Optimization of structure parameters in a coal pyrolysis filtration system based on CFD and quadratic regression orthogonal combination and a genetic algorithm

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ABSTRACT
An optimization method of structure parameters based on the quadratic regression orthogonal combination (QROC) and Genetic Algorithm (GA) is proposed in this work. The following work has been conducted to improve the performance of the coal pyrolysis filtration system and prolong the service life of the filter tubes based on QROC-GA method. Firstly, a simulation model is established and two factors always are chosen as optimization objectives. Then one single factor regression prediction algorithm is used to optimize each factor separately while the result was not satisfactory. Secondly, QROC is introduced to achieve the optimization of two factors in the filtration system. The regression relationship is obtained proved to be effective by statistical test and back propagation neural network (BPNN). Finally, a QROC-GA method is established to find the optimization points. Then a verification calculation is done with CFD again. The optimal result has the parameters that $\phi = 40^\circ$ and $\psi = 25^\circ$. From the simulation results, the mean square error is 0.401. The mean square error is 0.4992 by the QROC-GA results. The errors are within 0.1 between CFD and QROC-GA. The QROC-GA model has a good effect in the prediction of models under changing parameters, and the significance is also confirmed.

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1. Introduction
In recent years, environmental pollution has been getting worse due to the burning of fossil fuels (Ardabili et al., 2018), while the rational use of energy will greatly promote economic development and environmental protection (Lu et al., 2017). Coal, as the primal energy fuel, has an important role in the areas of electricity, heating and transportation (Xiong, 2006). Coal pyrolysis is a process of multi-stage transformation using the composition and structural characteristics of coal to replace oil and gas resources (Qu et al., 2010). In the process of coal pyrolysis, the pyrolysis gas is doped with particulate coal owing to combustion insufficiently. The filtration system is part of the coal pyrolysis process, and its main function is to filter out coal particles and to collect the coal pyrolysis gas. Coal particles can be recycled effectively by the filtration system (Liu et al., 2018). The filtration system is a complex structural system with a disordered flow field distribution. The filter tubes are easily blocked, which leads to shortened service life of the equipment and increased production costs. The accident rate and production costs can be reduced to a certain extent through the analysis and optimization of the internal flow field distribution (Amgad, 2020). So, the filtration efficiency must be considered. A uniform flow field distribution in the filtration system plays a crucial role in improving the efficiency (Yan et al., 2013). For this purpose, much work has been carried out based on parameter design optimization, computational fluid dynamics (CFD) methods, quadratic regression orthogonal combination (QROC) and intelligent algorithms in this article.

Some studies have used CFD to calculate filtration systems in different fields, and simulation results are in good agreement with experimental results. With the development of CFD, some intelligence algorithms have been used to obtain some hidden laws for corresponding theoretical research. Hoch et al. (2020) have studied the Euler–Lagrange model in CFD for the complex three-dimensional fiber structure of filter media. The simulation data were compared with the experimental data, verifying that the CFD calculation results were in good agreement with the experimental results. Azarafza et al. (2020) used the CFD method to simulate the filtration process of an engine. The error...
between the simulation results and the experimental results was less than 15%. It is effective to simulate the filtration process by the CFD method. Li et al. (2019) and Amgad (2018) have also proved the reliability of the CFD method for modeling filtration systems with consistency of the results between simulation calculation and experiment operation. Safikhani et al. (2011a) have studied pressure drop and cut-diameter. Their optimization function was obtained based on an artificial neural network. Elsayed and Lacor (2010) have studied the Muschelknautz method to optimize separator geometrical ratios. Kashani et al. (2018) have studied the separator using multi-gene genetic programming to obtain two efficiency equations that can optimize the preheater performance of a cyclone. Many intelligent methods have also been employed to good effect, such as convolutional neural networks (Chen, Liu, et al., 2020) and genetic algorithms (Ghalandari et al., 2019).

Some studies have used QROC design to analyze filtration systems in different fields. Hu et al. (2020) have used the QROC method to obtain an optimization scheme for the parallel seam welding processing parameters of a microcrystalline resonator. Gao et al. (2020) have used QROC design to analyze the effects of family origin and collection date on embryogenic callus retention and cell proliferation. The results show that the effect is significant. Qiang et al. (2020) have used the QROC method to study the effect of biochar on the yield of biogas. The results show that the regression equation model has a very significant variance result.

In addition, some other studies have been carried out. According to the analysis of parameters, changing three parameters has a great influence on the uniformity of the flow field in a coal pyrolysis heat exchanger (Bo et al., 2019). Chia and Shu (2011) have optimized the component parameters of a gas inlet, which achieved a more uniform distribution of gas velocity. Yildiz (2011) has studied the structural diameters and lengths of filter elements. The data were obtained from the analysis of variance using a second-order polynomial equation. It was proved that the separation efficiency was improved. The study of Zhan et al. (2018) has found that the superficial gas velocity, thickness of the granular layer and dust mass concentration parameters have a significant influence on the collection efficiency and pressure drop. Yu et al. (2018) have indicated that an increase in bed height and a decrease in granule size are beneficial for improving filtration efficiency. In the work of Sulaymon and Mustafa (2012), it has been revealed that the effect of deposition is an important factor, which should be taken seriously regarding the filtration rate. Paenpong et al. (2013) have proved that production efficiency was improved by increasing the size of filter media, mass flow rate and the number of filtration stages. It was found that geometric parameters are important variables affecting the internal flow characteristics and filtration efficiency. However, these works mainly focus on one part of the whole system and the results always deviate obviously from the actual situation. The research mentioned above mainly focuses on a single factor at a time and neglects correlation between factors. The present work not only studies the influence of a single factor on the uniformity of a filtration system, but also studies the influence of the correlation of multiple factors. The correlation between parameters cannot be ignored when studying filtration systems.

