

# A modified Johnson-Kendall-Roberts contact model for pavement engineering: Consideration of time-dependent surface energy

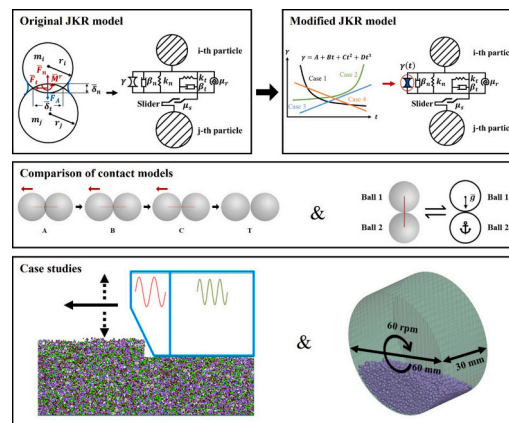
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## HIGHLIGHTS

- A modified JKR contact model variant is developed for pavement engineering.
- The differences between original and modified JKR contact models are investigated.
- Two cases of pavement engineering are studied using modified JKR contact model.

## GRAPHICAL ABSTRACT



## ARTICLE INFO

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## ABSTRACT

The Johnson-Kendall-Roberts (JKR) contact model is widely used in the discrete element method to simulate the dynamic behavior of particulate materials by assuming constant surface energy. However, under typical pavement conditions, such as asphalt mixture compaction and moist subgrade drying, particle surface energy varies with temperature and moisture content. This limits the accuracy of the traditional JKR model in capturing the evolution of inter-particle adhesion. To address this limitation, a time-dependent modified JKR contact model was proposed for pavement engineering applications. The modified model's performance was evaluated through a ball-ball pull-off test and validated via a ball gravity loading test based on the conservation of energy. Further, the case studies of pre-compaction and particle dewatering in pavement engineering were conducted using the modified JKR contact model. Results show that, under four different conditions, the compaction impulse increased by 15.57 %, 14.54 %, 13.04 %, and 14.87 %, indicating that the traditional model underestimates the additional compaction energy caused by enhanced adhesion and fails to accurately guide temperature control during compaction. For particle dewatering, the angle of repose decreased from 48.4° to 37.7°, reflecting the transition from a flowable to a stable particle structure. This enables better identification of the optimal construction window during the drying of subgrade materials. Overall, this study enhances the accuracy and

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applicability of the JKR contact model in pavement engineering by capturing dynamic adhesive behavior more realistically.

## 1. Introduction

The paving and compaction process of pavement directly determines the density and interlayer bonding performance of the pavement structure, which has a decisive impact on its long-term service performance and durability [1,2]. Insufficient or uneven compaction can easily lead to voids, cracks, and early damage [3,4]. In addition, the drainage performance of the subgrade and base layer plays a critical role in maintaining the structural integrity and service life of pavement systems. Inadequate drainage can result in water accumulation, weakening the bearing capacity of the base, accelerating material degradation, and eventually causing structural failures such as rutting and heaving [5,6]. Since both the base layer and paving processes involve complex granular material behavior, it is essential to clearly understand the particle-scale interactions and migration mechanisms during these stages. Without such understanding, the design and construction of pavement structures risk overlooking key factors that influence stability and durability under real-world conditions.

With the development of computational technology, the discrete element method (DEM) [7,8] has gradually become an important tool for studying asphalt pavement paving, compaction, and subbase degradation behavior due to its ability to reveal the internal structural evolution and microscopic mechanical mechanisms of materials at the particle scale [9–11]. DEM simulations can effectively capture fine-scale phenomena such as particle rearrangement, local stress concentration,

fragmentation, and shear failure, thereby providing theoretical support for optimizing construction processes and improving pavement performance [12,13]. In DEM, the contact model is the core component for simulating interparticle interactions. It is used to characterize the mechanical behavior between particles, which in turn determines the mechanical response and structural evolution of materials at the macro level. The selection of the contact model has a decisive impact on the simulation accuracy [14]. If the contact model fails to accurately reflect the actual particle contact behavior, it will be impossible to accurately predict the compaction density, shear failure mode, or structural stability, which in turn will affect the evaluation of pavement performance and design decisions. Traditional contact models mainly include the linear contact model [7] and the Hertz-Mindlin contact model [15], the former being suitable for elastic contact and the latter for describing nonlinear contact behavior. However, both contact models are only applicable to describing the interactions between non-viscous particles.

For materials with adhesive effects, such as asphalt mixtures or wet particle systems, the Johnson-Kendall Roberts (JKR) contact model [16] has been widely used to simulate interparticle adhesive behavior because it can take into account the attractive forces caused by surface energy. Existing studies based on the JKR model have achieved good application results in various fields. Xie et al. studied the adhesion mechanism of asphalt films based on the JKR contact model [17]. Xia et al. [18] and Zhou et al. [19] calibrated the discrete element parameters of wet coal particles and wet sand particles based on the JKR

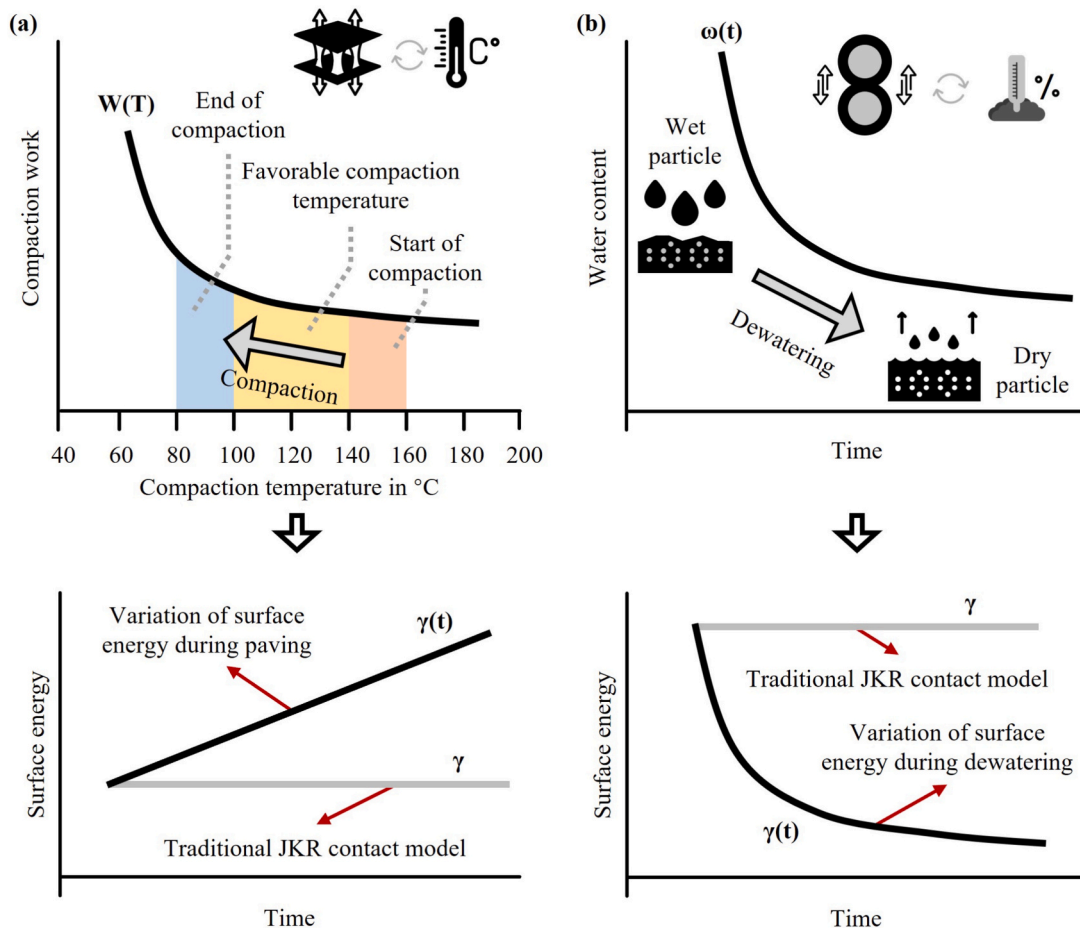


Fig. 1. Relationship between surface energy and time for (a) asphalt pavement compaction, (b) wet particles dewatering for subgrades.

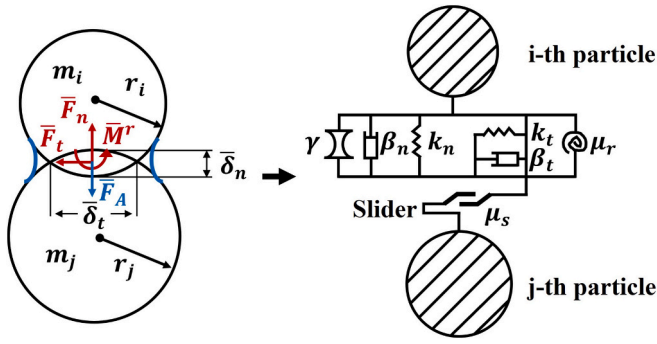


Fig. 2. Johnson-Kendall-Roberts (JKR) contact model.

contact model, respectively. Deng et al. [20] and Yan et al. [21] investigated the influence of JKR surface energy on the flow properties of fresh concrete in discrete element simulations. Zhao et al. evaluated the adhesion performance of high surface energy inorganic materials based on the JKR contact model [22]. Zhu et al. used JKR surface energy to characterize the macroscopic cohesion of lunar soil simulants [23]. In addition, the JKR contact model has also been successfully applied in characterizing capillary forces between wet particles [24,25].

