Effects of Mesoscopic Structure on Crack Resistance of Asphalt Mastic and Calibration of Contact Parameters

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Abstract. This paper investigated the effects of mesoscopic structure on crack resistance of asphalt mastic basing on the bending failure simulation with discrete element method. A Dynamic Link Library wrote by C++ is proposed for the modelling process of particle filling. Response surface and variance analysis are used to calibrate mesoscopic mechanical parameters of contact model, determine the influence of different parameters on deformation in bending failure test and the relationship between the parameters is fitted by mathematical formula. The effects of air void content and fine aggregate surface texture on crack resistance of asphalt mastic at -10 °C were studied then. It was proved that the adhesive strength and bonding area between fine aggregates co-influence the ultimate bending failure load, and the contact stiffness influences the ultimate bending deflection. Mathematical correlation formula between the radius of binding area and the critical stress that satisfies the ultimate load of asphalt mastic beam can be fitted in same form. The flexural strain energy density of asphalt mastic is increased with the decrease of air void content. The results are of positive significance for improving the mechanical properties of asphalt road in cold regions.

Keywords. Asphalt mastic, calibration, response surface analysis, mesoscopic structure, cracking, discrete element method.

1. Introduction
The cracking of asphalt road is a troublesome disease in cold climate areas, which has been the focus of the researchers for many years [1]. The direct manifestation of cracking is the separation of large minerals from binding material such as asphalt mastic [2]. Under the action of external force, this binding material is subjected to tensile-shear coupling loads meanwhile [3]. Improving the mechanical properties of the binding materials is necessary to reduce cracking risk of the asphalt road. In the current research, the research on matrix asphalt is more systematic. Commonly used experiments include bending beam rheology test (BBR), direct tensile test (DDT) [4]. Based on the grey correlation analysis, Zheng analyzed the ultimate bending failure strength of different kinds of binder materials at dissimilar temperature, and the effects of failure strain on the critical value of energy density, and obtained the intensity index of different materials [5].

With the development of computer technology, image processing technique and numerical analysis are more and more applied in scientific research. By using high resolution image processing technique, the heterogeneous fracture model is established and various fracture toughening mechanisms of
asphalt materials are studied by Kim [6]. Zhanping You [7] used X-ray computed tomography images that finished simulating the dynamic modulus of asphalt concrete. Compared with digital image processing analysis, numerical simulation is mainly divided into two categories, finite element method and discrete element method. DEM was originally proposed by Cundall and Strack in their paper published in 1979 [8]. Roozbahan proposed the compaction flow test, used DEM to study the possible influence of mold size, loading strip geometry and loading rate on CFT results, and studied the flow difference between asphalt mixture particles compacted in the laboratory and in the field [9]. Ding proposed a new modeling method, which used discrete element method to reconstruct the hollow shape of particles to accurately characterize the microstructure of aggregates and predict the mechanical properties of the aggregate skeletons [10].

In this study, by using the discrete element software, a 3D simulation model of asphalt mastic beam which composes of fine aggregate, asphalt mortar and air voids is established, bending failure test is conducted to analysis the influence of different variables on the mechanical properties of asphalt mastic. Response surface analysis and variance analysis are used during parameter calibration process. This study not only has some enlightening significance for the calibration of parameters in subsequent simulation experiments of multiphase mixture, but also provides some theoretical basis for reducing cracking risk of asphalt road in cold regions.

2. Materials and Laboratory Test

The properties of the asphalt which is selected for laboratory test are shown in table 1. The properties of mineral powder are shown in table 2. All the materials meet the specification requirements of Chinese code for Construction and Design of Highway Asphalt Pavement (JTG_F40-2004) (table 3). The asphalt mortar used in laboratory test is configured at a filler-asphalt ratio of 1:1.2 using shearing machine. Gradation of fine limestone aggregates is displayed in table 4. The asphalt content of asphalt mastic is 5%. The air void content is assumed to be zero to maximize the flowability.

