

RESEARCH ON DEM CALIBRATION OF CONTACT PARAMETERS OF COATED FERTILIZER

包膜肥料接触参数 DEM 标定研究

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ABSTRACT

To simulate the interactions between the coated fertilizer particles and the fertilizer discharging components accurately, the coated fertilizer contact parameters were calibrated using the discrete element method (DEM). Based on the angle of repose test, single-factor simulations were performed on the coefficient of restitution (COR), coefficient of static friction (COSF) and coefficient of rolling friction (CORF) between particles, and the internal relationship between the level change of each factor and the static angle of repose (SAOR) was determined. The CCD test was used to calibrate the contact parameters between particles. When the COR, COSF and CORF between particles are 0.625, 0.175, and 0.037, respectively, the simulation value of SAOR is 24.173°, and the relative error from the real value is 1.230%, which indicates that the calibrated fertilizer particle contact parameters are accurate and reliable.

摘要

为准确模拟包膜肥料颗粒与排肥部件之间的相互作用，采用离散元法校准了包膜肥料颗粒的接触参数。通过跌落试验、斜板滑动试验和斜板滚动试验测得肥料颗粒与 ABS 间的碰撞恢复系数、静摩擦系数和滚动摩擦系数分别为 0.47、0.42 和 0.095；基于休止角试验分别对颗粒间碰撞恢复系数、静摩擦系数和滚动摩擦系数进行单因素仿真，确定各因素水平范围与堆积角的作用关系。采用 CCD 试验标定颗粒间接触参数，对试验数据进行多元二次回归拟合，建立肥料颗粒堆积角与颗粒间接触参数的回归模型并进行最优参数求解，得到颗粒间碰撞恢复系数、静摩擦系数和滚动摩擦系数分别为 0.625、0.175 和 0.037 时，堆积角仿真值为 24.173°，与真实值相对误差为 1.230%，表明标定所得肥料颗粒接触参数准确可靠。

INTRODUCTION

Fertilizer is the "food" of crops and has an irreplaceable role in agricultural production (Chen *et al.*, 2014; Hvistendahl, 2010). To improve fertilizer utilization and reduce the environmental hazards of fertilizer loss, coated controlled-release fertilizers and variable amount fertilizer discharge application technologies have received widespread attention (Chojnacka *et al.*, 2020; Dimkpa *et al.*, 2020; Kornei, 2017). The outer groove wheel fertilizer discharger is a key carrier in the process of implementing precise variable fertilizer application, which has the advantages of simple structure and a large control range of fertilizer amount discharge but has problems such as large pulsation and poor stability of fertilizer discharge (Zhu *et al.*, 2018; Wang *et al.*, 2017). Therefore, it is of great importance to research the uniformity of fertilizer discharging by external slotted wheel dischargers.

Three methods are usually used to study the fertilizer discharge process of the outer groove wheel: experimental study, theoretical analysis, and numerical simulation. Experimental studies are the most direct and reliable research method, but it is difficult to obtain information on the internal forces and displacements of the particles. The theoretical analysis is often different from the actual results because it cannot fully consider all the practical complexities. Numerical simulation methods can make up for the shortcomings of theoretical analysis and experimental studies (Lv *et al.*, 2013; Zhao *et al.*, 2012; Landry *et al.*, 2006).

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The DEM method was proposed by *Cundall and Strack (1979)* and has been widely used to simulate the mixing, stirring, conveying, filling, and crushing of bulk materials in mining, geotechnical, pharmaceutical, chemical, and agricultural fields (*Lu et al., 2015; Shen et al., 2016; Gao et al., 2016*). To make the simulation match the real situation, it is necessary to calibrate its meso-parameters firstly. Most of the existing studies on the calibration of discrete element parameters of fertilizer particles are based on conventional fertilizers such as urea (*Liu et al., 2018*), compound fertilizers (*Wen et al., 2020*), and organic fertilizers (*Yuan et al., 2018; Han et al., 2021; Luo et al., 2018*), and there are few studies on the calibration of parameters of coated fertilizer particles. Coated fertilizers are influenced by the coating material and differ significantly from conventional fertilizers in terms of frictional characteristics. The improvement of the calibration process has been a subject of scientific research for many years (*Coetzee, 2017*). Researchers have tried several methods to calibrate or measure discrete element parameters, one is to directly measure the parameters of the particles through experiments, which is suitable for parameters that reflect the properties of the particles, such as Poisson's ratio, density, and shear modulus. One is to experimentally measure the macroscopic phenomena of the particles and then reverse calibrate them. In the inverse calibration process, the traditional method is "trial and error", which is inefficient and inaccurate (*Chen, 2017*). To make up for the above disadvantages, *Zhao (Zhao, et al., 2012)* tried to explore the complex relationship between micro and macro mechanical behavior and parameters through experience or theoretical formulas. In the calibration process, the method of experimental design is used to generate samples, such as Kevin (*Hanley et al., 2011*) used the Taguchi method and orthogonal experiment, and *Rackl (Rackl and Hanley, 2017)* used Latin hypercube sampling and Kriging method. Then, the optimized algorithm was used to process the data and get the calibration result, specifically, *Do (Do et al., 2018)* used genetic algorithm, *Benvenuti (Benvenuti et al., 2016)* used an artificial neural network, and *Zhou (Zhou et al., 2018)* used radial basis neural network method. Compared with the above methods, the experimental design based on response surface model theory has unique advantages in building regression models and analyzing the significance of factors. The method includes central combined design (CCD) and Box-Behnken design (BBD), and CCD is used in this study because it can fit the response surface better and with higher accuracy (*Myers et al., 2016*). Therefore, in this paper, a CCD-based repose angle test was chosen to calibrate the discrete element parameters of coated fertilizer particles and to study the uniformity of fertilizer discharge of the outer groove wheel discharger based on this.