Although the traditional JKR model can simulate the mechanical behavior of adhesive materials, one of its key assumptions—that surface energy is constant—is often not valid in dynamic engineering processes, particularly in the following two typical scenarios encountered in pavement engineering. In the first case (see Fig. 1 (a)), during the pre-compaction of asphalt mixtures [13,26,27], surface energy increases with decreasing temperature within a certain temperature range [28,29], leading to stronger particle adhesion. This directly affects compaction effort and final density. If surface energy is assumed constant, the model underestimates energy demand and misjudges the

effects of temperature on compaction quality. In the second case (see Fig. 1 (b)), during the dewatering of wet subgrades or base layers [30–32], surface energy gradually decreases as moisture content decreases and capillary forces weaken [33,34]. This weakens particle adhesion and causes the material to transition from a flowable to a stable granular structure. The JKR model cannot capture this evolution, making it difficult to assess the true state of the material. As a result, premature construction on undried layers may lead to structural voids or interlayer failure. These two scenarios highlight the necessity of incorporating variable surface energy into particle-scale models to improve accuracy in simulating thermal and moisture-dependent behaviors during pavement construction.

In summary, the absence of contact models capable of dynamically capturing the evolution of surface energy limits the ability of DEM to reflect realistic interparticle behavior, thereby restricting its applicability in critical pavement construction stages such as dynamic compaction and dewatering. To address this research gap, this study will propose a variant of the JKR contact model with time-dependent surface energy. The modified JKR contact model will be capable of dynamically adjusting the interparticle adhesive force according to changes in temperature or moisture content, thereby more accurately simulating the evolution behavior of particle systems under actual construction conditions. The modified JKR contact model will be validated through a ball-ball pull-off test and a gravity loading test, and will subsequently be applied to the pavement pre-compaction simulation and the dewatering simulation of wet particles.

## 2. JKR contact model with time-varying surface energy

The discrete element contact model describes the contact force between particles, achieved through the combination of different mechanical components. The visualization of the original JKR contact model [16] is shown in Fig. 2.

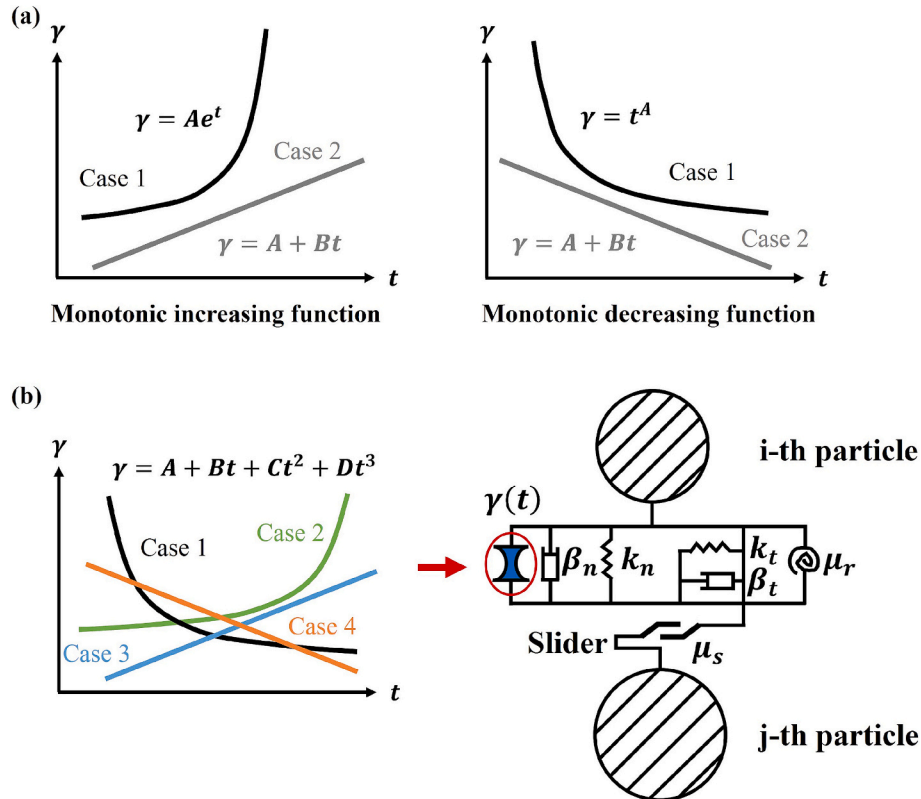


Fig. 3. Selection of fitting functions: (a) Fitting based on monotonic functions, (b) surface energy fitting based on cubic polynomials for the modified Johnson-Kendall-Roberts contact model.

In the contact model of the DEM, the forces are decomposed into contact  $\bar{F}^c$  and damping forces  $\bar{F}^d$ . The contact and damping forces can each be decomposed into normal  $\bar{F}_n$  and tangential forces  $\bar{F}_t$ . For the original JKR contact model, the normal contact force is:

$$\bar{F}_n = \frac{4E_{ij}\bar{a}^3}{3r_{ij}} - \sqrt{16\pi\gamma E_{ij}\bar{a}^3} \quad (1)$$

where  $E_{ij}$ ,  $\bar{a}$ ,  $r_{ij}$ , and  $\gamma$  are the effective Young's modulus, contact patch radius, contact effective radius, and surface energy, respectively.

The effective Young's modulus is given by:

$$E_{ij} = \left( \frac{(1-\nu_i^2)}{E_i} + \frac{(1-\nu_j^2)}{E_j} \right)^{-1} \quad (2)$$

where  $E_i$  and  $E_j$  are the Young's modulus of the two particles.  $\nu_i$  and  $\nu_j$  are the corresponding Poisson's ratios.

The contact patch radius  $\bar{a}$  is related to the normal overlap at the contact  $\bar{\delta}_n$  according to the following non-linear expression:

$$\bar{\delta}_n = \frac{\bar{a}^2}{r_{ij}} - \sqrt{\frac{4\pi\gamma\bar{a}}{E_{ij}}} \quad (3)$$

where the normal overlap at the contact  $\bar{\delta}_n$  is updated after each computational step of the DEM, and the analytical solution for the contact patch radius  $\bar{a}$  can be found according to [35].

The contact effective radius is given by:

$$r_{ij} = \left( \frac{1}{r_i} + \frac{1}{r_j} \right)^{-1} = \frac{r_i r_j}{r_i + r_j} \quad (4)$$

where  $r_i$  and  $r_j$  are the radius of the two particles.

The tangential contact force is:

$$\bar{F}_t = \begin{cases} \bar{S}_t \bar{\delta}_t, & \|\bar{S}_t \bar{\delta}_t\| \leq |\mu_s (\bar{F}_n + 6\pi\gamma r_{ij})| \\ \mu_s (\bar{F}_n + 6\pi\gamma r_{ij}), & \text{otherwise} \end{cases}$$

$$\text{with } \bar{S}_t = 8G_{ij}\bar{a} \quad (5)$$

where  $\bar{\delta}_t$ ,  $\mu_s$ , and  $G_{ij}$  are the tangential overlap at the contact, coefficient of static friction, and effective shear modulus, respectively.

The effective shear modulus is given by:

$$G_{ij} = \left( \frac{2-\nu_i}{G_i} + \frac{2-\nu_j}{G_j} \right)^{-1} \quad (6)$$

where  $G_i$  and  $G_j$  are the shear modulus of the two particles.

For the modified JKR contact model in this study, the surface energy was considered as a function of time  $\gamma(t)$  rather than a constant  $\gamma$ . Therefore, the normal contact force in Eq. (1) can be rewritten as:

$$\bar{F}_n = \frac{4E_{ij}\bar{a}^3}{3r_{ij}} - \sqrt{16\pi\gamma(t)E_{ij}\bar{a}^3} \quad (7)$$

In practical engineering applications, the surface energy–time relationship is typically monotonic, such as increasing during asphalt cooling or decreasing during particle dewatering. Theoretically, various models can be employed to fit the surface energy–time relationship, such as linear functions, exponential functions, and power functions (see Fig. 3 (a)). However, the rate of change is usually nonlinear and may vary across different stages of the process. Linear functions fail to capture this nonlinearity, while exponential and power functions are constrained by their single-curvature characteristics, which limits their ability to represent complex variations in the change rate. By contrast, a cubic polynomial provides greater flexibility: it can degenerate into a linear form, effectively capture monotonic nonlinear behaviors, and even accommodate non-monotonic trends if they occur (see Fig. 3 (b)).