| Category    | Penetration/mm 5 °C | Penetration/mm 25 °C | Ductility at 15 °C(mm) | Softening point(°C) | Viscosity(Pa·s) 60 °C | Viscosity(Pa·s) 90 °C |
|-------------|---------------------|-----------------------|------------------------|----------------------|------------------------|------------------------|
| CNOOC 70#   | 0.72                | 7.13                  | 51.5                   | 46.6                 | 4862                   | 2981                   |

| Density(Kg/m³) | The water content (%) | Roughness(μm) | Sand equivalent (%) |
|----------------|------------------------|---------------|---------------------|
| 2737           | 0.141                  | 2.237         | 65.6                |

| Range (mm) | <0.6 | <0.15 | <0.075 |
|------------|------|-------|--------|
| Pass (%)   | 100  | 90-99 | 75-99  |

| Sizes(mm)  | 2.36 | 1.18  | 0.60  | 0.30  | 0.15  | 0.075  |
|------------|------|-------|-------|-------|-------|--------|
| Percentage (%) | 33   | 27    | 19    | 14    | 10    | 6      |

The analysis of the failure mechanism of asphalt mixture is the basis of understanding the damage law of asphalt road, structure simulation analysis, asphalt mixture design optimization and repair [11]. Three points bending test is commonly selected to measure the mechanical property of asphalt beam in bending failure of under dissimilar temperature. According to the requirements in the code (JTJ052-2000), prepare the asphalt mastic beams in four duplicates and parallel tests to evaluate the deformation behaviors at the temperature of -10 °C using the LX-II automatic bending tester. The
manual uniformly distributed load is applied to the middle at a rate of 50 mm/min (figure 1). The dimension is 250 ± 2.0 mm in length with a cross section 30±2 mm in width and 35±2 mm in height (figure 2). Results in laboratory are used to calibrate the parameters in the following modeling section and to be compared with results of simulation.

3. Simulation Modeling

3.1. Modeling Procedure

The asphalt mastic beam, as a multiphase composite, includes fine aggregates, mortar, and air. In the laboratory tests, the air void content was assumed to be 0% to maximize the flow ability. So the asphalt mortar is considered the a homogeneous material fully filled between aggregates in simulation models of asphalt mastic by setting the contact radius of particle to be a little greater than the physical radius as shown in figure 3.

The specific modeling process is as follows. The beam with the dimension of 250 mm×30 mm×35 mm is meshed by Gambit, which was divided into 262500 blocks, the grid file is imported into FEM software, get the center coordinates of the particles by loading user defined functions. Write Dynamic Link Library code by using C++ and load it into DEM software. All the process mentioned above is for rapidly filling the particle factory. This method avoids the disadvantage of the conventional compression method and the radius expansion method causing local stress is too excessive to reach balance for a long time. Discrete element simulation model is constructed as shown in figure 4.
3.2. Selection of Mesoscopic Mechanical Model

Zhanping You pointed out in his doctoral dissertation research paper that the contact between aggregates in asphalt mixture has cohesive strength when aggregate are fully coated with asphalt, aggregates can slide freely when they are not coated with asphalt and their surface is absolutely smooth [12]. Consider the factors mentioned above, Hertz-Mindlin contact model and Particle Bonded model are selected for coupling analysis in this paper (figure 3). As early as 1882, Hertz had given the solution of the normal force at the contact overlap of elastic material particles [13]. Tangential force is based on the research done by Mindlin and Deresiewicz [14]. The Bonded Particle Model was proposed by Potyondy and Cundall in 2004 to simulate rock breakage [15]. The principle of the Bonded Particle model is that the asphalt between aggregates is simplified as a bonding beam, all the mesoscopic information and the mechanical deformation among the particles is reflected by the bonding beam.

4. Calibration and Simulation

Due to the idealisation used in the most DEM simulation models regarding the size distribution, form and stiffness of particle. It is necessary to undertake the calibration process to determine, that the selection of mesoscopic mechanical contact model parameters results in the realistic macroscopic behavior of the virtual bulk material.

4.1. Calibration of Hertz-Mindlin Model Parameter

Hertz-Mindlin model characterizes a conventional non-viscous contact between fine aggregates. After setting the physical property of fine aggregates particle, users only need to set the coefficient of restitution, coefficient of static friction, coefficient of rolling friction in DEM software. There are many scenarios in which the Hertz-Mindlin contact model can be applied. In this part, angle of repose test for fine aggregate was selected to calibrate the parameter. Three different parameters were set for parallel simulation, and the optimal parameters matching the macroscopic laboratory test were selected combining the response surface analysis and variance analysis. Process is shown in figure 5.