In this study, in order to obtain an effective method for the analysis and optimization of a coal pyrolysis filtration system, and to overcome the defects mentioned above, the following work was studied and completed. In Section 2, a simulation model is established to optimize the flow field in a filtration system with real equipment in a domestic enterprise. Two factors are chosen as optimization objectives. In Section 3, one single-factor regression prediction is used to optimize the factors and verify the influence on the flow field distribution. However, analysis based only on a single factor cannot achieve a reliable optimization result, and may even result in a worse performance. In Section 4, QROC is used to realize a joint optimization in filtration based on CFD; an two-factor quadratic regression prediction equation is obtained. Twenty-five models are compared with predicted results for a back propagation neural network (BPNN). It is used to verify the reliability and accuracy of calculation and simulation. The final optimal result is obtained based on the QROC-GA. Meanwhile, its authenticity and correctness are verified by the CFD again with the optimization factor. Finally, the main conclusions are summarized and discussed in Section 5.

2. Modeling approach
2.1. Computational model

In this study, the motion of an internal flow field in a filtration system is calculated and analyzed. The flow state is always determined by the Reynolds number according to the structural characteristics of the filtration system. The Reynolds number is expressed by Equation (1) (Kovacs, 1981):

\[
Re = \frac{\rho u d_k}{\mu}
\]

where \(\mu\) is the kinematic viscosity of the flow; \(\rho\) is the fluid density of the flow; \(d_k\) is the diameter of the characteristic length; \(u\) is the fluid velocity, which is defined as
$u = q/A; q$ is the flow rate; and $A$ is the cross section of the tube, defined as $A = \pi (d_k/2)^2$. In ordinary conditions, the flow is always laminar when the Reynolds number is less than 2000, with turbulent flow for Reynolds numbers larger than 4000 (Jin et al., 2013). In this article, the porous flow model is used in the filter tubes regions of the filtration system, the other parts of the filtration system are free flowing using the turbulence model. The standard $k$–$\varepsilon$ equation is used in the turbulence model (Chen, Liang, et al., 2020; Slack et al., 2000). The air phase is generally used to measure the dissipation rating; $u_i$ is the velocity component along $x$, $y$- and $z$-axes; $G_k$ and $G_b$ mean the velocity gradient and buoyancy, respectively; $Y_M$ is the contribution to the turbulent pulsating pressure expansion; $C_{1\varepsilon} = 1.44$, $C_{2\varepsilon} = 1.92$ and $C_{3\varepsilon} = 1$ are empirical constants; $\sigma_k$ and $\sigma_\varepsilon$ are Prandtl numbers, and we have $\sigma_k = 1.3$ and $\sigma_\varepsilon = 1.0$ (Drainy et al., 2009).

In this article, the porous flow model shares the same continuity and momentum equations with the turbulent flow model except that the velocity in the porous flow model is the superficial velocity. The superficial velocity is defined as

$$u_{\text{super}} = u \otimes \varepsilon$$

where $\varepsilon$ is the porosity. The pressure is discontinuous at the interface between porous flow and the turbulent flow domains according to the porous velocity formulation. The porous flow is modeled by the momentum source term in ANSYS® Fluent®. Darcy’s law is used to describe the relationship between flow rate and pressure drop at low flow rate in porous media. The expression is as follows:

$$\frac{\Delta p}{L} = \frac{Q}{\alpha A}$$

where the $Q$ is the flow rate; $A$ is the cross-sectional area of the filter tubes, and $\alpha$ is the permeability.

For porous media with a high flow rate, the flow rate and pressure drop relationship is expressed by the Forchheimer equation:

$$-\frac{\Delta p}{L} = \frac{\mu}{\alpha} u + \frac{1}{2} C_2 \rho u^2$$

where $\alpha$ is the permeability; $C_2$ is the inertial resistance factor; $\mu u_i/\alpha$ is the viscous loss term; and $C_2 \mu u^2$ is an inertial loss term (Ambreen et al., 2020). The equation can be simplified to the Darcy equation without the quadratic term on the right-hand side of Equation (9).

For the first term of the equation, $\alpha$ changes significantly with different geometric shapes, which has a great influence on the interior flow. Darcy’s law is generally used to measure $\alpha$. According to Kozeny theory (Kozeny, 1927), the $\varepsilon$ of porous media is related to $\alpha$. The expression is as follows:

$$a = \frac{d_k^2 \varepsilon^3}{150(1 - \varepsilon)^2}$$

The best empirical correlation between $\alpha$ and $C_2$ can be yielded as (Zhou et al., 2019)

$$C_2 = c_1 \alpha^{c_2}$$
The $c_1$ and $c_2$ are empirical constants. Zhou et al. (2019) have obtained the empirical values of $c_1$ and $c_2$.

$$C_2 = 10^{10} a^{-(3/2)}$$ (12)

The Equation (10) is imported into Equation (12), the $C_2$ can be calculated by

$$C_2 = 10^{10} \left( \frac{d^2 e^{9/2}}{150^{3/2}(1 - \varepsilon)^3} \right)$$ (13)

The Darcy friction factor is $64/Re$ in fully developed laminar flow in a circular tube (Cheng & Todreas, 1986). The porous flow parameters for laminar flows can be obtained as $1/\alpha = 32/(\varepsilon D^2)$ and $C_2 = 0$ (Wang et al., 2021). In this study, we propose using Equations (10) and (13) for turbulent flow; a series values of $c_1$ and $c_2$ were tested until the values were appropriate for turbulent flow. The parameter values for $C_2$ and $\alpha$ are recorded in Table 2.

In the filter tube area of the filtration system, the flow direction from the turbulent flow area to the porous flow area is in the $x$- and $z$-directions. Therefore, the permeability and inertial drag coefficient aren’t needed in the $y$-direction. The permeability in the $y$-direction can be assumed to be infinitely small to prevent unphysical fluid longitudinal flow. The permeability along the $x$- and $z$-directions is assumed to be 1000 times that in the $y$-direction to avoid convergence difficulties.

