | 10.437       | 10.290     | 10.443   |
| $k_3$ | 11.197       | 10.883       | 10.920     | 11.517   |
| $R$   | 1.030        | 0.446        | 0.677      | 1.300    |

5. Optimization design and simulation analysis

5.1. Range Analysis

The analysis results for collision times between particle and blade wall are shown in Table 5. $K_i$ represents the sum of factor values under level $i$; $k_i$ represents the mean value of $K_i$, and $R$ represents the range of $k_i$. Based on the $R$ values, it is observed that the order of the impact of each parameter on the collision times is $A>D>C>B$. So the most critical factor affecting collision times is blade outlet angle, while the second is outlet width. Therefore, the most favorable sequence of main parameters to reduce collision times is $A_1B_2C_2D_1$. On the other hand, the range analysis of Table 6 shows that the order of parameters affecting the pump head is $D>A>C>B$. The most favorable sequence of parameters to keep a higher pump head is $A_3B_3C_1D_3$.

The purpose of this orthogonal design is to reduce the collision times between crystal particles and blades as many as possible, so as to reduce the probability of particles adhering to the surface of blades. Therefore, ensuring pump sufficient pump head, the final optimal parameters can be determined are $A_1B_2C_1D_1$, namely $\beta_2=25^\circ$, $\beta_1=29^\circ$, $\phi=110^\circ$, and $b_2=8mm$.

5.2. Optimal results

The flow fields in the optimal impeller were obtained by the CFD-DEM coupling method. The pump head calculated by the numerical method is 10.14m, which meets the head design. Meanwhile, the number of particle-blade collisions within a unit time step is 138, less than any of the nine test schemes. Figure 5 presents the particle-blade contact force distribution of the optimal impeller (Fig. 5(a)) and the original one (Fig. 5(b)). By comparison, the optimal impeller model could significantly reduce collisions between particles and blades so that the probability of the crystal particles adhering to the impeller can be declined. Moreover, the collisions between particles and blades at the inlet edge are still severe, and the contact force is more significant compared with contact force on the pressure side of blade, which indicates that this phenomenon is a universal law of crystal particles in centrifugal pumps.
According to the similarity between liquid and particle flow fields, the law that the movement of particles is mainly subject to the liquid phase still holds. In the original impeller (refer to Fig. 4(a)), the boundary layer creates a low-speed region near the blade pressure side. As a result, the velocities of particles get a decline with the consequent drag force getting smaller, leading to increasing collisions between particles and blades (Fig. 5(b)). However, in the optimal impeller (see Fig. 6(a)), the low-speed region has been significantly reduced. This change allows the particles to flow more smoothly through the impeller passage, reducing the number of collisions (Fig. 5(a)).

6. Conclusions
According to the four factors and three levels mentioned, the $L_9(3^4)$ orthogonal array has been designed. The CFD-DEM coupling method is utilized to predict inner flow in the pump with crystal particles. The best program for the least collision between parties and blades was obtained. Under the design condition, the number of collisions experienced a dramatic decrease, and the optimal head still meets the requirement. The low-speed flow areas near pressure sides of the blades in the optimal impeller have been reduced. Thus, the optimization has declined the probability of the crystal particles adhering to the impeller, and the final optimal impeller accomplished better pump performance.
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