In addition, the polynomial form is computationally simple, numerically stable, and well-suited for stepwise DEM simulations. Therefore, once the surface energy values at different temperatures or moisture contents are obtained, the surface energy–time curve can be fitted using the cubic polynomial function. It is noteworthy that for the pre-compaction process, the relationship between surface energy and time is essentially a mapping of the relationship between surface energy and temperature. For the wet particle dewatering process, the relationship between surface energy and time is essentially a mapping of the relationship between surface energy and moisture content. This is because temperature-dependent or moisture-dependent surface energy cannot be directly described in DEM. Therefore, the relevant issues need to be reformulated as the process of surface energy changing with time. Since DEM calculations proceed stepwise in time, constructing a time-dependent surface energy function provides a practical and implementable solution. In this study, the following cubic polynomial function was used to describe the time-varying surface energy:

$$\gamma(t) = A + Bt + Ct^2 + Dt^3 \quad (8)$$

where  $A$ ,  $B$ ,  $C$ , and  $D$  are the parameters to be fitted.

The damping forces for both JKR contact models are:

$$\bar{F}_n^d = -2\beta_n \bar{u}_n^{\text{rel}} \sqrt{\bar{S}_n m_{ij}}$$

$$\bar{F}_t^d = -2\beta_t \bar{u}_t^{\text{rel}} \sqrt{\bar{S}_t m_{ij}}$$

$$\text{with } \bar{S}_n = 2E_{ij}\bar{a} \quad (9)$$

where  $\beta_n$ ,  $\beta_t$ ,  $\bar{u}_n^{\text{rel}}$ ,  $\bar{u}_t^{\text{rel}}$ , and  $m_{ij}$  are the normal critical damping ratio, shear critical damping ratio, relative normal translational velocity, relative tangential translational velocity, and equivalent mass of the particle, respectively.

The critical damping ratio  $\beta$  is related to the coefficient of restitution (COR)  $e$ , and the relationship between them is as follows:

$$\beta = \frac{-\ln(e)}{\sqrt{\pi^2 + (\ln(e))^2}} \quad (10)$$

The equivalent mass of the particle is given by:

$$m_{ij} = \left( \frac{1}{m_i} + \frac{1}{m_j} \right)^{-1} = \frac{m_i m_j}{m_i + m_j} \quad (11)$$

where  $m_i$  and  $m_j$  are the mass of the two particles.

For both JKR contact models, the external moment is created by the rolling resistance moment:

$$\bar{M}^r = \begin{cases} -\bar{S}_t r_{ij}^2 \bar{\theta}^{\text{rel}}, & \|\bar{M}^r\| \leq |\mu_r r_{ij} (\bar{F}_n + 6\pi\gamma r_{ij})| \\ \mu_r r_{ij} (\bar{F}_n + 6\pi\gamma r_{ij}), & \text{otherwise} \end{cases} \quad (12)$$

where  $\bar{\theta}^{\text{rel}}$  and  $\mu_r$  are the relative rotation angle and rolling friction coefficient, respectively. In DEM, mechanical energy consists of body energy  $E_{\text{body}}$  and contact energy  $E_{\text{contact}}$ :

$$E_{\text{mechanical}} = E_{\text{body}} + E_{\text{contact}} \quad (13)$$

Mechanical body energy is the energy related to body motion. These include the energy due to body forces, where body forces are defined to be gravity loading and applied forces and moments, the energy dissipated by local damping, and the kinetic energy:

$$E_{\text{body}} = E_{\text{body\_forces}} + E_{\text{local\_damping}} + E_{\text{kinetic}} \quad (14)$$

For both JKR contact models, the contact energy consists of five components: strain energy  $E_k$ , slip energy  $E_\mu$ , dashpot energy  $E_\beta$ , rolling strain energy  $E_{k_r}$ , and rolling slip energy  $E_{\mu_r}$ :



$$E_{\text{contact}} = E_k + E_\mu + E_\beta + E_{k_r} + E_{\mu_r} \quad (15)$$

The strain energy is stored in nonlinear springs and is defined as the energy dissipated due to contact deformation:

$$E_k = \frac{1}{2} (\bar{F}_{n_0}^c + \bar{F}_n^c) \bar{\delta}_n + \frac{1}{2} (\bar{F}_{t_0}^c + \bar{F}_t^c) \bar{\delta}_t^k$$

with  $\bar{\delta}_t^k = \frac{\bar{F}_t^c - \bar{F}_{t_0}^c}{\bar{S}_t}$  (16)

where  $\bar{F}_{n_0}^c$  and  $\bar{F}_{t_0}^c$  are the JKR normal and shear forces at the beginning of the time step.

The slip energy is defined as the total energy dissipated by frictional slip:

$$E_\mu = -\frac{\bar{F}_{t_0}^c}{2\bar{S}_t} (\bar{F}_{t_0}^c + \bar{F}_t^c) \quad (17)$$

The dashpot energy is defined as the total energy dissipated by the dashpots:

$$E_\beta = -\bar{F}^{\text{d-rel}} \bar{u} \Delta t \quad (18)$$

where  $\Delta t$  is the time step.

The rolling strain energy is stored in rolling springs and is defined as the energy dissipated due to rolling deformation:

$$E_{k_r} = \frac{\|\bar{M}^r\|^2}{16G_{ij}\bar{a}r_{ij}^2} \quad (19)$$

The rolling slip energy is defined as the total energy dissipated by rolling slip:

$$E_{\mu_r} = -\frac{1}{2} (\bar{M}_0^r + \bar{M}^r) \bar{\theta}^r$$

with  $\bar{\theta}^r = \bar{\theta}^{\text{rel}} - \left( \frac{\bar{M}^r - \bar{M}_0^r}{8G_{ij}\bar{a}r_{ij}^2} \right)$  (20)

where  $\bar{M}_0^r$  is the rolling resistance moment at the beginning of the time step.

The above content introduced the equations for calculating the relevant parameters of the two JKR contact models. The significant differences between the two models arise from the formulation of the normal contact force (cf. Eq. (1) and Eq. (7)). In the modified JKR contact model, the surface energy is time-dependent, making the normal contact force a dynamic quantity. Consequently, all parameters associated with the normal contact force are also affected. As a result, the formulations of Eqs. (5), (12), (16), (17), (19), and (20) differ from those in the original JKR model when the modified version is applied. These distinctions form the basis for the comparison, validation, and application of the proposed model.

### 3. Comparison of contact models

In this study, a user-defined model based on the original JKR contact model was recoded using Particle Flow Code (PFC) 3D. The time-varying surface energy  $\gamma(t)$  (cf. Eq. (8)) replaced the constant surface energy  $\gamma$  to characterize the time-dependent adhesion between particles.

#### 3.1. Ball-ball pull-off test

To clearly illustrate the significant differences between the modified JKR contact model and the original JKR contact model, a normal ball-ball pull-off test was used as a benchmark example. This test provides a controlled, idealized scenario that highlights the differences in the behavior of the two models under the same conditions, and has been widely used in previous theoretical studies of contact models [36,37].

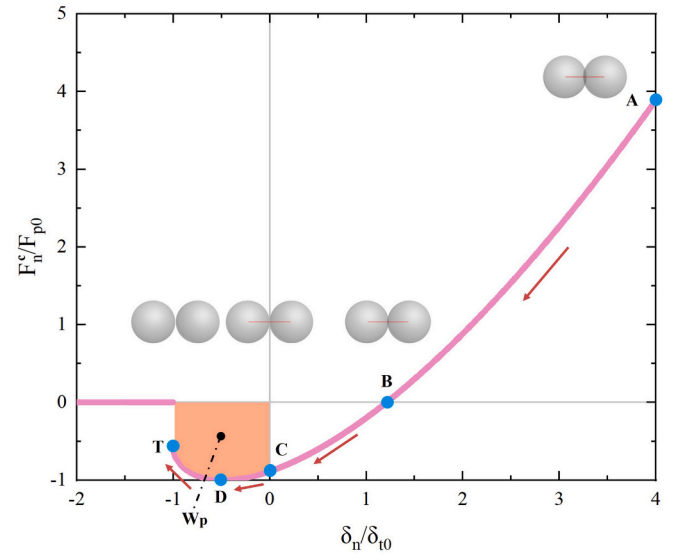


Fig. 4. Contact force-displacement relationship for the original JKR contact model.

For convenience of description, the following symbols took the form of scalars in the normal direction. They should be distinguished from the vector forms that appeared in the previous section. Fig. 4 shows the relationship between contact force and displacement in the original JKR contact model for the normal pull-off test between two balls.