In this study, the coated fertilizer particles were used as the research object, and the actual static angle of repose (SAOR) of the coated fertilizer particles was measured by the image processing method, and the contact parameters of the coated fertilizer particles in the discrete element simulation software EDEM were reverse-calibrated based on the actual SAOR. The simulated SAOR of the coated fertilizer particles in EDEM was quickly determined by the EDEMPy post-processing procedure.

MATERIALS AND METHODS

DEM MODELING OF FERTILIZER GRANULES

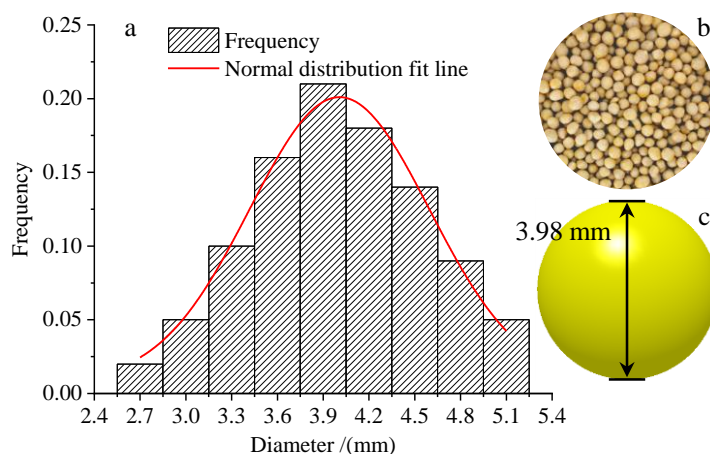


Fig. 1 - Fertilizers and discrete element model

In this paper, the coated controlled-release fertilizers were sourced from Shandong Nongyang Biological Technology Co., Ltd., China. (Fig.1b), 100 randomly selected fertilizer granule samples were measured in three directions: length, width, and thickness using digital calipers (accuracy 0.01 mm), and the average triaxial dimensions of fertilizer particles were 4.08 mm×3.97 mm×3.89 mm.

The equivalent diameter D and sphericity S_p were calculated using Equation (1), the equivalent diameter and sphericity are 3.98 mm and 0.975, respectively, and its size distribution is shown in Fig. 1a. A single sphere with a diameter of 3.98 mm was used in the DEM simulation to build the fertilizer granule simulation model (Fig.1c).

$$\begin{cases} D = \sqrt[3]{LWT} \\ S_p = \frac{D}{L} \end{cases} \quad (1)$$

Where:

D is the equivalent diameter of fertilizer granules, [mm]; L is the length of fertilizer granules, [mm]; W is the width of fertilizer granules, [mm]; T is the thickness of fertilizer granules, [mm]; S_p is the sphericity.

A random sample of 300 fertilizer granules was selected, and the mass and volume were measured using a digital balance (accuracy 0.001 g) and a measuring cylinder (accuracy 0.01 mL), respectively (drainage method), and the true density of fertilizer granules was calculated as 1.46 g/cm³ using equation (2). The moisture content of fertilizer granules was measured as 0.88% using a rapid moisture analyzer (accuracy 0.001 g).

$$\rho_{real} = \frac{m_0}{V_1 - V_0} \quad (2)$$

Where:

ρ_{real} is the true density of fertilizer particles, [g/cm³]; m_0 is the mass of fertilizer particles, [g]; V_1 is the total volume of fertilizer particles and water in the measuring cylinder, [cm³]; V_0 is the volume of water in the measuring cylinder, [cm³].

Due to the extremely low moisture content of the coated fertilizer particles and the lack of adhesion between the particles, the Hertz-Mindlin model was used in the EDEM software for DEM parameter calibration. Based on the drop test, the inclined plate sliding test and the inclined plate rolling test, the COR, COSF and CORF between the fertilizer particles and the ABS were measured to be 0.47, 0.42 and 0.095, respectively. Due to the limited space of the article, the process of determining the contact parameters between fertilizer particles and ABS will not be explained. Other parameters used in the simulation are Poisson's ratio 0.225 and shear modulus 1.528×10⁸ Pa.