![Figure 4. Discrete element model.](image)

![Figure 5. Simulation of angle of repose test.](image)
divide each array into 4 equal parts, identify the highest particle in every part, fit the centroid coordinates of these particles approximately with the straight line, and measure the angle between the fitting line and the horizontal line, taking the average value of 4 groups as simulation result. The principle of calculation is shown in figure 6 [16].

Figure 6. Calculation of angle of repose.

4.1.1. Response Surface Analysis and Variance Analysis. Box-Behnken Design in response surface analysis was used to establish mathematical model, take the angle of repose (AoR) as the index. Select coefficient of restitution (A), coefficient of static friction (B) and coefficient of rolling friction (C) to design the three-factor and three-level response surface experiment (table 5). Take the results in table 6 for regression analysis; the regression equation is AoR=11.3422-2.42976× A-0.81227+95.14584× C. After fitting, variance analysis for regression equation is shown in table 7.

| Table 5. Variables and levels of Box-Behnken Design. |
|------------------------------------------------------|
| level | A  | B  | C   |
|-------|----|----|-----|
| -1    | 0.2| 0.6| 0.10|
| 0     | 0.5| 0.8| 0.15|
| -1    | 0.8| 1.0| 0.20|

| Table 6. Experiment design and results of Box-Behnken. |
|-------------------------------------------------------|
| Experiment | A  | B  | C  | AoR (°) |
|------------|----|----|----|---------|
| 3          | -1 | 1  | 0  | 24.5661 |
| 15         | 0  | 0  | 0  | 23.9051 |
| 16         | 0  | 0  | 0  | 23.9051 |
| 2          | 1  | -1 | 0  | 22.2836 |
| 14         | 0  | 0  | 0  | 23.9051 |
| 12         | 0  | 1  | 1  | 27.9799 |
| 4          | 1  | 1  | 0  | 21.9730 |
| 5          | -1 | 0  | -1 | 18.9684 |
| 13         | 0  | 0  | 0  | 23.9051 |
| 7          | -1 | 0  | 1  | 28.6990 |
| 1          | -1 | -1 | 0  | 24.6823 |
| 6          | 1  | 0  | -1 | 18.8960 |
| 10         | 0  | 1  | -1 | 19.6906 |
| 9          | 0  | -1 | -1 | 18.7703 |
| 7          | 0  | 0  | 0  | 23.9051 |
| 11         | 0  | -1 | 1  | 29.7729 |
| 8          | 1  | 0  | 1  | 27.9319 |
Table 7. Variance analysis for the regression.

| Source      | Sum of Squares | Degree of Freedom | Mean Square | F value | P value | Significance |
|-------------|----------------|-------------------|-------------|---------|---------|--------------|
| Model       | 185.52         | 3                 | 61.84       | 151.79  | <0.0001 | significant  |
| A           | 4.25           | 1                 | 4.25        | 10.43   | 0.0066  |              |
| B           | 0.21           | 1                 | 0.21        | 0.52    | 0.4843  |              |
| C           | 181.05         | 1                 | 181.05      | 444.41  | <0.0001 |              |
| Residual    | 5.30           | 13                | 0.41        |         |         |              |
| Lack of Fit | 5.30           | 9                 | 0.59        |         |         |              |
| Pure Error  | 0.00           | 4                 | 0.00        |         |         |              |
| Cor Total   | 190.81         | 16                |             |         |         |              |

From the results, the significance level of the model is $P<0.0001$, indicating a high significance degree of the selected model. Comparing the F value, the order of the influence of each factor on AoR is $C>A>B$. And this also supports the conclusion proposed by Bharadwaj that coefficient of restitution hardly affects the calculation result when the material is in dense phase stacking motion without collision rebound [17]. The interaction of rolling friction and coefficient of restitution with AoR is shown in figure 7.

Figure 7. (a) Interaction of various factors on 3D surface diagram; (b) Contour fitting curve.

4.1.2. Determination of Optimal Parameters. The fluidity of bulk materials is good; the internal friction angle is considered equal to the angle of repose. The value of angle of repose tested laboratory is 35.4°. Calculate the coefficient of static friction using the AoR based on the formula: $B=\tan 35.4^\circ=0.711$. From figure 8, it proved that AoR changes with the isogradient of restitution and rolling friction. There are several collocation combinations that can make the value of AoR 35.4°.