To facilitate description, all values were normalized first. The maximum tensile force between the balls is defined as the pull-off force [38]:

$$F_{p0} = 3\pi\gamma r_{ij} \quad (21)$$

The pull-off force  $F_{p0}$  is independent of the elastic properties and is only dependent on the particle size and surface energy. The normal contact force  $F_n^c$  can be normalized using  $F_{p0}$ . In addition, the tear-off distance  $\delta_{t0}$  is defined for normalization of the normal contact overlap  $\delta_n$ . The tear-off distance is the separation distance at which the contact breaks under tension:

$$\delta_{t0} = \frac{a_0^2}{2\sqrt{6}r_{ij}} \quad (22)$$

where  $a_0$  is the contact patch radius at which  $F_n^c = 0$ , i.e., the point of equilibrium when no external forces are acting:

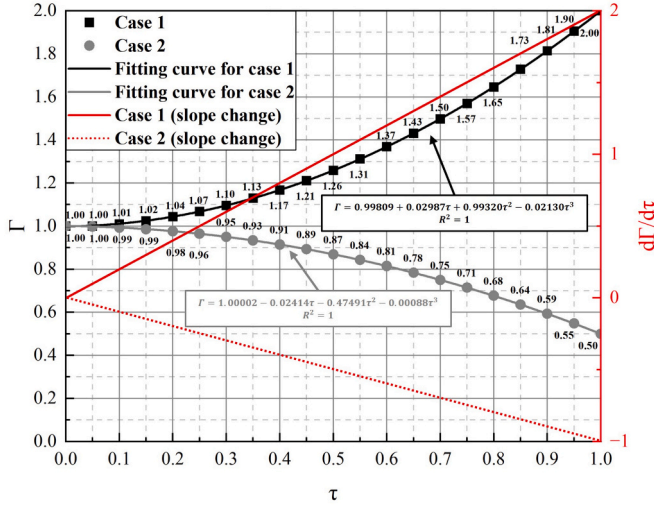
$$a_0 = \sqrt[3]{\frac{9\pi\gamma r_{ij}^2}{E_{ij}}} \quad (23)$$

Two overlapping balls were created: one remained static, while the other moved at a uniform speed in the opposite direction. At the starting point A, the contact deformation reached its maximum value, while the repulsive force was also maximum. As the ball moved, the overlap gradually decreased, and the repulsive force also decreased. The contact force reached equilibrium at point B, i.e., the repulsive force was equal to the attractive force. At this point,  $a = a_0$ . The ball continued to move until the overlap at point C was zero. According to the JKR theory [16], the contact force at point C corresponds to a specific value,  $F_C = -\frac{8}{9}F_{p0}$ . The elastic energy of the ball was converted into kinetic energy as it moved from point A to point C. At point C, all elastic energy was converted to kinetic energy. The ball continued to move, but it was no longer affected by the repulsive force because there was no direct ball-ball contact; the interaction between the two balls was influenced only by van der Waals attraction. At point D, the attractive force will be at its maximum due to the necking effect, i.e.,  $F_D = F_{p0}$ . Until the tear-off

**Table 1**

Contact force, overlap, contact patch radius at points B, C, D, T.

| Point | $F_n^c$                         | $\delta_n$                                               | $a$                                             |
|-------|---------------------------------|----------------------------------------------------------|-------------------------------------------------|
| B     | 0                               | $\sqrt[3]{\frac{3\pi^2\gamma^2 r_{ij}^2}{E_{ij}^2}}$     | $\sqrt[3]{\frac{9\pi\gamma r_{ij}^2}{E_{ij}}}$  |
| C     | $-\frac{24}{9}\pi\gamma r_{ij}$ | 0                                                        | $\sqrt[3]{\frac{4\pi\gamma r_{ij}^2}{E_{ij}}}$  |
| D     | $-3\pi\gamma r_{ij}$            | $-\sqrt[3]{\frac{3\pi^2\gamma^2 r_{ij}^2}{16E_{ij}^2}}$  | $\sqrt[3]{\frac{9\pi\gamma r_{ij}^2}{4E_{ij}}}$ |
| T     | $-\frac{15}{9}\pi\gamma r_{ij}$ | $-\sqrt[3]{\frac{27\pi^2\gamma^2 r_{ij}^2}{16E_{ij}^2}}$ | $\sqrt[3]{\frac{\pi\gamma r_{ij}^2}{4E_{ij}}}$  |

**Fig. 5.** Surface energy-time relationship.

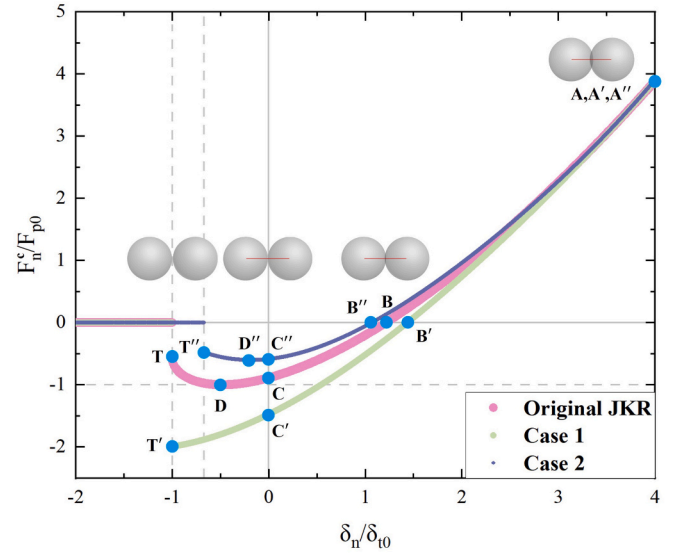
point T, there was an attractive force between the balls. After the tear-off point T, the contact force mutated to 0, i.e., there was no more attractive force between the balls. The contact force at the tear-off point T corresponded to a specific value,  $F_T = -\frac{5}{9}F_{p0}$ . The contact force, overlap, and contact patch radius at points B, C, D, and T can be calculated analytically. They are provided in Table 1.

$W_p$  denotes the work of adhesive peeling, i.e., the work required to pull two adhered balls apart to create new surfaces. This work of adhesive peeling can be quantified by calculating the area above the curve CDT and is given by:

$$W_p = \int_{\delta_c}^{\delta_T} F_n^c d\delta = \int_{a_c}^{a_T} \left( \frac{4E_{ij}a^3}{3r_{ij}} - \sqrt{16\pi\gamma E_{ij}a^3} \right) \left( \frac{2a}{r_{ij}} - \sqrt{\frac{\pi\gamma}{E_{ij}a}} \right) da$$

$$= \frac{\sqrt[3]{4\pi^5} + 12\sqrt[3]{2\pi^5}}{5} \sqrt[3]{\frac{\gamma^5 r_{ij}^4}{E_{ij}^2}} \approx 22.516 \sqrt[3]{\frac{\gamma^5 r_{ij}^4}{E_{ij}^2}} \approx 0.936 F_{p0} \delta_{t0} \quad (24)$$

To compare the significant differences between the modified JKR contact model and the original JKR contact model, two different cases of time-varying surface energy were considered: with increasing time, the surface energy eventually increased to twice the initial value and decreased to half of the initial value (see Fig. 5). During this process, the slope of the curve continuously changes, representing the rate of change of the surface energy. Based on the slopes at different times, the corresponding surface energy values can be determined. Finally, the scattered data points were fitted using Eq. (8) to obtain the parameters of the function. In this process, since the slope variation is linear, the corresponding discrete points are unique. The following equation was used to normalize the values:

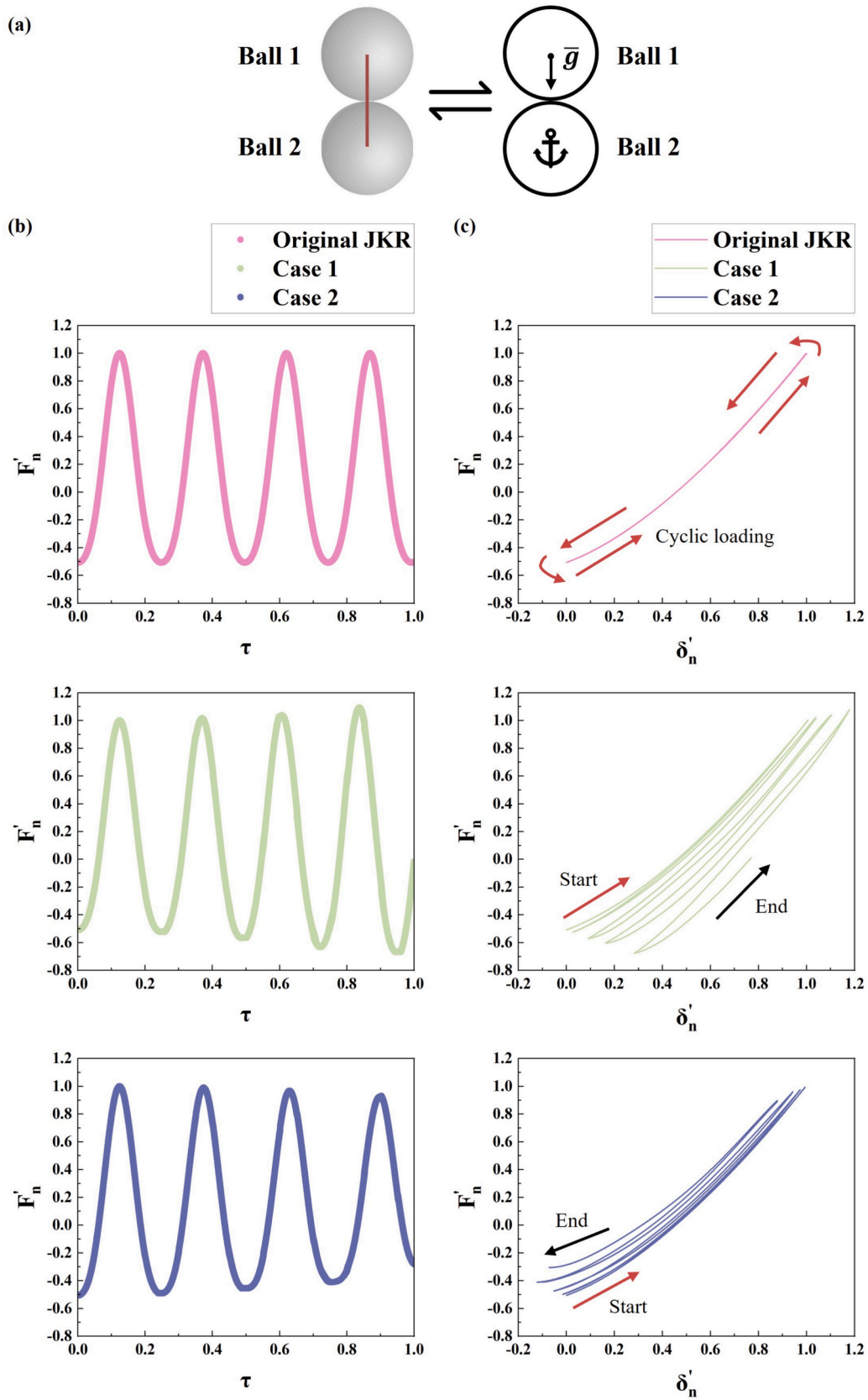
**Fig. 6.** Comparison of the contact force-displacement relationship for the original JKR contact model and the JKR contact model with time-dependent surface energy.