### 2.2. Simulation model

The filtration system consists of: an upper chamber, six venturis, and a lower chamber including 288 filter tubes. The diameters of both inlet and outside are 400 mm. The structure and size of the filtration system is shown in Figure 1. The angle between the centerlines of the inlet and the horizontal direction is $45^\circ$. The gas is inserted from the inlet to the lower chamber. The size of the chamber is: $l_{\text{length}} = 3230$ mm; $W_{\text{width}} = 2210$ mm; and $H_{\text{height}} = 8250$ mm. The flow velocity of the gas at the inlet will decreased seriously due to the expansion volume of the upper chamber (Liu et al., 2018). Additionally, the length of the filter tubes is 1820 mm and the height of the upper chamber is 3250 mm. The model, in accordance with a real coal pyrolysis filtration system, is shown in Figure 1.

The backflush port is shown in the Figure 1(a). Gas at high pressure is injected into the backflush port. The function of the backflush port is to remove particles that had been adsorbed on the filter tubes, so as not to affect the secondary use of the filter tubes. In this article, the flow field uniformity of the filter tubes in the filtration system is analyzed to get the optimal structure design scheme. The backwash process is simplified to reduce the influence factors. Therefore, the backflush port is set as the wall surface. Media porosity has a great influence on the filtration system flow (Pashchenko, 2019).

The fluid domain of the filtration system was meshed with GAMBIT®. The number of grids can be calculated.
according to the interval size, which represents the size of the spacing between grids. A smaller value of interval size means a bigger number of grids. In order to get a reliable result, four models with different interval sizes were calculated to know whether there was an obvious influence on the CFD results due to mesh numbers.

In Table 1, the results of four models (called Models 1–4) are recorded. It can be seen clearly that the mean square error varies within only 4.5% from Model 1 to Model 4 when the number of models is increased. Since the calculation will not be affected obviously by the number of grids, a smaller number should be a better choice in this work, having a higher computational efficiency and lower computational cost.

However, the calculation accuracy is always higher with a larger number of the grids, and more complex and important flow fields should have more meshes, up to a certain maximum number. Taking into account the above, the total grid number of Model 1 was taken to be 20,1526 meshes with an inlet angle of 45° and a baffle angle of 25.4°. Some adjustments were also made: the interval size in the filter tubes fluid domain was reduced to 20 mm and the meshes were enhanced. Since both the upper cavity and the inferior cavity have simpler structures compared to the filter tubes, the interval size was set to 30 and 50 mm, respectively.

The boundary parameter settings are shown in Table 2. The reference temperature was the room temperature, and the turbine kinetic energy and turbine dispersion rate were set from Fluent. In this article, the porosity of the filter tubes was assumed to be 0.5. The porous medium thickness was set to 5 mm. The turbulence model was also adopted and compounded with a porous media model based on a continuous pressure solver. The viscous resistance and the inertial resistance were calculated with Equations (10) and (13).

After the fluid domain was meshed with GAMBIT, the velocity uniformity of the filter tubes in the filtration system was calculated with CFD in the ANSYS environment. The fluid flow in Fluent accords with the conservation of mass and energy. ANSYS is industry-leading fluid simulation software known for its advanced physics modeling capabilities and industry leading accuracy. It is not only widely used to solve the Navier–Stokes equations, but also problems in fluid flow (John et al., 1985). The finite volume method was used to make a spatial discretization in all fluid domains of the filtration system. The computational domain was divided into a series of non-repetitive control bodies, with a control body around each grid point. The differential equations to be solved could be integrated for each control volume. Thus, discrete equations were obtained and the corresponding parameters recorded in Table 3.

### 3. Experiments based on one factor design

In order to study the influence of the baffle angle ($\psi$) factor on the uniformity of the flow field in the filtration system, baffles were always added to the original structure model. The inlet angle ($\psi$) was changed. Comparative experimental cases were carried out. Figure 2 shows that the models with baffles had a longer rotation time and longer path in the lower cavity trace of the filter system than those of models with no baffle. The main function of the filtration system is to filter coal particles. The long path of the flow field is conducive to the deposition of particles. So baffles have a greater impact on the flow field of the filtration system. Table 4 shows the mean square deviations of the velocity values of five slices in the Z-direction in the filtration system. The slice positions of five slices are shown in Figure 3. The Z-positions were as follows: $Z_1 = 0.255$ m was recorded as slice 1; $Z_2 = 0.657$ m was recorded as slice 2; $Z_3 = 1.150$ m was recorded as slice 3; $Z_4 = 1.515$ m was recorded as slice 4; and $Z_5 = 1.725$ m was recorded as slice 5.

It can be seen from Table 4 that the mean square deviation value of each slice in the models with baffles is less than that of the models without baffles. So the baffle is one of the main factors affecting the flow field of the filtration system.

Figure 4 shows that the air flow field is mainly in the lower chamber of the filtration system with the 45° inlet angle. However, the gas flow field mainly rushes to the

### Table 1. The analysis of grid independence.

| Computational grid | Mesh 1 | Mesh 2 | Mesh 3 | Mesh 4 |
|--------------------|-------|-------|-------|-------|
| Number of grids    | 201,526 | 205,561 | 208,533 | 215,837 |
| Mean square error  | 0.3592 | 0.3560 | 0.3556 | 0.3429 |

### Table 2. Parameters of multiphase flow and porous area.

| Parameter                                | Value    |
|------------------------------------------|----------|
| Inlet pressure (Pa)                      | 100,325  |
| Outlet pressure (Pa)                     | 98,325   |
| Reference temperature (K)                | 298.15   |
| Turbulent kinetic energy (m$^2$/s$^2$)   | 1        |
| Turbulent dissipation rate (m$^3$/s$^3$) | 1        |
| Porous permeability (-)                  | 0.5      |
| Viscous resistance (m$^{-1}$)            | 3.00e+06 |
| Inertial resistance (m$^{-2}$)           | 5.77     |
| Porous medium thickness (mm)             | 5        |

### Table 3. Parameters in spatial discretization.

| Gradient pressure | Least squares cell based standard |
|-------------------|----------------------------------|
| Momentum          | Second order upwind              |
| Turbulent kinetic energy (m$^2$/s) | First order upwind              |
| Turbulent dissipation rate (m$^3$/s$^3$) | First order upwind              |
opposite chamber wall when the inlet angle is 0°, so the size of the inlet angle is another factor affecting the flow field distribution of the filtration system.