THE STATIC ANGLE OF REPOSE (SAOR) TEST

The inter-particle contact coefficient was calibrated using the SAOR test, and the actual SAOR of the fertilizer particles was measured first (as shown in Fig. 2), and the Fiji-ImageJ image processing software was used to process the fertilizer particles and extract the contour line after the stacked particles were stabilized, and the actual SAOR of the fertilizer particles was deduced from the slope of the contour line, and the test was repeated 10 times to take the average value.

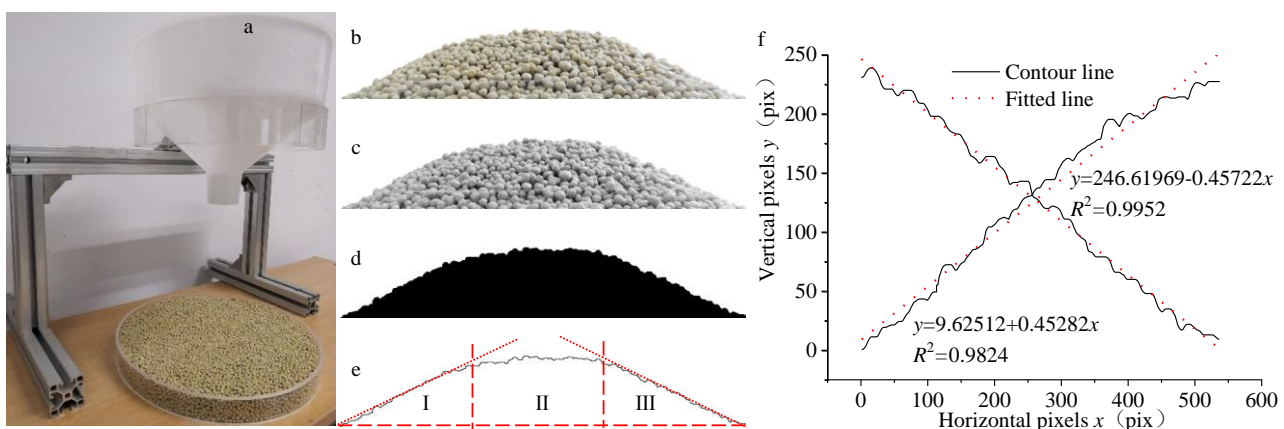


Fig. 2 - Schematic diagram of SAR of fertilizer particles

EDEM2018 was used to numerically simulate the SAOR of fertilizer particles (Fig.3). To accurately reflect the interaction between fertilizer particles, the funnel shown in Fig. 3a was used to perform SAOR test on the fertilizer particles. The total amount of particles in the bottom cylinder was 2500 g, and the total amount of particles in the funnel is 1000 g, the total simulation time is 4 s, and the time step is 5×10^{-6} s. After the simulation has been completed, use Python 3.6 to call the EDEMPy library, run the SAOR post-processing program, as shown in Fig. 3b, set up 18 sampling surfaces on the fertilizer particle surface, read the fertilizer particle position information on the accumulation surface and perform linear fitting, output the average and standard deviation of the SAOR.