$$\tau = \frac{t}{t_{end}}$$

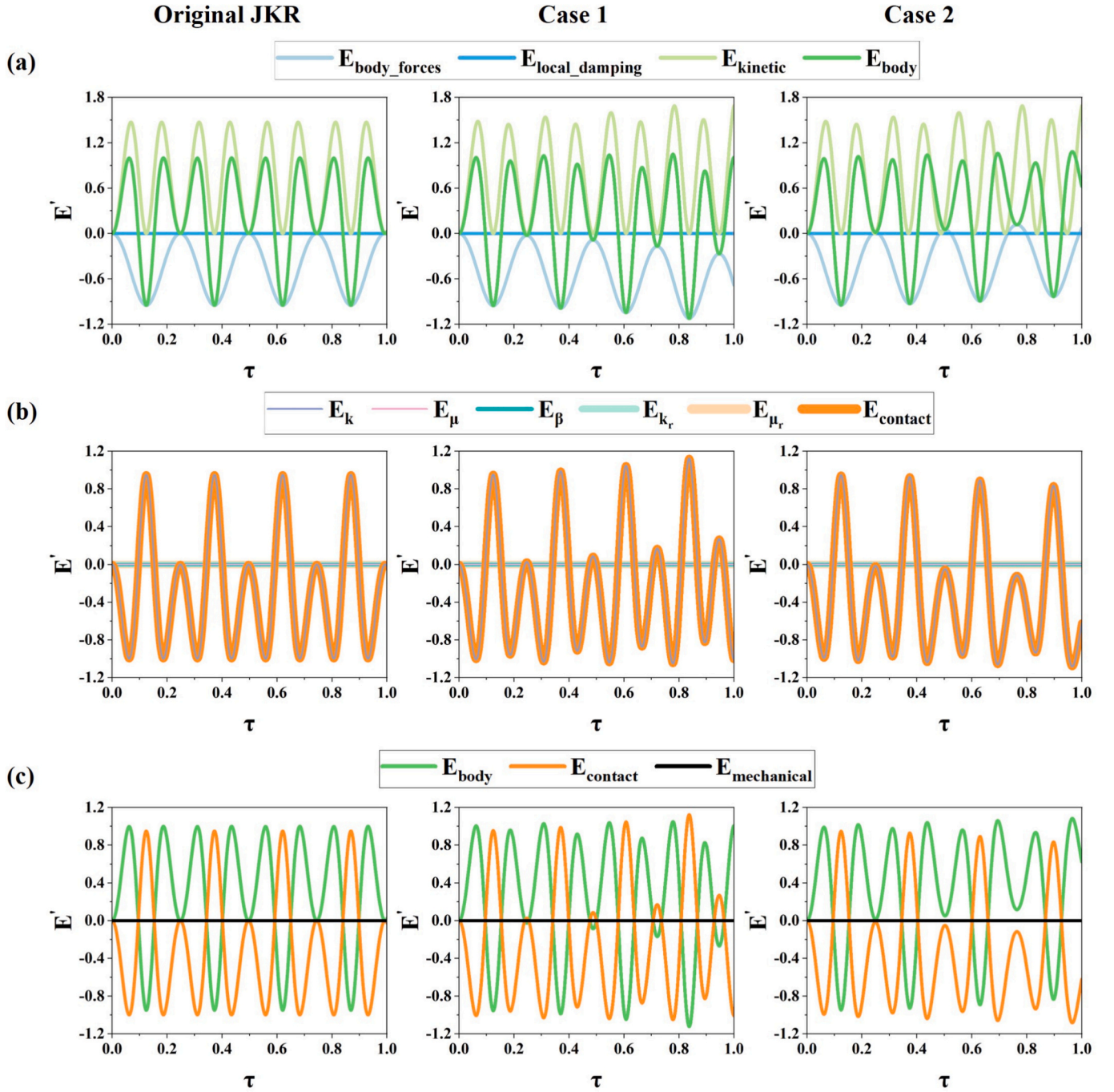
$$\Gamma(\tau) = \frac{\gamma(t)}{\gamma} \quad (25)$$

where  $t_{end}$  and  $\gamma$  are the total time and constant surface energy of the simulation using the original JKR contact model, respectively.  $\tau = 0$  and  $\tau = 1$  correspond to the times at the beginning of the simulation (point A in Fig. 4) and balls tear-off (point T in Fig. 4), respectively.

According to the relationship of surface energy-time in Fig. 5, the same simulation of normal pull-off between balls was performed. As shown in Fig. 6, the curves of contact force-displacement for the modified JKR contact model and the original JKR contact model were plotted together. At the starting points A, A', and A'', there was no difference between the three cases since the surface energies were the same. As the ball moved, the slope of the curve decreased at the slowest rate for Case 1; the slope of the curve decreased at the fastest rate for Case 2; and the slope of the curve for the original JKR contact model decreased at a rate between the above two cases. Points B'' and B' were distributed on the left and right sides of point B. Point B'' corresponded to the case of smaller overlap, i.e., less repulsive force; therefore, it corresponded to a smaller attractive force at force equilibrium (lower surface energy). Point B' corresponded to the case of larger overlap; therefore, it corresponded to a larger attractive force at force equilibrium (higher surface energy). On the same vertical coordinate, from top to bottom, this was Case 2, the original JKR contact model, and Case 1. This is because, for the same overlap, the repulsive force is the same; then, for the same overlap, the greater the surface energy, the greater the attractive force. At zero overlap, from top to bottom, the points C'', C, and C' were in order. For Case 2, the attractive force will reach its maximum at point D'' due to the necking effect; at the tear point T'', the tear-off force between the balls reached its limit when  $F_{T''} = -\frac{5}{9}F_{D''}$ . For Case 1, the tear-off of the balls was different from the other two cases: there was no necking effect between the balls because the limit distance of attraction (point T') was reached before the necking effect. Further, numerical integration was employed to quantify the work of adhesive peeling for Case 1 and Case 2. The CT curve corresponding to the work of adhesive peeling was  $1.778F_{p0}\delta_{t0}$ ; the C'D''T'' curve corresponding to the work of adhesive peeling was  $0.379F_{p0}\delta_{t0}$ . Both values are 1.899 and 0.405 times the work



**Fig. 7.** Ball gravity loading test without considering damping: (a) Boundary conditions for ball gravity loading, (b) normal contact force-time curves, (c) normal contact force-overlap curves.



**Fig. 8.** Ball gravity loading test without considering damping: (a) Body energy curves for different cases, (b) contact energy curves for different cases, (c) mechanical energy for different cases.

of adhesive peeling in the original JKR contact model, respectively.

### 3.2. Gravitational loading test of ball

As shown in Fig. 7 (a), the gravitational loading test of the ball was used to illustrate the difference between the modified JKR contact model and the original JKR contact model. At the beginning of the simulation, ball 1 and ball 2 just started to make contact (zero contact overlap); both balls had a radius of 0.05 m and a density of 1000 kg/m<sup>3</sup>. Ball 2 was completely fixed, and ball 1 was only affected by gravity. For the original JKR contact model, the surface energy of ball 1 was set to 100 J/m<sup>2</sup>. For the modified JKR contact model, the surface energy of ball 1 was scaled using the functional relationship in Fig. 5. The effect of damping