### 3.1. The selection of parameters to be optimized

In order to get close to the actual situation, the model of a coal pyrolysis filtration system based on real equipment in a domestic enterprise was established to optimize its flow field. Since it is hard to perform calculations on a large number of models with very small parameter changes by the CFD method, we selected a few groups of parameters with equal intervals to obtain a relatively better result based on the quadratic regression orthogonal combination method, and then made a further optimization with GA. In order to complete the above work, a reasonable selection of parameters in cases A and B was very important.

The inlet angle was 45° in the original design and a similar value was always used in actuality, so the parameter range studied was around 45°, and case B3 was set to 45° as a middle scheme. From the structure of the filtration system, it can be seen that the inlet angle cannot be 90°, otherwise air will be blown to the bottom directly and the system will lose its function of gas filtration. Meanwhile, an inlet angle of 0° should also be avoided in engineering because the filter tubes will face many more particles from the impaction directly from the inlet – this can be seen in Figure 4(b) – tubes have to work under a harsh situation where particles will spread around the whole area inside. According the analyses above, both 0° and 90° should be avoided, therefore we take parameters around 45° with the same interval value of 5° here.

In this study of baffle angles, it can be found that the baffle is one of the main factors affecting and improving the flow field in the filtration system. Similar to the inlet angle, proper values of baffle angles should also be away from 0° since baffles would not be effective in this condition. Additionally, once the baffle angle is too large, the air flow find it difficult to pass through the space on the left, as shown in Figure 5, and its value should be an acute angle and far from 90°. Therefore, angles 25° to 35° were taken as cases A1–A4.

### 3.2. The influencing factor design of the baffles

The scheme for baffle design optimization is listed in Figure 5. There were five baffle scheme cases. The baffle sizes were: \( h_{\text{height}} = 300 \text{ mm} \); \( t_{\text{thickness}} = 10 \text{ mm} \). The distances between adjacent baffles were 510 mm. The position of the bottom end of the first baffle was marked as point O. The horizontal distance OA was 2090 mm. The vertical distance between point A and point B was 1000 mm (\( l_{AB} \)). The angle between OA and OB was 25°. This model was called case A1. The vertical distance from
point B to point C was 160 mm ($l_{BC}$). The angle between OA and OC was 29°. The bottom ends of all the baffles in case 1 were extended to the position of the line OC. This design model was called case A2. Similarly, the vertical distance from point C to point D was 1160 mm ($l_{CD}$). The angle between lines OA and OD was 32°. This model was called case A3. The angle between lines OA and OE was 35°. This model was called case A4. All cases are recorded in Table 5.

The data were obtained in the directions of the $Y$- and $Z$-axes. The $Y$-positions are shown in Figures 3 and 6. The three $Y$-positions are as follows: $Y_1 = 8.05$ m; $Y_2 = 7.25$ m; and $Y_3 = 6.6$ m.

The 20 velocity values were selected at each section for further calculation. The fluctuation of the flow field was represented by the mean square deviation ($y$) as in Equation (14), where $a_i$ is the variable, $\gamma$ is the overall mean value, and $N$ is the total amount of data:

$$y = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (a_i - \gamma)^2} \quad (14)$$

Numerical analysis was carried out to obtain the mean square deviation of the velocity. The $x$-axis in Figure 7 is the $Z$-direction in the filtration system, and the following rules were found from Figure 7. First, as to the $Y$-sections, the $y$-value of the velocity fluctuated more seriously in slices 1, 2, 4 and 5 than the $y$-value in slice 3. In the $Y_3$ position, the fluctuation value of $y$ was least in the four cases in $Z$-positions other than those of the positions $Y_1$ and $Y_2$. The value of $y$ was about 0.5. The $y$-value of case A4 was always more stable than the other cases according to Figures 7(a)–7(c). Therefore, case 4 seemed to be the optimal design scheme for this part. Secondly, as to the $Z$-sections, there was a symmetrical distribution. Slice 3 is along the centerline and out of the filter tubes; its structure is much simpler than those of the other sections and there is no filter tube area in $Z_3$. The velocity flow field was not affected by the viscous resistance or inertial resistance in slice 3. Thus, it always had the lowest mean square deviation. The other four sections were all across the filter tubes area, slices 2 and 4 always fluctuated more obviously since they were in the asymmetrical part of the tubes. Thus, the distribution was non-uniform. While $Z_1$ and $Z_5$ were much more uniform than $Z_2$ and $Z_4$, this may be caused by the fact that they were across the filters in the middle. From these two groups, it can be seen that it was more uniform in the central part of filter tubes.

In order to analyze the influence of a single factor for the experimental design, a single-factor partial regression model was obtained by fixing other factors. We define the baffle angle $\varphi$ and the inlet angle $\psi$ as factors of the partial regression model. The single-factor partial regression model of $\varphi$ is shown in Figure 8, where $\bar{Y}$ means the mean value of $y$ from $Y_1$ to $Y_3$.

The result shows that the best value of $y$ is 0.475 in the filter tubes area with $\varphi = 35^\circ$. The regression coefficient of $\varphi$ is 0.4121, thus $\varphi$ has a significant influence on the flow field of the filtration system. The mean square deviation of case A4 is smaller than those of the other cases.