Coefficient of restitution is calculated by the equation: $C = \sqrt{H_B/H_A}$. The principle of this conventional measurement is shown in figure 8. Particle A is free dropped down from height A. At the lowest point, the collision with the base made by particle material. According to the law of conservation of energy, particle A bounces to height B and transmits some of its energy to the base. Due to the fast collision process, use high-speed camera to capture. Refer to the similar experiment done by Qin [18], select $A=0.208$ as the coefficient of restitution. According to the regression equation obtained above, determine $C=0.26$ as the optimal parameters for Hertz-Mindlin contact model. The parameters can be considered to meet the requirements of the selected contact model when the mesoscopic behavior of particles is amplified to obtain the same state as the macroscopic angle of repose test in laboratory.
4.2. Calibration of Bonded Particle Model Parameter

Based on the above-mentioned modeling for entity, the simulated bending failure test of mastic beam was conducted by using software. The parameters of Hertz-Mindlin contact model obtained in the previous section are applied to the Bonded Particle model, further calibrate other uncertain parameters. The process is shown in figure 9.

4.2.1. Response Surface Analysis and Variance Analysis. Box-Behnken Design in response surface analysis was used to establish mathematical model for calibrating the Bonded Particle Model parameters used in bending failure simulation. Take the ultimate bending failure load (FL) as the index. Select normal stiffness per unit area (Sn), critical normal stress (σ_{max}) and bonded disk radius (σ_{bond}) to design the three-factor and three-level response surface experiment (table 8). Other parameters such as St can be calculated or inverse calculated by referring to the formula listed in section 3.2. Take the results in table 9 for regression analysis, after fitting, the results of variance analysis are shown in table 10.

| Level | Sn (×10^11 N/m^3) | σ_{max} (×10 MPa) | σ_{bond} (mm) |
|-------|-------------------|------------------|--------------|
| -1    | 3.4188            | 1.25             | 0.3          |
| 0     | 5.6980            | 1.50             | 0.4          |
| -1    | 7.9772            | 1.75             | 0.5          |
Table 9. Experiment design and results of Box-Behnken.

| Experiment | Sn | $\sigma_{\text{max}}$ | $R_{\text{bond}}$ | FL(N) |
|------------|----|----------------------|------------------|-------|
| 15         | 0  | 0                    | 0                | 1065  |
| 2          | 1  | -1                   | 0                | 870   |
| 9          | 0  | -1                   | -1               | 480   |
| 3          | -1 | 1                    | 0                | 1229  |
| 1          | -1 | -1                   | 0                | 760   |
| 12         | 0  | 1                    | 1                | 1393  |
| 4          | 1  | 1                    | 0                | 1100  |
| 10         | 0  | 1                    | -1               | 580   |
| 7          | -1 | 0                    | 1                | 1233  |
| 16         | 0  | 0                    | 0                | 1065  |
| 14         | 0  | 0                    | 0                | 1065  |
| 17         | 0  | 0                    | 0                | 1065  |
| 13         | 0  | 0                    | 0                | 1065  |
| 11         | 0  | -1                   | 1                | 1110  |
| 6          | 1  | 0                    | -1               | 500   |
| 8          | 1  | 0                    | 1                | 1258  |
| 5          | -1 | 0                    | -1               | 596   |

Table 10. Variance Analysis for the regression.