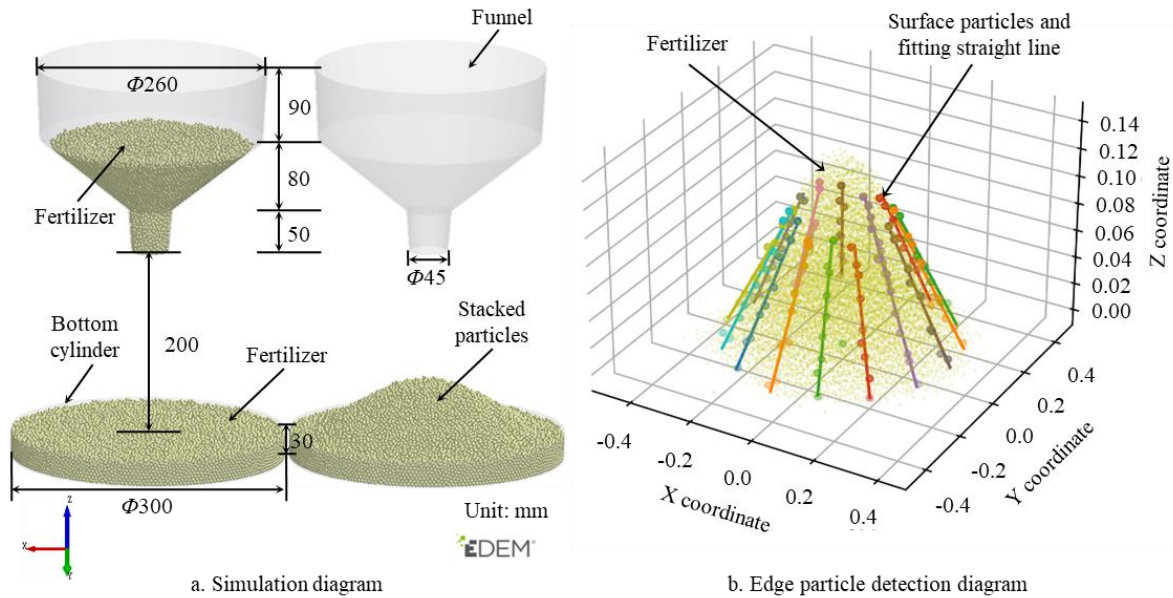


Fig. 3 – Simulation test diagram

Coefficient of restitution (COR)

Set the coefficient of static friction (COSF) and coefficient of rolling friction (CORF) between fertilizer particles 0.18 and 0.035, respectively. The horizontal range of the COR is 0.3 to 0.7, and the horizontal gradient is 0.1.

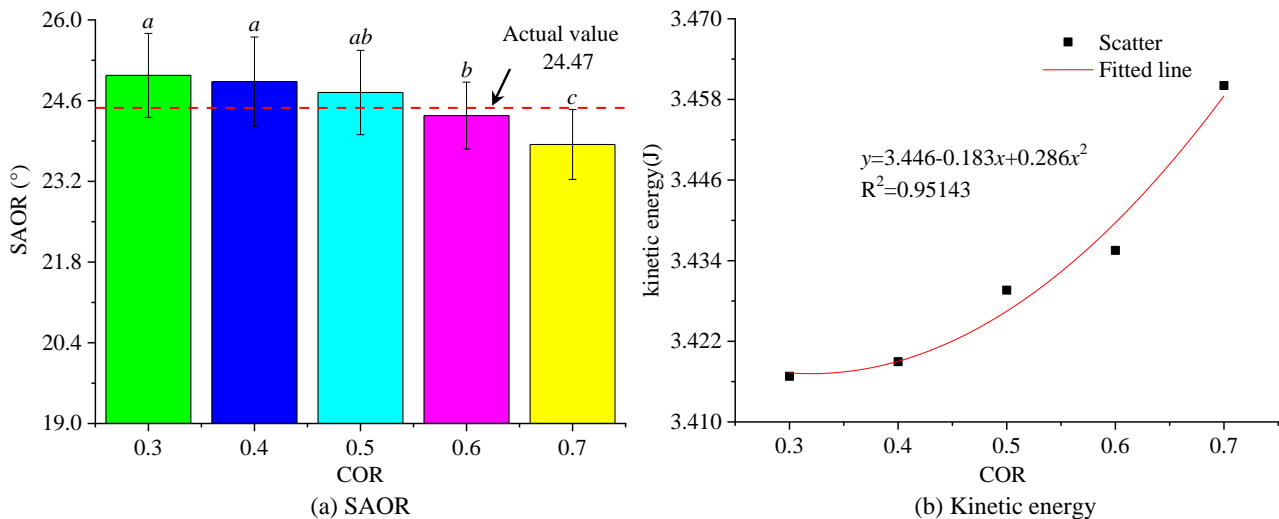


Fig. 4 – Effects of COR on SAOR and total kinetic energy of particles

The variation of SAOR of fertilizer particles under each COR gradient between fertilizer particles is shown in Fig. 4(a). One-way ANOVA was performed using SPSS 25.0, and the homogeneity of the variance test result was significant at $0.694 > 0.05$, the analysis of variance could be performed; ANOVA results showed $P < 0.0001$, indicating significant differences in the effects of different inter-granule COR on the SAOR.

From Fig. 4(a), it can be seen that the SAOR decreases with the increase of the inter-particle COR, and the difference between the SAOR groups is not significant when the inter-particle COR is 0.3, 0.4, and 0.5, and the difference between the SAOR groups is significant when the inter-particle COR is 0.6 and 0.7, and the COR corresponding to the actual value of the SAOR is between 0.5 and 0.6.

The variation of the total kinetic energy of fertilizer particles with the inter-particle COR is shown in Fig. 4(b). The larger COR, the greater the total kinetic energy of fertilizer particles, indicating that as the COR increases, the particles increase their collision bounce and fall more easily to a position far from the center of the fertilizer pile, and the particles on the surface of the fertilizer pile become more dispersed, resulting in a smaller pile-up angle.

Coefficient of static friction (COSF)

Set the COR and CORF between fertilizer particles to 0.5 and 0.035, respectively. The COSF between fertilizer particles ranges from 0.12 to 0.24, and the horizontal gradient is 0.03.