![Figure 5. Optimization of baffle design.](image1)

![Figure 6. Position of $Y$.](image2)

**Table 5.** Experimental design of the baffles.

| Cases | Angle $\psi$ (°) | Length (mm) |
|-------|-----------------|-------------|
| A1    | 25              | 1000        |
| A2    | 29              | 1160        |
| A3    | 32              | 1320        |
| A4    | 35              | 1480        |
Figure 7. Mean square deviations of angle $\psi$: (a) $Y_1 = 8.05$ m; (b) $Y_2 = 7.25$ m; (c) $Y_3 = 6.6$ m.

Figure 8. Function diagram of angle $\psi$.

3.3. The influencing factor design of the air inlet angle

The angle of the air inlet ($\psi$) has a big influence on the flow distribution in the filtration system, thus it is important to choose an appropriate value. The factor $\psi$ is increased or decreased by 5° without changing $\varphi$. The cases are listed in Table 6. Figure 9 is the air inlet angle diagram.

The total $y$-values of $Y_1$ to $Y_3$ in five Z-sections are shown together in Figure 10. Figure 11 shows the single-factor partial regression model of $\psi$; $y$ is the mean value of the mean square deviations of velocities in all the Z-sections in here. Figure 10 shows that the $y$-value fluctuation in cases B1, B3 and B5 was smaller than in cases B2 and B4, which shows gentle fluctuations in the Z-direction. From Figure 11, it is known that the regression coefficient of $\varphi$ is 0.5778. The trend in $y$-values was increasing at first, and then decreasing. The optimal case was B1 with $\psi = 35^\circ$ in that part. The optimal $y$-value was 0.356 when $\psi = 0.356$. So $\varphi$ had a great influence on the uniformity of the flow field.

Table 6. Experimental design of the air inlet angle.

| B cases | Angle $\psi$ (°) |
|---------|------------------|
| B1      | 35               |
| B2      | 40               |
| B3      | 45               |
| B4      | 50               |
| B5      | 55               |

Figure 9. Diagram of air inlet angle.

Figure 10. Mean square deviation of angle $\psi$. 
3.4. Combination calculation of single-factor design

The two groups of single-factor designs of $\psi$ and $\phi$ had the optimal angles $\psi = 35^\circ$ and $\phi = 35^\circ$ according to Sections 3.2 and 3.3. Therefore, a new model was established with $\psi = 35^\circ$ and $\phi = 35^\circ$ combined with cases A4 and B1 based on single-factor design, and a CFD model was also established to prove its advance.

However, the result was poor with $y = 0.571$, worse than $y = 0.475$ in case A4 and $y = 0.356$ in case B1. These poor values mean that the flow field was more disordered in the whole filter tube area. Therefore, it was ineffective to optimize the flow field by only a single-factor partial regression model since the parameters in a coal pyrolysis filtration system always have complex correlations. To solve this problem, a quadratic regression orthogonal combination model with a genetic algorithm (QROC-GA) is given in Section 4.

4. Experiments based on the quadratic regression orthogonal combination

In this section, the optimal solution is found and the flow chart could be described as shown in Figure 12. In Section 4.1, nine models were used to establish a model based on QROC in a given range. The prediction equation was obtained as in Equation (16) and then two kinds of validation method were used to keep the effectiveness of result. First, a significance regression test was used to keep the relationship significant in Section 4.2. Secondly, 27 CFD models were calculated to make sure that the regression result was near the result of the CFD method. Each model was established to obtain a $y$-value. The boundary condition settings and mesh sizes were nearly the same. The selected positions of all data were consistent. Additionally, a BPNN model was also introduced to make a regression comparable with QROC.

4.1. The experimental design

In order to get a better effect of gas purification with specific $\psi$ and $\phi$, the QROC method was used to realize the analysis and optimize the structural design of the filtration system. QROC design is a scientific optimization method for dealing with multi-factor experiments. The parameters are optimized with a limited number of tests based on probability theory and mathematical statistics. The influence of multiple factors is analyzed together and then a quantitative model is established from complex interacting conditions by QROC.

Compared with the all-level factor method, QROC has the advantages of fewer test times and enough residual degrees of freedom. Once the design result of the orthogonal regression has no significance, more experiments can be done at the ‘asterisk point’ (see below) and the center point based on the orthogonal regression test. The quadratic polynomial regression equation model is expressed as Equation (15) (Cha & Kang, 2018):

$$\hat{y} = b_0 + \sum_{j=1}^{F} b_j x_j + \sum_{i<j} \sum_{j=1}^{F} b_{ij} x_i x_j + \sum_{j=1}^{F} b_{jj} x_j^2$$  (15)

where $b_0$, $b_j$, $b_{ij}$, $b_{jj}$ represents the regression coefficients; $F$ is the number of factors; $x_i$ and $x_j$ are the factor variables; and $\hat{y}$ means the test result.

The design of the quadratic regression experiment consists of factor points, coordinate axis points and center points. Figure 13 shows the combination distribution of the characteristic points, where the factor point is called the corner point and its value is 1 or $-1$. The coordinate axis point is called the asterisk point. The distance
between the coordinate origin and the asterisk point is \( r \), which is also called the axis arm. These values are determined according to the requirements of orthogonal or rotary experimental design. There are nine test points related to two selected variables in this study.

According to the characteristics of rotation and non-degradation, the experimental processing formulas are designed as Equation (16):

\[
\begin{align*}
N &= m_c + 2F + m_0 \\
m_c &= \frac{2^{F-a}}{2} \\
r &= 2^{(F-a)/4} \\
(m_c + 2r^2)^2 - Nm_c &= 0
\end{align*}
\]

where \( N \) means the total number of points in the experiment; \( m_c \) is the number of test points in all-factor test at two-levels; \( a \) represents the degree of test implementation – \( a = 0 \) means full implementation, \( a = 1 \) means half of full implementation, \( a = 2 \) means four quarters of full implementation; \( r \) is the distance between the asterisk point and the center point, the value is determined by the number of factors and the degree of implementation; \( 2F \) represents the number of asterisk points; \( m_0 \) represents the repetition number of the center test point.