| Source     | Sum of Squares | Degree of Freedom | Mean Square | F value | P value | Significance |
|------------|----------------|-------------------|-------------|---------|---------|--------------|
| Model      | 1.272E+6       | 9                 | 1.413E+5    | 76.00   | <0.0001 | significant  |
| Sn         | 990.13         | 1                 | 990.13      | 0.53    | 0.4893  |              |
| $\sigma_{\text{max}}$ | 1.466E+5   | 1                 | 1.466E+5    | 78.85   | <0.0001 |              |
| $R_{\text{bond}}$ | 1.005E+6   | 1                 | 1.005E+6    | 540.67  | <0.0001 |              |
| Sn$\times$$\sigma_{\text{max}}$ | 14280.25   | 1                 | 14280.25    | 7.68    | 0.0276  |              |
| Sn$\times$$R_{\text{bond}}$ | 3600.00    | 1                 | 3600.00     | 1.94    | 0.2076  |              |
| R$\times$$\sigma_{\text{max}}$ | 8281.00    | 1                 | 8281.00     | 4.45    | 0.0728  |              |
| Sn2        | 5047.96       | 1                 | 5047.96     | 2.71    | 0.1434  |              |
| $\sigma_{\text{max}}^2$ | 6949.01    | 1                 | 6949.01     | 3.74    | 0.0945  |              |
| $R_{\text{bond}}^2$ | 74900.59   | 1                 | 74900.59    | 40.28   | 0.0004  |              |
| Residual   | 13016.25      | 7                 | 1859.46     |         |         |              |
| Lack of Fit| 13016.25      | 3                 | 4338.75     |         |         |              |
| Pure Error | 0.00          | 4                 | 0.00        |         |         |              |
| Cor Total  | 1.285E+6      | 16                |             |         |         |              |

From table 10, the significance level of the model is P<0.0001, indicating a high significance degree of the selected model. Comparing the F value, the order of the influence of each factor on ultimate bending failure load is: $R_{\text{bond}} > \sigma_{\text{max}} > \text{Sn}$. Among the P value, P(Sn)=0.4893 indicates that the stiffness per unit area has no significant influence on ultimate bending failure load. Only consider the interaction of stiffness per unit area, bonded disk radius with the failure load as shown in figure 10.
4.2.2. Determination of Optimal Parameters. Ultimate load of bending failure test for asphalt mastic in laboratory at -10°C is 1201 N; extract contour data for obtaining the formula of fitting curve, shown as below.

\[ R_{bond} = \frac{89.6}{\sigma_{\text{max}}} + 0.3743 \quad R^2=0.9934 \quad 0.3743 < R_{bond} \leq 0.5 \]  

(1)

The variation trend of the fitting curve corresponding to the relationship between bonded disk radius and critical normal stress that satisfy the different ultimate bending failure load values is consistent. Deduce that all the relationship can be calculated in such form \( R_{bond} = A/\sigma_{\text{max}} + B + C \).

Jingsong Shan pointed out that the ultimate strain was affected by different stiffness in the splitting experiment of asphalt mixture [19]. It is found that the value of different stiffness also affects the ultimate strain of the bending failure simulation test above. Using the formula of fitting curve, select \( R_{\text{bond}} = 0.45 \) mm, \( \sigma_{\text{max}} = 1.70175 \times 10^6 \) MPa as fixed values, modify Sn respectively 3.1339×10^11 N/m^3, 3.4188×10^11 N/m^3, 3.7037×10^11 N/m^3, conduct asphalt mastic bending failure simulation additionally. The flexural stress-strain curve was obtained and compared with laboratory test (figure 11). The ultimate flexural stress is approximately the same, and the ultimate bending failure load of all specimens remain around 1200 N in figure 11(b). The results support the validity of the response surface analysis that the ultimate bending failure load is related to the critical stress and bonded disk radius. Deflection is related to stiffness curve of Sn=3.4188×10^11 N/m^3, of which is closest to the laboratory test result, and difference of flexural strain energy density is small (figure 12). Sn=3.4188×10^11 N/m^3, \( R_{\text{bond}} = 0.45 \) mm, \( \sigma_{\text{max}} = 1.70175 \times 10^6 \) MPa are selected as the Bonded Particle model parameters.

Figure 10. (a) Interaction of various factors on 3D surface diagram; (b) Contour fitting curve.

Figure 11. (a) Flexural stress-strain curve; (b) Ultimate bending failure load.
5. Results and Discussion

5.1. Mesoscopic Behavior of the Bending Failure Simulation

The cracking of asphalt mastic beam at low temperature can be regarded as a process of energy dissipation [20]. During bending failure test simulation, the manual uniformly distributed load is applied initially, a fraction of particles in the upper portion of the beam contacted with punch appeared extrusion sliding. Color particles green according to the distribution and magnitude of the unbalanced force in figure 9. It can be seen that although the load is applied vertically to the top, not all the force passes vertically down, some diffuses laterally. The reason why the upper part of beam to be crushed is that some force does not diffuse in time, causing bonding beam colored pink broken, but negligible compared to the number of intact bonding beam. This internal phenomenon is not observed clearly in macroscopic laboratory test. At this point, some of the work done by external force is converted into the fracture energy, the other is stored in asphalt mastic beam as flexural strain energy until there is no bonding beam broken on the upper side of the neutral surface. Continue loading, all work done by the punch is completely stored as flexural strain energy with no bonding beam broken. When the ultimate deflection occurs, the bonding beams at the bottom of the span start to be broken. Macroscopically it appears as a fracture which goes through bottom and expands upwards and the distribution of the unbalanced force diffuses from mid to both sides, but the unbalance force at the crack tip is always the largest. Flexural strain energy is converted to surface energy release at last.