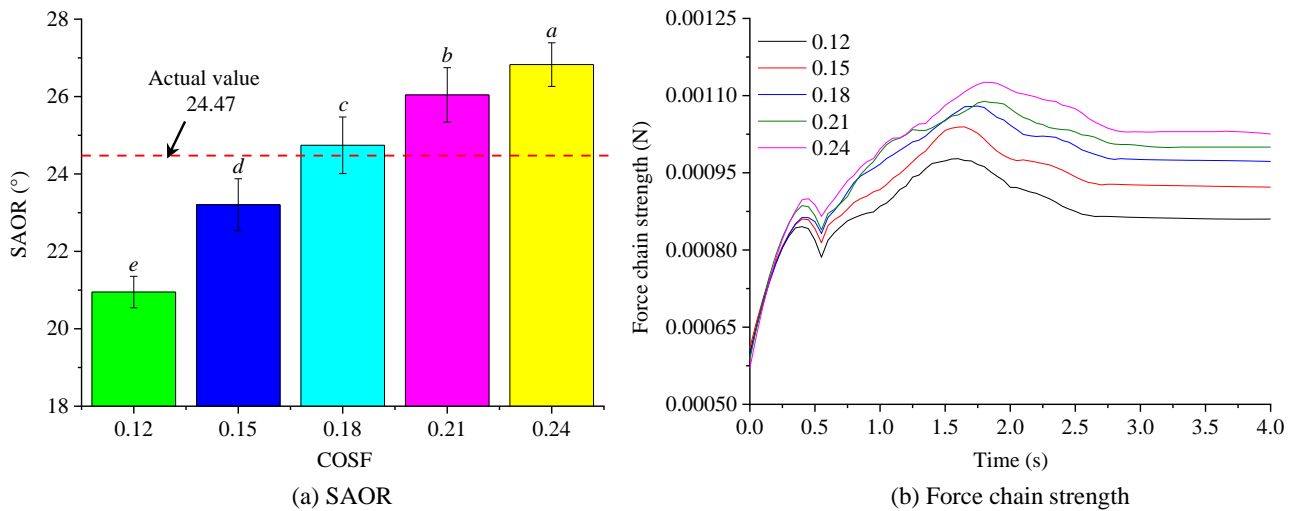


Fig. 5 – Effects of COSF on SAOR and force chain strength of particles

The variation of the SAOR of fertilizer particles under each COSF gradient between fertilizer particles is shown in Fig. 5(a). One-way ANOVA was performed using SPSS 25.0, and the homogeneity of the variance test result was significant at $0.265 > 0.05$, the analysis of variance could be performed; ANOVA results showed $P < 0.0001$, indicating significant differences in the effects of different inter-granule COSF on the SAOR.

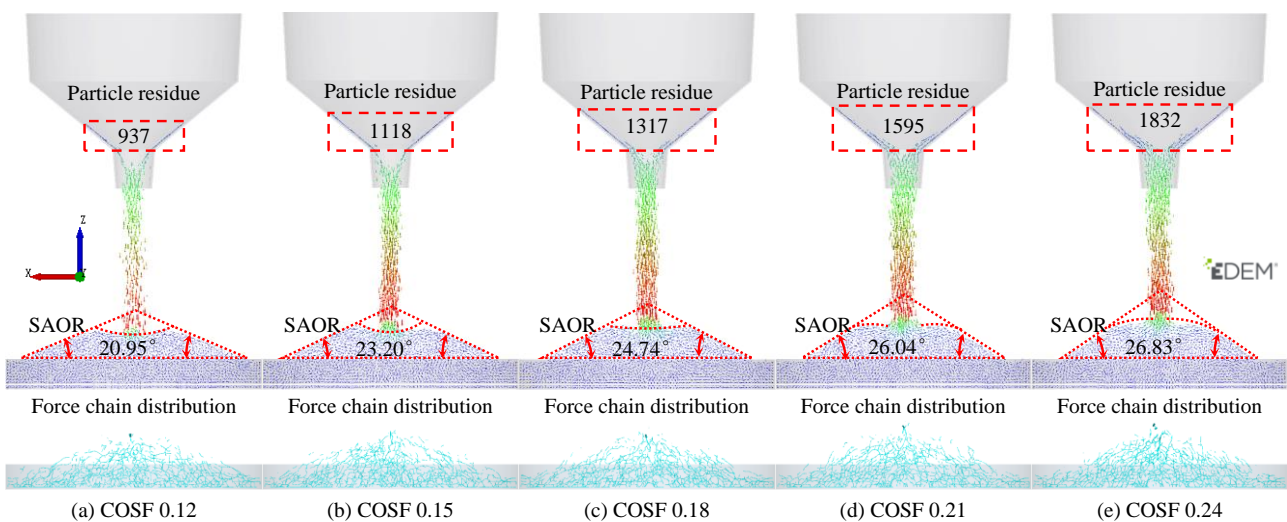


Fig. 6 – Schematic diagram of fertilizer particle retention, bottom particle repose and force chain distribution in the funnel with different inter-particle COSF

It can be seen that the SAOR increases with the increase of the COSF between the particles (Fig.5), and the effect of each factor level on the SAOR is significant, and the COSF corresponding to the actual value of the SAOR is between 0.15 and 0.18. The variation of the force chain distribution strength of the bottom fertilizer particles with the inter-particle COSF is shown in Fig. 5(b).