In accordance with statistical principles, the structure matrix of the two variable combination is recorded in Table 7. The structure matrix of the QROC design is recorded in Table 8, and the factor level coding table is shown in Table 9 (Wang et al., 2017).

The test design scheme and calculation results are shown in Table 10. In accordance with the QROC design, the 27 groups of models are replaced by the 9 groups of experiments.

\[ \chi (x) = \frac{1}{1 + e^{-x}} \]  

To ensure the rationality of the regression equation, the BPNN was used to compare with the CFD model. The BP network is a powerful tool for establishing a mathematical model. The relationship between the input and the output of a system can be stored in the BP network by sample training (Song et al., 2020). Previous studies have shown that a three layer BP network can express arbitrary nonlinear mapping (Hagan et al., 2002).

Considering the quadratic polynomial regression equation as a system, then \( \psi^\circ \) and \( \varphi^\circ \), and \( y \) is the input and output of the system, respectively. To endow the network with the ability of nonlinear calculation, a sigmoid function is taken as the transfer function in this fitting mission as in Equation (17), where \( x \) means the input and then a value between 0 and 1 will be the output. A sigmoid function is always chosen in a BP net to achieve good symmetry:

\[ \chi (x) = \frac{1}{1 + e^{-x}} \]  

Table 7. Matrix structure of the quadratic combination.

| Case | \( X_0 \) | \( X_1 \) | \( X_2 \) | \( X_1' \) | \( X_2' \) |
|------|--------|--------|--------|--------|--------|
| 1    | 1      | 1      | 1      | 1      | 1      |
| 2    | 1      | 1      | -1     | -1     | 1      |
| 3    | 1      | -1     | 1      | -1     | 1      |
| 4    | 1      | -1     | -1     | 1      | 1      |
| 5    | 1      | \( r \) | 0      | 0      | \( r^2 \) |
| 6    | 1      | -\( r \)| 0      | 0      | \( r^2 \) |
| 7    | 1      | 0      | \( r \)| 0      | \( r^2 \) |
| 8    | 1      | 0      | -\( r \)| 0      | \( r^2 \) |
| 9    | 1      | 0      | 0      | 0      | 0      |

Table 8. Structure matrix of QROC.

| Case | \( X_0 \) | \( X_1 \) | \( X_2 \) | \( X_1' \) | \( X_2' \) |
|------|--------|--------|--------|--------|--------|
| 1    | 1      | 1      | 1      | 1      | 1      |
| 2    | 1      | 1      | -1     | -1     | 1      |
| 3    | 1      | -1     | 1      | -1     | 1      |
| 4    | 1      | -1     | -1     | 1      | 1      |
| 5    | 1      | \( r \) | 0      | 0      | \( r^2 \) |
| 6    | 1      | -\( r \)| 0      | 0      | \( r^2 \) |
| 7    | 1      | 0      | \( r \)| 0      | \( r^2 \) |
| 8    | 1      | 0      | -\( r \)| 0      | \( r^2 \) |
| 9    | 1      | 0      | 0      | 0      | 0      |

Table 9. Coding values of factor level.

| \( X_0 \) | \( X_1' \) | \( X_2' \) |
|---------|---------|---------|
| Upper asterisk arm, \( r \) | 60 | 38 |
| Upper level, 1 | 52.5 | 34.75 |
| Zero level, 0 | 50 | 31.5 |
| Lower level, \( -1 \) | 47.5 | 28.25 |
| Lower asterisk arm, \( -r \) | 40 | 25 |

Table 10. Experimental and statistical results.

| Case | \( Z_1 \) | \( Z_2 \) | \( X_1' (\psi) \) | \( X_2' (\psi) \) | Mean square deviation (\( y \)) |
|------|-------|-------|--------|--------|-----------------|
| 1    | 1     | 1     | 52.5   | 34.75  | 0.6398          |
| 2    | 1     | -1    | 52.5   | 28.25  | 0.7521          |
| 3    | -1    | 1     | 47.5   | 34.75  | 0.6879          |
| 4    | -1    | -1    | 47.5   | 28.25  | 0.6572          |
| 5    | 1     | 0     | 60     | 31.5   | 0.8666          |
| 6    | -1    | 0     | 40     | 31.5   | 0.5112          |
| 7    | 0     | 1     | 50     | 38     | 0.5855          |
| 8    | 0     | -1    | 50     | 25     | 0.7317          |
| 9    | 0     | 0     | 50     | 31.5   | 0.7152          |
supplemented to compare with results predicted by the neural network. The result is recorded in Table 11 and the relative error is chosen to evaluate the deviation and accuracy. The relative error is used to evaluate the uniformity as in Equation (18). From Table 11, it can be seen that relative error ranges from 1.70% to 35.07%, and has an average value of 17.44%. Thus, it can be inferred that the CFD model has a certain accuracy and reliability, since a BPNN is always considered to be one of the most effective prediction models.

\[
error = \left| \frac{\hat{y}_{\text{CFD}} - \hat{y}_{\text{BPNet}}}{\hat{y}_{\text{CFD}}} \right| \times 100\% \tag{18}
\]