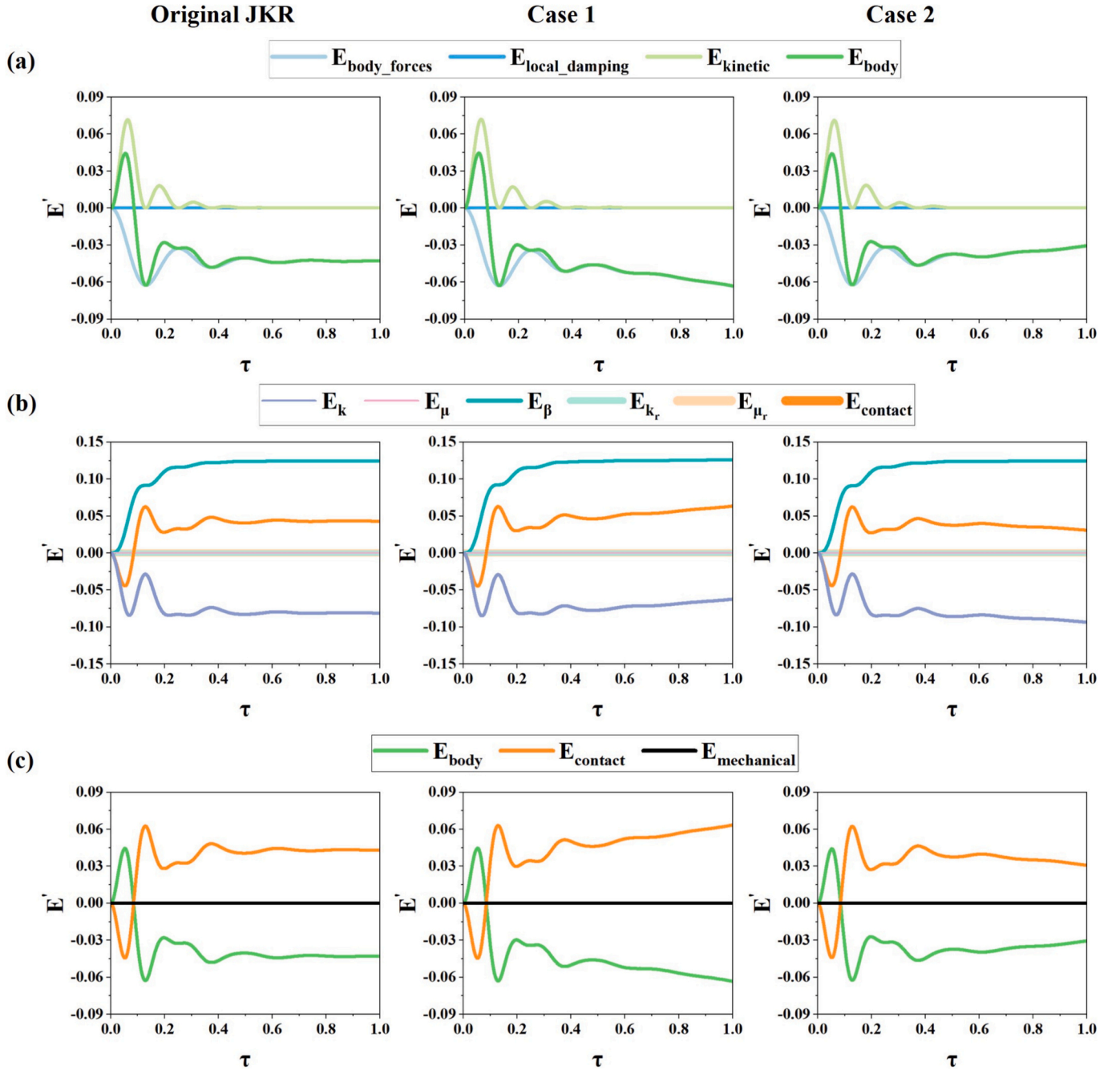
forces on the balls was not considered. The simulations for all cases used the same time, which was normalized according to Eq. (25). In addition, normal contact force and normal overlap were normalized using the following equations:

$$F'_n = \frac{F_n^c}{F_{nO\_JKR\_max}^c}$$

$$\delta'_n = \frac{\delta_n}{\delta_{nO\_JKR\_max}}$$
(26)

where  $F_{nO\_JKR\_max}^c$  is the peak of normal contact force in the original JKR contact model and  $\delta_{nO\_JKR\_max}$  is the maximum value of normal overlap in the original JKR contact model.





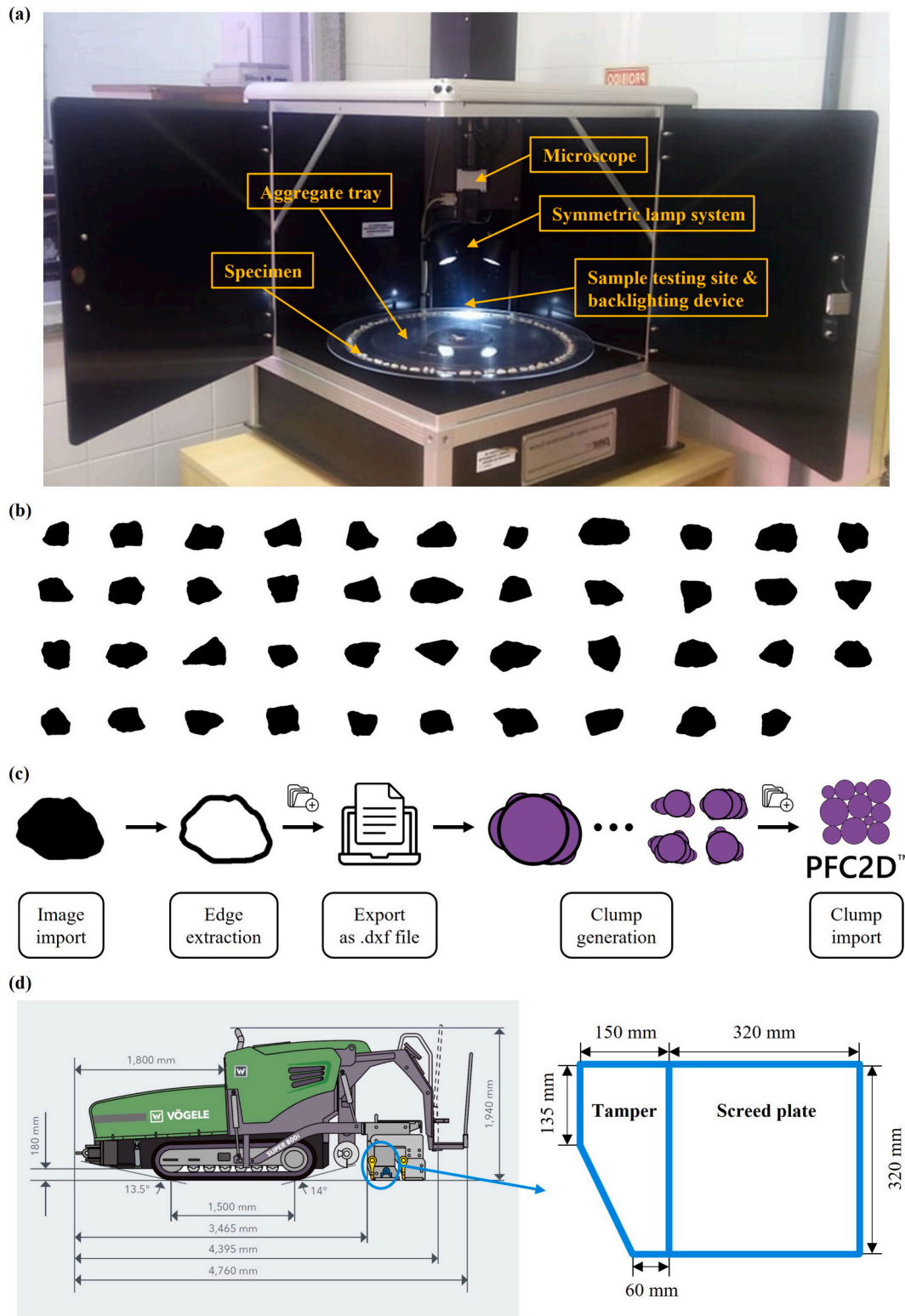
**Fig. 9.** Ball gravity loading test considering damping: (a) Body energy curves for different cases, (b) contact energy curves for different cases, (c) mechanical energy for different cases.

Fig. 7 (b) and Fig. 7 (c) show the normal contact force-time curves and normal contact force-overlap curves for three cases. The red arrows in the 1st plot of Fig. 7 (c) represent cyclic loading paths; the red arrows in the 2nd and 3rd plots of Fig. 7 (c) represent loading paths at the beginning of the simulation, and the black arrows represent loading paths at the end of the simulation. For the original JKR contact model, the normal overlap was zero at the start of loading. Under the effect of gravity, ball 1 was in contact with ball 2, and the normal overlap increased. At the maximum of normal overlap  $\delta'_n = 1$ , ball 1 rebounded and moved in the reverse direction until it reached  $\delta'_n = 0$ . The above steps were repeated until the end of the simulation. According to the curve in the 1st plot of Fig. 7 (b), it was known that a total of 4 full cycles were sustained.

Compared to the original JKR contact model, the maximum normal

overlap in Case 1 increased; the distance between the ball and the starting point during rebound also increased. The above process was repeated until the end of the simulation. According to the curve in the 2nd plot of Fig. 7 (b), it can be seen that the peak of the curve was continuously increasing and continued for more than four cycles. This is attributed to the fact that the increase in attraction has advanced the time point for equilibrating the repulsive forces; therefore, the loading cycle has shrunk. Compared to the original JKR contact model, the maximum normal overlap in Case 2 decreased; the ball exceeded the starting point during the rebound, and the distance increased. According to the curve in the 3rd plot of Fig. 7 (b), it can be seen that the peak of the curve was continuously decreasing and continued for less than four cycles. This is attributed to the fact that the decrease in attraction has lagged the time point for equilibrating the repulsive forces; therefore,





**Fig. 10.** Preparation of numeric model for pre-compaction simulation: (a) The Aggregate Imaging System (AIMS), (b) shape of 2D aggregates, (c) discrete element representation of 2D aggregates, (d) 2D geometry of the paver.

the loading cycle has expanded.