The smaller the inter-particle COSF is the weaker the strength of the force chain generated by the bottom particles stacking. Combined with Fig. 6, it can be seen that the fertilizer granules flow from the funnel impacts the surface layer of the fertilizer pile, and the weak force chain on the cone surface is easily broken to trigger the slippage of the granules on the surface layer of the fertilizer pile, which in turn leads to a smaller

piling angle. The retention amount of fertilizer particles in the funnel and the accumulation state of the bottom particles at each level at the time of 1.8 s are shown in Fig. 6. The inter-particle COSF has a significant effect on the number of fertilizer particles remaining in the funnel, and the number of fertilizer particles remaining in the funnel increases with the increase of the inter-particle COSF, indicating that the increase of the inter-particle COSF leads to the poor mobility of fertilizer particles; the SAOR of the bottom particles increases with the pile angle at the bottom increased with the increase of inter-granular COSF, and the shape of the intersection of fertilizer pile and fertilizer flow gradually changed from concave to flat and to convex.

Coefficient of rolling friction (CORF)

Set the COR and COSF between fertilizer particles to 0.5 and 0.18, respectively. The CORF between fertilizer particles ranges from 0.025 to 0.045, and the horizontal gradient is 0.005.

The variation of the SAOR of fertilizer particles under each CORF gradient between fertilizer particles is shown in Fig. 7(a). One-way ANOVA was performed using SPSS 25.0, and the homogeneity of the variance test result was significant at $0.875 > 0.05$, the analysis of variance could be performed; ANOVA results showed $P < 0.0001$, indicating significant differences in the effects of different inter-granule CORF on the SAOR.

From Fig. 7(a), it can be seen that the SAOR increases with the increase of CORF between particles, and the effect of each factor level on the SAOR is significant, and the CORF corresponding to the true value of the stacking angle is between 0.30 and 0.35.

The variation of the average rotational energy of the particles with the CORF is shown in Fig. 7(b). The average rotational energy of particles decreases with the increase of CORF, and the larger the rotational energy is, the more likely the particles falling on the surface layer of the fertilizer pile will roll, which in turn destroys the stable accumulation state between the particles on the surface layer of the cone and causes the surface particles to roll off and the accumulation angle becomes smaller.

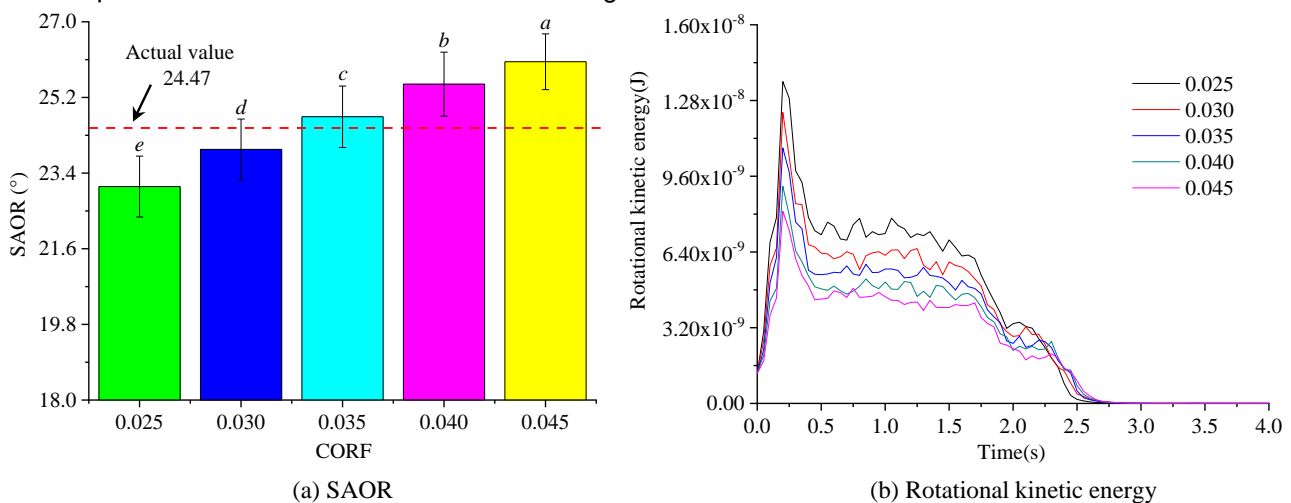


Fig. 7 – Effect of RFC and average rotational energy of granules on repose angle

CCD CALIBRATION TEST

According to the results of pre-experiment and single-factor analysis, the CCD test was carried out on the COR, COSF, and CORF between particles, and the test results are shown in Table 1.