Assuming that the failure mode of the material corresponds to the energy state per unit volume, the fracture of the material can be represented by the function of the strain energy density, which is as follow [21].

\[
\frac{dW}{dV} = \int_0^{\varepsilon_{\text{max}}} \sigma \varepsilon \, d\varepsilon
\]

where \(dW/dV\) is the energy density; \(\varepsilon_{\text{max}}\) is the limiting strain; \(\sigma\) and \(\varepsilon\) are the components of stress and strain.

The value of \(dW/dV\) is the area of integral envelop under the curve before fracture. Calculate the flexural strain energy density in figure 11 (a). From the results shown in the figure 12, the greater the value of stiffness is, the smaller the index is at the low temperature. It shows that stiffness is an important factor affecting the crack resistance at low temperature.

5.2. Effect of Void Content

The deformation and damage of asphalt mastic with different air void contents are different. It is difficult to calculate the void distribution and void content accurately in conventional laboratory experiments. Simulation experiment can solve this problem effectively, greatly save time and material input. The shape of particle most commonly used in DEM simulation is spherical. The particle can't be shrunk down to fully fill indefinitely regardless of the simulation time. Therefore, it is necessary to
convert the void content, the conversion formula used is as follows.

\[
VC_{conv} = 1 - \frac{VC_{phys} - VC_{targ}}{0.5236}
\]  

(3)

where \(VC_{phys}\) is void content on physical macroscopic scale; \(VC_{targ}\) is equivalent to void content on mesoscopic mechanical scale after applying the contact model; 0.5236 is the value of volume of inscribed sphere \((r=0.5 \text{ mm})\) divided by the volume of cube \((1 \text{ mm} \times 1 \text{ mm} \times 1 \text{ mm})\).

Remove different number of particles in the random position, obtain the asphalt mastic for bending simulation with 4%; 6%; 8% void content. The void distribution is shown in figure 13.

![Figure 13: Void distribution.](image)

It can be seen from the results of bending failure tests with the increase of air void content in figure 14, the number of contact bonding points reduces, the bending failure load decreases, maximum deflection of the mid-span decreases but it is not obvious, the flexural strain energy density decreases, the low-temperature crack resistance weakens accordingly. Therefore, during the preparation of the asphalt mixture, asphalt mastic as a binding filling between the coarse aggregate, the mixing uniformity, sufficient or not has a strong influence on the low-temperature crack resistance of asphalt road.

![Figure 14: Variations with void content.](image)

6. Conclusion

1. Constructed discrete element model by using Hertz-Mindlin contact model coupling Bonded Particle contact model could accurately capture the mesoscopic structure of asphalt mastic. Visualization of mesoscopic mechanical behavior such as the distribution of force and bonding broken state is achieved.

2. Response surface analysis and variance analysis are effective for calibrating the parameters of mesoscopic contact model. Through the calibration process, determine that the adhesive strength and bonding area between particles co-influence the ultimate bending failure load, the contact stiffness per unit area influence the ultimate bending deflection.

3. Mathematical correlation formula between bonded disk radius and critical stress and that
satisfies the ultimate failure load of asphalt mastic beam at different temperatures can be fitted by such form $R_{\text{bond}}=A/\sigma_{\text{max}}B+C$. In this study, only list one formula fitting for asphalt mastic at -10°C. Other correlation formulas satisfying different materials at different temperature are similar, no need to elaborate here.

(4) The low-temperature crack resistance of asphalt mastic is weakened with the increase of void content. On the mesoscopic level, owing to the insufficient and uneven mixing of asphalt mortar such a binder between fine aggregates, the flexural strain energy density decreases with the contact bonding point reduction.

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