### 4.2. The significance test of regression

The regression coefficients are calculated as in Equation (19) and the quadratic polynomial regression prediction equation is obtained as in Equation (20):

\[
\begin{align*}
b_0 &= \frac{1}{N} \sum_{i=1}^{N} y_i \\
b_j &= \frac{1}{N} \sum_{i=1}^{N} x_{ij} y_i, \quad (i = 1, 2, \ldots, N, j = 1, 2, \ldots, p) \\
b_{kj} &= \frac{1}{N} \sum_{i=1}^{N} x_{ik} x_{ij} y_i, \quad k \neq j \\
b_{ij} &= \frac{1}{N} \sum_{i=1}^{N} x_{ij}^2 y_i, \quad (i = 1, 2, \ldots, N, j = 1, 2, \ldots, p)
\end{align*}
\tag{19}
\]

\[
\hat{y} = 0.001x_1^2 - 0.002x_2^2 + 0.034x_1 + 0.341x_2 - 0.004x_1 x_2 - 6.007 \tag{20}
\]

Then a test can be made based on the significance test value of variance by Equation (21):

\[
F_R = \frac{SSR/dfr}{SSR/dfr} \tag{21}
\]

where \(dfr\) is the number of degrees of freedom of regression; \(dfr\) is the number of degrees of freedom of the residual square; \(SSR\) means the sum of squares of residuals; and \(SS\) means the sum of squares of regression. Here \(F_R\) in the two factors regression equation is 0.9258. The regression relationship is significant when the value of \(F_R\) is bigger than \(F(dfr, dfr)\). Here the \(F(dfr, dfr)\) is 0.0029 under a significance level of 0.05, and \(F_R > F(dfr, dfr)\).

In summary, the results from the analysis of a single factor cannot be used to make a real design because of low regression coefficients and no obvious significances: \(F_{AA} = 0.475\) and \(F_{B1} = 0.3560.475\), while QROC has a high regression coefficient of \(F_R = 0.9258\). Therefore, the optimal result is available here. The factors can be predicted and selected for uniformity optimization in a flow field distribution.

### 4.3. Optimal structural design and verification

Since it is difficult to build a general model by CFD modeling, many advanced intelligence methods are widely used to obtain the relationships and laws hidden in the parameters. These methods always have a strong ability to optimize structure parameters. A genetic algorithm (GA) was also used here, in combination with QROC. The genetic algorithm is a computational model to simulate the natural selection and genetic mechanism of Darwinian biological evolution. It is a method of obtaining the optimal solution by simulating the natural evolution process (Safikhani et al., 2011b).

In this article, GA was used to find the optimal scheme for the filtration system and to obtain two parameters based on Equation (20), which is set as a fitness function. Then the result was also verified by the CFD method. The algorithm starts from an initial population that is generated randomly. Each set of the population is encoded with binary form and combined. The new fitness individuals are found by selection, crossover and mutation. Finally, the optimal population is evolved, which is the optimal solution of the problem (Fang et al., 2017). The flow chart used here is shown in Figure 14.

The constraints of the parameters \(\varphi\) and \(\psi\) were given from the model structure, i.e. [40, 60] and [25, 38].

### Table 11. Comparison based on CFD method.

| \(\psi^\ast\) | \(\varphi^\ast\) | Numerical simulation | BPNN | Relative error (%) | QROC | Relative error (%) |
|---|---|---|---|---|---|---|
| 40 | 25.4 | 0.555 | 0.400 | 27.88 | 0.282 | 49.12 |
| 40 | 28.9 | 0.441 | 0.404 | 8.42 | 0.49 | 1.09 |
| 40 | 32.1 | 0.445 | 0.478 | 7.52 | 0.576 | 29.43 |
| 40 | 35.1 | 0.574 | 0.472 | 17.76 | 0.646 | 12.58 |
| 40 | 37.9 | 0.535 | 0.383 | 28.45 | 0.679 | 26.83 |
| 45 | 25.4 | 0.395 | 0.533 | 35.07 | 0.451 | 14.26 |
| 45 | 28.9 | 0.487 | 0.584 | 19.76 | 0.550 | 12.98 |
| 45 | 32.1 | 0.519 | 0.650 | 25.36 | 0.597 | 15.07 |
| 45 | 35.1 | 0.556 | 0.655 | 17.70 | 0.601 | 8.10 |
| 45 | 37.9 | 0.575 | 0.420 | 26.91 | 0.572 | 0.48 |
| 50 | 25.4 | 0.795 | 0.712 | 10.47 | 0.666 | 13.71 |
| 50 | 28.9 | 0.767 | 0.736 | 3.98 | 0.708 | 7.61 |
| 50 | 32.1 | 0.629 | 0.709 | 12.80 | 0.664 | 8.87 |
| 50 | 35.1 | 0.660 | 0.671 | 1.70 | 0.623 | 5.52 |
| 50 | 37.9 | 0.618 | 0.588 | 4.84 | 0.532 | 13.91 |
| 55 | 25.4 | 0.900 | 0.844 | 6.28 | 0.988 | 9.71 |
| 55 | 28.9 | 0.920 | 0.730 | 20.64 | 0.933 | 1.41 |
| 55 | 32.1 | 0.829 | 0.577 | 30.36 | 0.838 | 1.12 |
| 55 | 35.1 | 0.636 | 0.707 | 11.20 | 0.711 | 11.79 |
| 55 | 37.9 | 0.545 | 0.698 | 28.12 | 0.559 | 2.52 |
| 60 | 25.4 | 1.049 | 0.961 | 8.40 | 1.355 | 29.18 |
| 60 | 28.9 | 0.838 | 0.926 | 10.59 | 1.224 | 46.09 |
| 60 | 32.1 | 0.796 | 0.880 | 10.49 | 1.059 | 32.94 |
| 60 | 35.1 | 0.863 | 0.999 | 15.71 | 0.865 | 0.230 |
| 60 | 37.9 | 0.702 | 1.022 | 45.61 | 0.651 | 7.16 |
| Average | 0.6651 | 0.670 | 17.44 | 0.713 | 14.76 |
The results of the optimal solution design scheme were calculated by writing the genetic algorithm program in MATLAB®. The optimal structure parameters $\phi = 40^\circ$ and $\psi = 25^\circ$ were obtained by the GA. The value of $y$ is 0.4992 for the optimal structure parameters, which were calculated based on Equation (20).