Table 1

CCD test plan and results

Number	COR x_1	COSF x_2	CORF x_3	SAOR y (°)
1	0.40	0.15	0.0300	22.8850
2	0.70	0.15	0.0300	21.9785
3	0.40	0.21	0.0300	25.2489
4	0.70	0.21	0.0300	23.8707
5	0.40	0.15	0.0400	23.5763
5	0.40	0.15	0.0400	23.5763
6	0.70	0.15	0.0400	23.4178
7	0.40	0.21	0.0400	27.0148

Table 1
(continuation)

Number	COR x_1	COSF x_2	CORF x_3	SAOR y (°)
8	0.70	0.21	0.0400	25.6742
9	0.30	0.18	0.0350	24.8131
10	0.80	0.18	0.0350	22.9109
11	0.55	0.13	0.0350	21.7858
12	0.55	0.23	0.0350	26.5836
13	0.55	0.18	0.0266	23.1235
14	0.55	0.18	0.0434	25.6804
15	0.55	0.18	0.0350	24.7499
16	0.55	0.18	0.0350	24.6826
17	0.55	0.18	0.0350	24.5547
18	0.55	0.18	0.0350	24.4386
19	0.55	0.18	0.0350	24.8903
20	0.55	0.18	0.0350	24.7471
21	0.55	0.18	0.0350	25.0695
22	0.55	0.18	0.0350	24.9396
23	0.55	0.18	0.0350	25.1522

Using Design-Expert 10.0 software to perform multiple quadratic regression fitting on the experimental data, a regression model of the SAOR of fertilizer particles and the contact parameters between the particles was established, and the regression equation y was obtained as:

$$y = 1.8853 + 15.5406x_1 + 106.5343x_2 + 198.2651x_3 - 45.9381x_1x_2 + 130.9310x_1x_3 + 1198.9543x_2x_3 - 13.8756x_1^2 - 220.1364x_2^2 - 4851.9527x_3^2 \quad (3)$$

The significance test of the regression equation is shown in Table 2. It can be seen from the table that the degree of fit of the model is extremely significant ($P < 0.0001$), and the lack of fit term is not significant ($P > 0.05$), indicating that the equation fits well, and the regression model can be used to express the relationship between response indicators and various experimental factors.

Table 2

Analysis of variance table

Source	Sum of Squares	df	Mean Square	F-Value	P-Value
Model	37.7275	9	4.1919	80.8013	< 0.0001**
X_1	3.5705	1	3.5705	68.8222	< 0.0001**
X_2	23.7769	1	23.7769	458.3093	< 0.0001**
X_3	7.3229	1	7.3229	141.1515	< 0.0001**
$X_1 X_2$	0.3419	1	0.3419	6.5897	0.0234*
$X_1 X_3$	0.0771	1	0.0771	1.4870	0.2444
$X_2 X_3$	0.2587	1	0.2587	4.9875	0.0437*
X_1^2	1.5487	1	1.5487	29.8522	0.0001**
X_2^2	0.6237	1	0.6237	12.0221	0.0042**
X_3^2	0.2338	1	0.2338	4.5063	0.0535
Residual	0.6744	13	0.0519		
Lack of Fit	0.2403	5	0.0481	0.8857	0.5322
Pure Error	0.4341	8	0.0543		
Cor Total	38.4019	22			

$R^2=0.9824$; $CV\%=0.93$

Note: ** means extremely significant impact ($P < 0.01$), * means significant impact ($P < 0.05$).

It can be seen from Table 2 that the impact COR, COSF, and CORF of fertilizer particles in the first item have a significant impact on the SAOR; in the interaction item, the impact COR-COSF and COSF-CORF have significant effects on the SAOR; Fig. 8 shows the response surface for interactive factors.