In addition to the normal contact force curves, different energy-time curves were also demonstrated, as shown in Fig. 8. The following equation was used to normalize the energy:

$$E' = \frac{E_{\phi}}{E_{body0\_JKR\_max}} \quad (27)$$

where  $E_{\phi}$  is any energy and  $E_{body0\_JKR\_max}$  is the maximum body energy in the original JKR contact model.

Fig. 8 (a) shows the body energy curves for different cases. For the

original JKR contact model, the ball returned to the starting point after each loading, so each energy curve showed a periodic variation. For Case 1, the ball returned further away from the starting point each time; this resulted in less gravitational potential energy at the furthest return position, i.e., the peak value of the body force energy was decreasing. Since the waveform of the body force energy was no longer symmetrical, the waveform of the kinetic energy for each set of two also exhibited an irregular shape. The peak of kinetic energy increased with every other wave. For Case 2, the ball rebounded past the starting point, moving farther away with each return; this resulted in greater gravitational potential energy at the furthest return position, i.e., the peak value of the body force energy was increasing. The pattern of change in kinetic energy was similar to Case 1. For each of these three cases, the energy change continued for four cycles, greater than four cycles, and less than four cycles (see above for reasons).

Fig. 8 (b) shows the contact energy curves for different cases. Since no damping was considered and no rolling occurs, the contact energy consisted only of strain energy (cf. Eq. (16)). For the original JKR contact model, the contact energy showed a periodic variation pattern. Due to the gradual increase and decrease in surface energy, the contact energy for Case 1 and Case 2 showed an overall upward and downward trend, respectively. Fig. 8 (c) shows the mechanical energy curves for different cases. The mechanical energy consisted of body and contact energy (cf. Eq. (13)). During the loading process, there was always an inter-conversion between body and contact energy. In Fig. 8 (c), mechanical energy remained constant at 0, indicating that the conservation of energy was satisfied.

Furthermore, to assess the effectiveness and feasibility of the modified JKR contact model under actual conditions, a gravitational loading test of ball considering damping was additionally considered. The test parameters and loading conditions remained unchanged, with only the normal critical damping ratio  $\beta_n$  being additionally set to 0.3. Fig. 9 shows the different energy-time curves for the gravitational loading test of ball considering damping.

Fig. 9 (a) shows the body energy curves for different cases. For all cases, due to the presence of damping, the kinetic energy of the ball rapidly decayed; in steady state, the body energy was contributed solely by gravitational potential energy. For the original JKR contact model, due to the constant surface energy, the body energy also remained constant in steady state. For case 1, due to the continuous increase in surface energy, the increased repulsive force caused the body energy to decrease. For case 2, due to the continuous decrease in surface energy, the decreased repulsive force caused the body energy to increase.

Fig. 9 (b) shows the contact energy curves for different cases. Due to the consideration of damping, contact energy consists of strain energy and dashpot energy. For all cases, dashpot energy tended to stabilize as the ball gravity loading test progressed. In the three cases, differences in surface energy led to distinct trends in the late loading stage: strain energy remained constant, while contact energy exhibited increasing and decreasing tendencies, respectively. Fig. 9 (c) shows the mechanical energy curves for different cases. During the loading process, there was always a mutual conversion between body energy and contact energy, and the mechanical energy remained at 0. This indicates that the conservation of energy remains satisfied even when damping is considered, demonstrating the broad applicability of the modified JKR contact model under practical conditions.

#### 4. Case studies

To investigate the applicability of the modified JKR contact model and compare it with the original JKR contact model, two case studies were provided for different application scenarios. One was used for the study of pre-compaction: during the pre-compaction process, the surface energy increased with time. The other was used for the study of particle dewatering: during the particle dewatering process, the surface energy decreased with time.

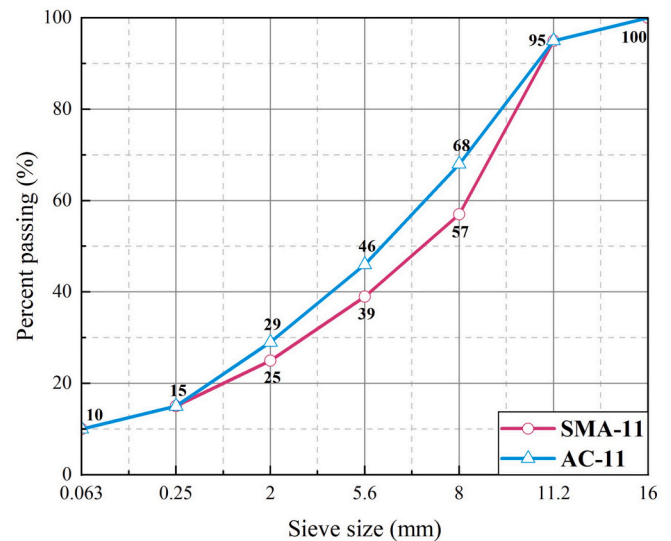


Fig. 11. Gradation curve of SMA-11 and AC-11.

#### 4.1. Simulation of pre-compaction during paving

The Aggregate Imaging System (AIMS) is a computer-controlled device used to capture images of grain particles and measure the texture of different types of particles [39]. In this case study, to model the particles more realistically, AIMS was used to capture the shape of the aggregates (see Fig. 10 (a) for the construction of AIMS). The aggregates used for the image measurements were taken from a quarry near Hünnerberg, Germany. The type of aggregate was basalt. A total of 42 aggregates were selected for DEM simulations (see Fig. 10 (b)). The images captured by AIMS were in 2D. Therefore, the simulations were performed next using PFC 2D. Fig. 10 (c) shows the processing of the aggregate images used to import the PFC 2D: The aggregate images were read using MATLAB, and the edges were extracted; the binarized data were exported to files in .dxf format, which was recognized in PFC 2D for creating clumps; then, the clumps were created using the bubble pack algorithm [40], which was built into PFC, i.e., several spheres were used to approximate the real shape of the particles; finally, the clump templates were imported into PFC 2D for use in simulations. Fig. 10 (d) shows the paver geometry model used for the pre-compaction simulation. The paver consisted of a tamper and a screed plate, which were modeled independently to load different working conditions. In this study, SMA-11 and AC-11 gradations were selected to study the process of pre-compaction. The curves of the gradations can be seen in Fig. 11.

The high computational cost renders full-scale 3D pre-compaction simulations impractical. Therefore, this study considered only the 2D case. However, the simplification of aggregates to 2D can influence the results. Accordingly, the error associated with dimensional reduction was first quantified based on the indirect tensile test (IDT). The image acquisition of 2D virtual aggregates was already described in Fig. 10, whereas the reconstruction of 3D virtual aggregates was performed using a 3D scanner. As shown in Fig. 12 (a), 40 representative aggregates were selected for IDT simulations, and clumps were generated using the bubble pack method. Marshall specimens with various gradations, 63.5 mm in height and 100 mm in diameter, were then produced, as illustrated in Fig. 12 (b). Loading and support strips were placed at the two ends of each specimen; the loading rate was set to 50 mm/min; and the contact model parameters were assigned according to [41]. Subsequently, ITD simulations were conducted on the specimens until failure. Fig. 12 (c) compares the tensile stress–tensile strain curves for specimens of different dimensions and gradations. For SMA-11, the peak stresses in 2D and 3D simulations were 1.66 MPa and 1.95 MPa, respectively. For AC-11, the corresponding values were 1.63 MPa and 1.81 MPa. The