To make a validation directly, a new model was established with $\phi = 40^\circ$ and $\psi = 25^\circ$. The numerical simulation was finished with Fluent and the mean square deviation was 0.401. The error data for $y$ were within 0.1 between the results of numerical simulation and calculation. Thus, the method has been verified effectively to find the optimal solution.

4.4. Robustness of the QROC-GA method

Robustness means that the model can keep its characteristic behavior when it is disturbed or uncertain. QROC design is a scientific optimization method of dealing with multi-factor experiments. As the number of experiments increases, the robustness of the regression will certainly improve. However, CFD model results are always the same and there is no significance to be achieved by repeating them many times, whereas the QROC design will be stable in work of a similar kind to CFD, and so the $m_0$ is one in Equation (19). This is also the advantage of QROC based on a CFD model.

As for the GA, it will obtain a negative number near zero during calculation, since it is finding a global optimal result. A negative number has no significance in optimization and should be avoided. In order to improve the robustness, a constant correction value is added to Equation (20). This constant value can be set as a very small positive number (0.001 here by experience), and thus a negative number between 0.001 and zero can be avoided. The correction prevents the QROC-GA giving a result of no significance to some degree.

5. Conclusions

In order to optimize the flow field distribution in the filtration system, this study mainly focused on the key factors, through structural design, to obtain the optimal design scheme. After a series of related research to solve this work, a QROC-GA method was proposed here and solved the problem effectively. This work could be also used for other similar multi-parameter optimization where many models based on CFD need to be calculated, especially for complex fluid equipment in the energy field. The main conclusions are as follows.

(1) In order to obtain and understand the properties of the flow field in a coal pyrolysis filtration system, a series of models drawn from real equipment were established to realize CFD calculations with various sections. With a series of comparisons and calculation results, the inlet angle and baffle angle ($\psi$ and $\phi$) were selected as important parameters to be studied, since they have an obvious influence on the uniformity of the flow distribution and need to be optimized within a certain range. Additionally, they are much easier to change for a given structure.

(2) In order to find the optimal scheme, a series of models with different parameters were established and calculated with CFD. To save costs in terms of time and resources in the calculation, regression methods were introduced here to obtain a prediction model. One single-factor regression was used at first for both $\psi$ and $\phi$, but it could not find an effective optimal scheme since the parameters affect each other. Therefore, a quadratic regression orthogonal combination was adopted to establish a multi-parameter model. The QROC model can represent the relation between the angles $\phi$ and $\psi$ and the flow distribution within a certain range well enough with only a few models. The results were checked with both statistical tests and a BPNN.

(3) For further optimization, a structure parameters optimization method based on quadratic regression orthogonal combination (QROC) and a genetic algorithm (GA) was proposed in this work, and used to find optimization points having smaller standard deviations. The proposed QROC-GA model was used to obtain an optimized scheme for a filtration system having a more uniform flow field distribution. When within a certain range, more than one optimization scheme was obtained by the GA; thus, a verification calculation was repeated with CFD, and it was proved that the QROC-GA model has a strong capability in optimization work.

(4) The QROC-GA method can be used with CFD models to obtain a regression and an optimization for multi-parameter optimization problems. Once there is more than one factor in a CFD problem needing to be optimized, and they have an obvious impact for each
other, a quadratic regression orthogonal combination can be introduced to establish a model to predict the results within a certain range. As to multiparameter optimization with CFD, many models and calculations with changing parameters are always needed, while using our method it can be simplified in a large degree. Still, as to complex solutions in QROC models, the GA was proved to have very reliable results. The main conclusions have great significance not only for designing the coal cracking filtration systems, but for other similar equipment as well.

**Nomenclature**

| Symbol | Definition |
|--------|------------|
| ρ      | Density (kg/m³) |
| u      | Flow velocity (m/s) |
| A      | Cross section of tube (m²) |
| μ      | Kinematic viscosity (kg/m·s) |
| q      | Flow rate (m³/s) |
| d_k    | Diameter (m) |
| Re     | Reynolds number (–) |
| k      | Turbulent kinetic energy (m²/s²) |
| ε_i    | Dissipation rate (m²/s³) |
| u_x, u_y, u_z | Velocity components (m/s) |
| x, y, z | Cartesian coordinates (m) |
| t      | Time (s) |
| ∇      | Divergence (–) |
| p      | Mean pressure (Pa) |
| G_k    | Velocity gradient (–) |
| G_b    | Velocity buoyancy (–) |
| Y_M    | Contribution to the turbulent pulsating pressure expansion (–) |
| C_1, C_2, C_3_e | Empirical constants (–) |
| σ_k, σ_ε | Prandtl numbers (–) |
| ε      | Porosity (–) |
| α      | Permeability (m) |
| C_2    | Inertial resistance factor (m⁻²) |
| L      | Length (m) |
| c_1, c_2 | Constants (–) |
| a_i    | Variable (–) |
| γ      | Overall mean value (m/s) |
| N      | Total amount of data (–) |
| y      | Mean square deviation (m/s) |
| b_0, b_j, b_ij, b_jj | Regression coefficients (–) |
| F      | Factor number (–) |
| ŷ     | Test result (–) |
| a     | Degree of test implementation (–) |
| r     | Distance to asterisk and center points (–) |
| m_0   | Number of center test points (–) |
| m_c   | Number of test points (–) |
| ψ     | Angle of air inlet (°) |
| φ     | Angle of baffle (°) |

| df_r | Degrees of freedom of regression (–) |
| df_R | Degrees of freedom of residual square (–) |
| SS_R | Sum of squares of residuals (–) |
| SS_r | Sum of squares of regression (–) |
| F_R  | Significance test (–) |

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