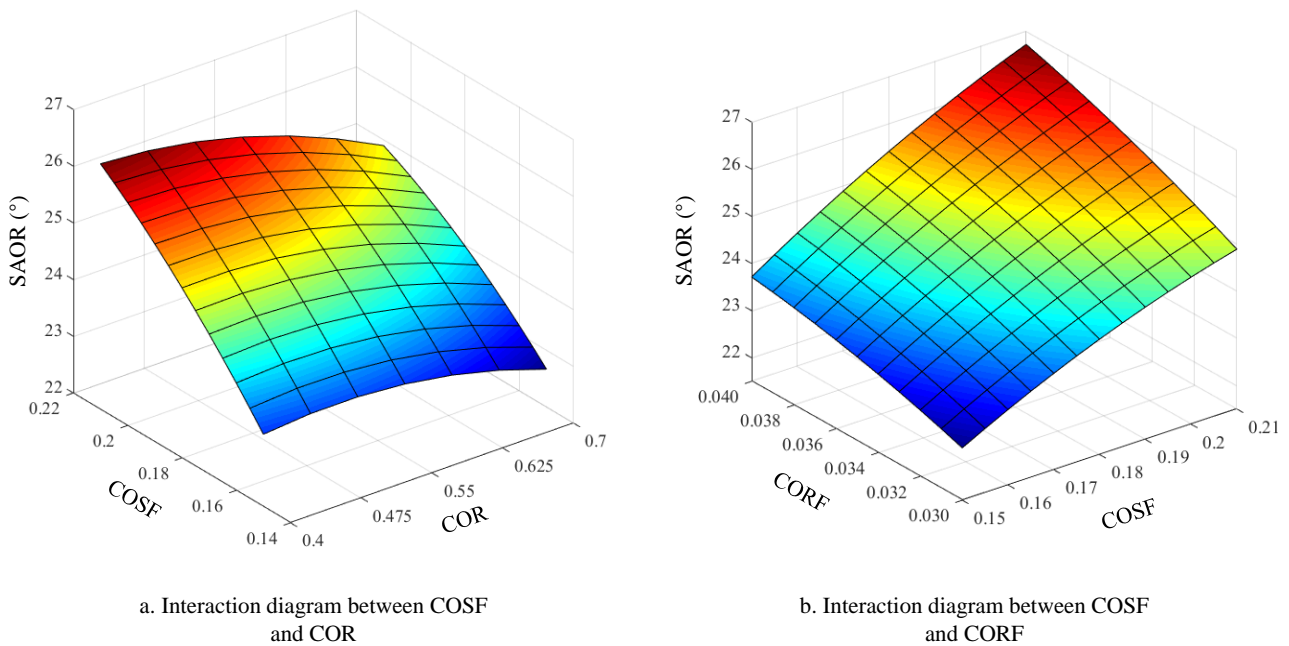


Fig. 8 – Response surface diagram

It can be seen from Fig. 8a that the SAOR increases with the increase of the COSF, and decreases with the increase of the COR, which is consistent with the results of the analysis of variance; The slope of the response surface curve of the crash COR and the COSF at each level is lower than the slope at the interaction level, indicating that the interaction is significant. It can be seen from Fig. 8b that the SAOR increases with the increase of the COSF, and with the increase of the CORF, which is consistent with the results of the analysis of variance; The slope of the response surface curve of the CORF and the COSF at each level is lower than the slope at the interaction level, indicating that the interaction is significant.

Use the optimization module of Design-Expert 10.0 software to solve the optimal parameters of the regression model, and select the constraint condition of the objective function as:

$$\begin{cases} y=24.47415 \\ \text{s.t.} \begin{cases} 0.40 \leq x_1 \leq 0.70 \\ 0.15 \leq x_2 \leq 0.21 \\ 0.03 \leq x_3 \leq 0.04 \end{cases} \end{cases} \quad (4)$$

According to the constraints, the objective function is optimized and the combined parameters are obtained: the COR, the COSF, and the CORF are 0.625, 0.175, and 0.037, respectively, and the SAOR is 24.474°. The simulation test is carried out under this parameter, and the SAOR of simulation is 24.173°, and the relative error from the true value is 1.230%. A comparison of the simulation and actual SAOR profiles is shown in Fig. 9.

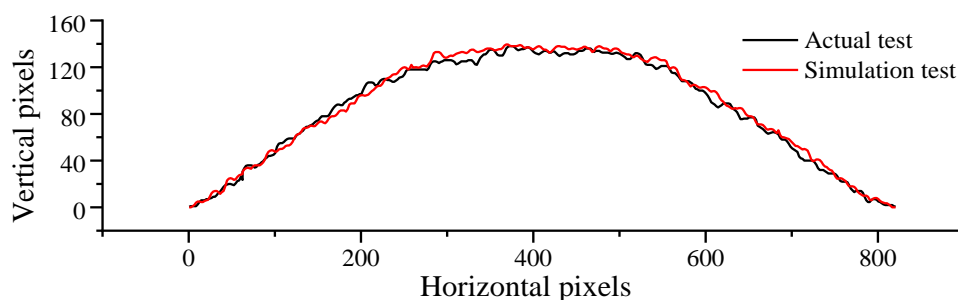


Fig. 9 – Comparison of actual and simulation SAOR profiles

CONCLUSIONS

The COR, COEF and CORF between fertilizer granules and ABS were 0.47, 0.42, and 0.095, respectively, measured and calibrated by the drop test, sliding test, and rolling test of the sloped plate. Through single-factor experiments, it is obtained that the COR, COSF and CORF of fertilizer particles have a direct effect on the total kinetic energy of the particles, the strength of the force chain, and the rotation energy of the particles, respectively, and then change the accumulation state between the particles and cause the SAOR change. The regression model of the SAOR of fertilizer particles and the contact parameters between the particles was established by the CCD test and the optimal parameters were solved. The COR, COSF and CORF were 0.625, 0.175 and 0.037, respectively, and the SAOR is 24.474° . The simulation test is carried out under this parameter, and the SAOR of simulation is 24.173° , and the relative error from the true value is 1.230%.

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