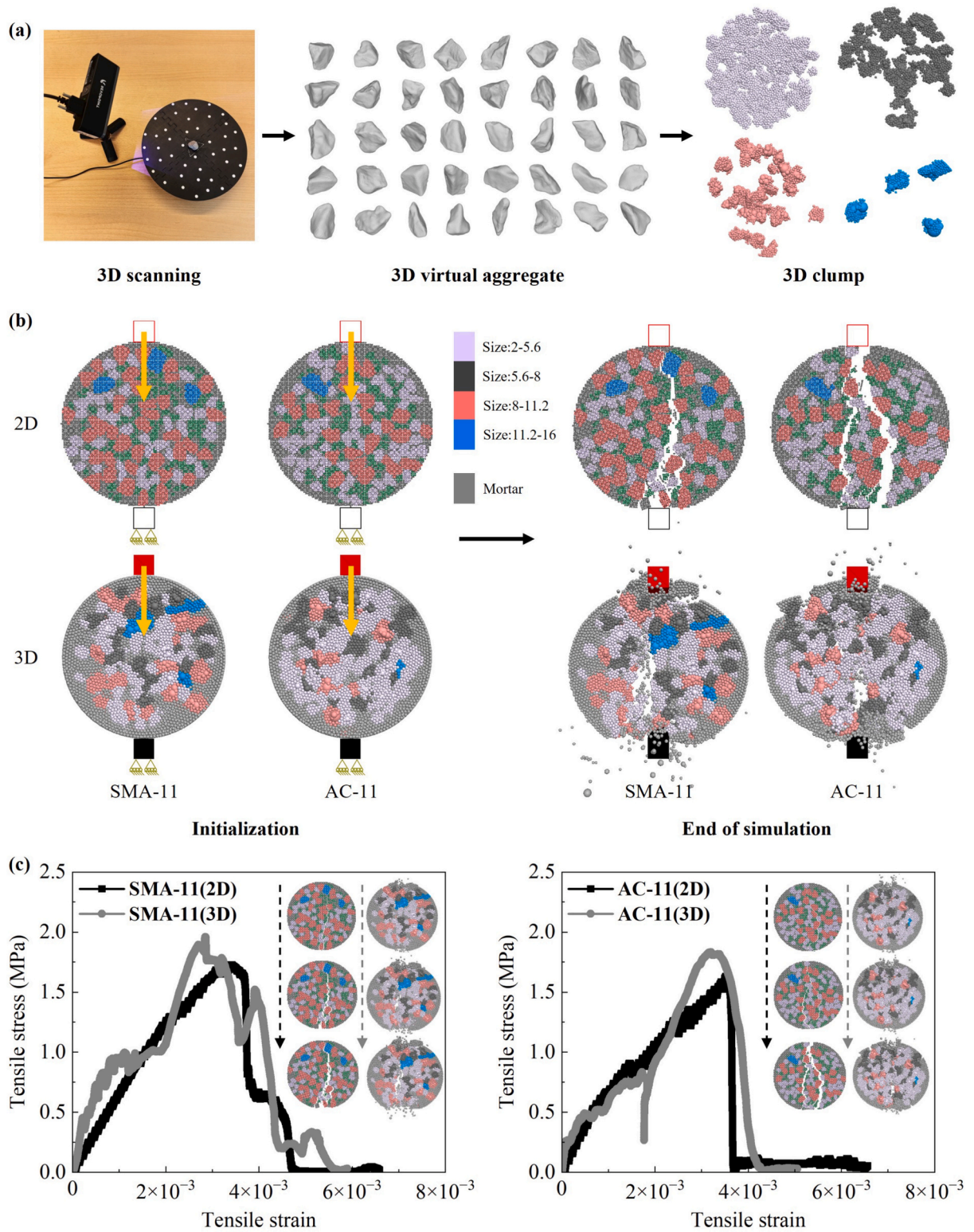


Fig. 12. Indirect tensile test: (a) Reconstruction of 3D virtual aggregates, (b) indirect tensile tests in different dimensions, (c) comparison of results.

resulting errors of 17.47 % and 11.04 % fall within an acceptable range. Therefore, although the 2D simplification of aggregates introduces some error, it substantially improves computational efficiency. Considering this balance between accuracy and efficiency, all subsequent pre-compaction simulations are carried out in two dimensions.

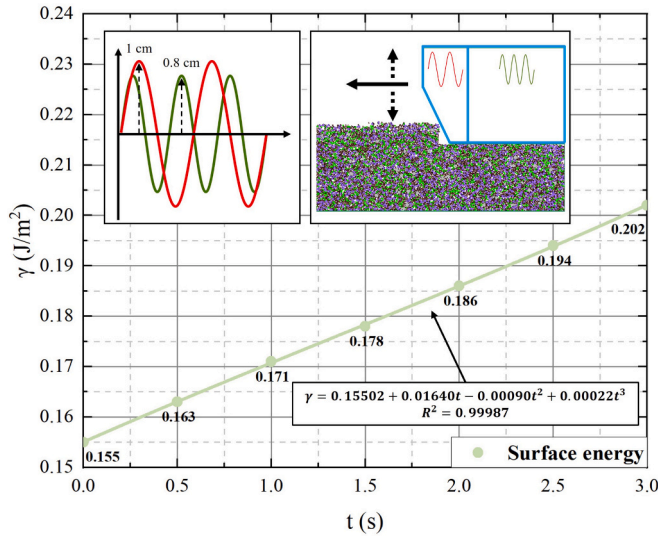
Table 2 shows the parameters used in the pre-compaction simulation for particles. These parameters were determined with reference to

previous literature [27,42,43] and practical situations. According to previous studies, the surface energy of the aggregates coated with asphalt film, i.e., the work of peeling between bitumen and aggregates [44], was calibrated to  $0.155 \text{ J/m}^2$  at  $130^\circ\text{C}$  for DEM simulations [17]. The experimental results in previous studies showed that the surface energy of bitumen had an approximately linear relationship with temperature over the range of compaction temperatures [45,46]. In this



**Table 2**  
Simulation parameters for pre-compaction.

| Young's modulus [Pa] | Density [kg/m <sup>3</sup> ]                 | Stiffness ratio                             | Poisson's ratio                            | Coefficient of restitution                |
|----------------------|----------------------------------------------|---------------------------------------------|--------------------------------------------|-------------------------------------------|
| $5.5 \times 10^{10}$ | 2650                                         | 2.6                                         | 0.3                                        | 0.2                                       |
| Local damping        | Coefficient of static friction (clump-clump) | Coefficient of static friction (wall-clump) | Rolling friction coefficient (clump-clump) | Rolling friction coefficient (wall-clump) |
| 0                    | 0.5                                          | 0.7                                         | 0.5                                        | 0.7                                       |



**Fig. 13.** Surface energy-time relationship for pre-compaction.

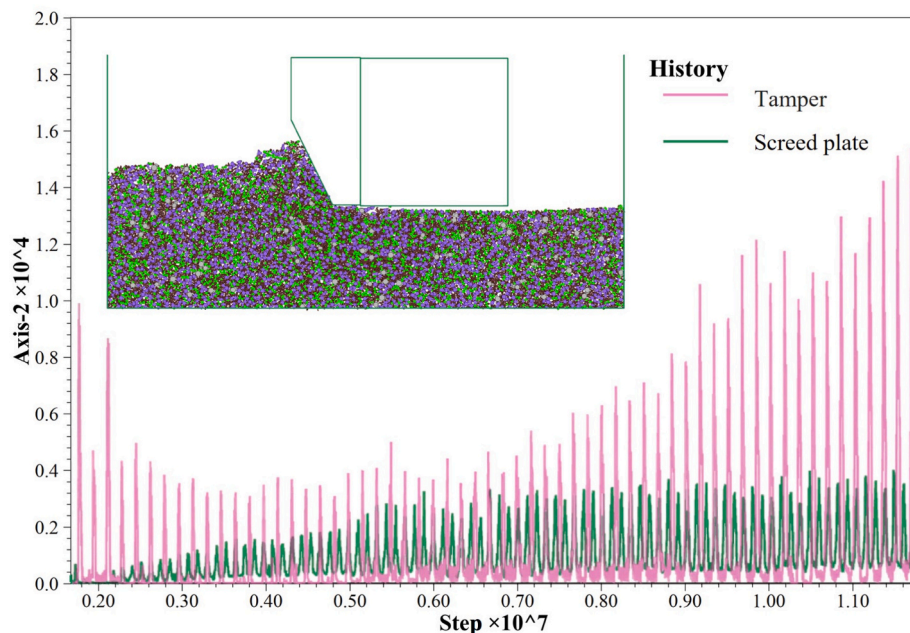
study, it was assumed that there was also a linear relationship between the surface energy of the aggregates coated with asphalt film and temperature; then, the linear relationship in [46] was scaled up equivalently for use in representing the change in surface energy as it decreased from 130 °C to 80 °C according to [46]. The simulations continued for a total of 3 s. Due to the high computational cost of DEM simulation, it was not realistic to simulate the increase in surface energy on a realistic time-scale; therefore, it was assumed that the process of increasing surface

energy was completed within 3 s. The relationship between surface energy and time was shown in Fig. 13. The paver was set to run at a speed of 5 m/min. The tamper and screed plate were set to periodic uniform amplitudes of 1 cm and 0.8 cm with frequencies of 20 Hz and 30 Hz, respectively. In addition, in PFC 2D, the thickness of the particles was defaulted to a unit length of the column. To compensate for the unit scaling relationship, the surface energy values shown in Fig. 13 were amplified by a factor of 1000 in the actual simulations. This is because, in PFC 2D, the column thickness is by default set to 1 m, and a compensation factor is required to correct this relationship when scaling from the millimeter scale to the meter scale [47]. The following scaling relationship applies to the conversion of surface energy between PFC 2D and PFC 3D:

$$\gamma_{2D} = \gamma_{3D} t \quad (28)$$

where  $\gamma_{3D}$  is the surface energy (J/m<sup>2</sup>) in the 3D simulation,  $\gamma_{2D}$  is the surface-energy-per-length (J/m) used in the 2D simulation, and  $t$  is the effective thickness.

Fig. 14 shows a screenshot at the end of the pre-compaction simulation. Further, the timesteps were converted to time to facilitate the presentation of the results. Fig. 15 shows the contact force-time relationship between the tamper (screed plate) and the particles for different gradations. To enable the quantification of the values, the impulses during compaction were calculated using numerical integration. Compared to the AC-11 gradation, the compaction impulses using the SMA-11 gradation were greater for both tamper and screed plate; compared to the AC-11 gradation, the paver needed to compact and move coarser aggregates when compacting the SMA-11 gradation, which made the compaction process more difficult. Wang et al. [27] analyzed the difference between the above two gradations for pre-



**Fig. 14.** End of pre-compaction simulation.



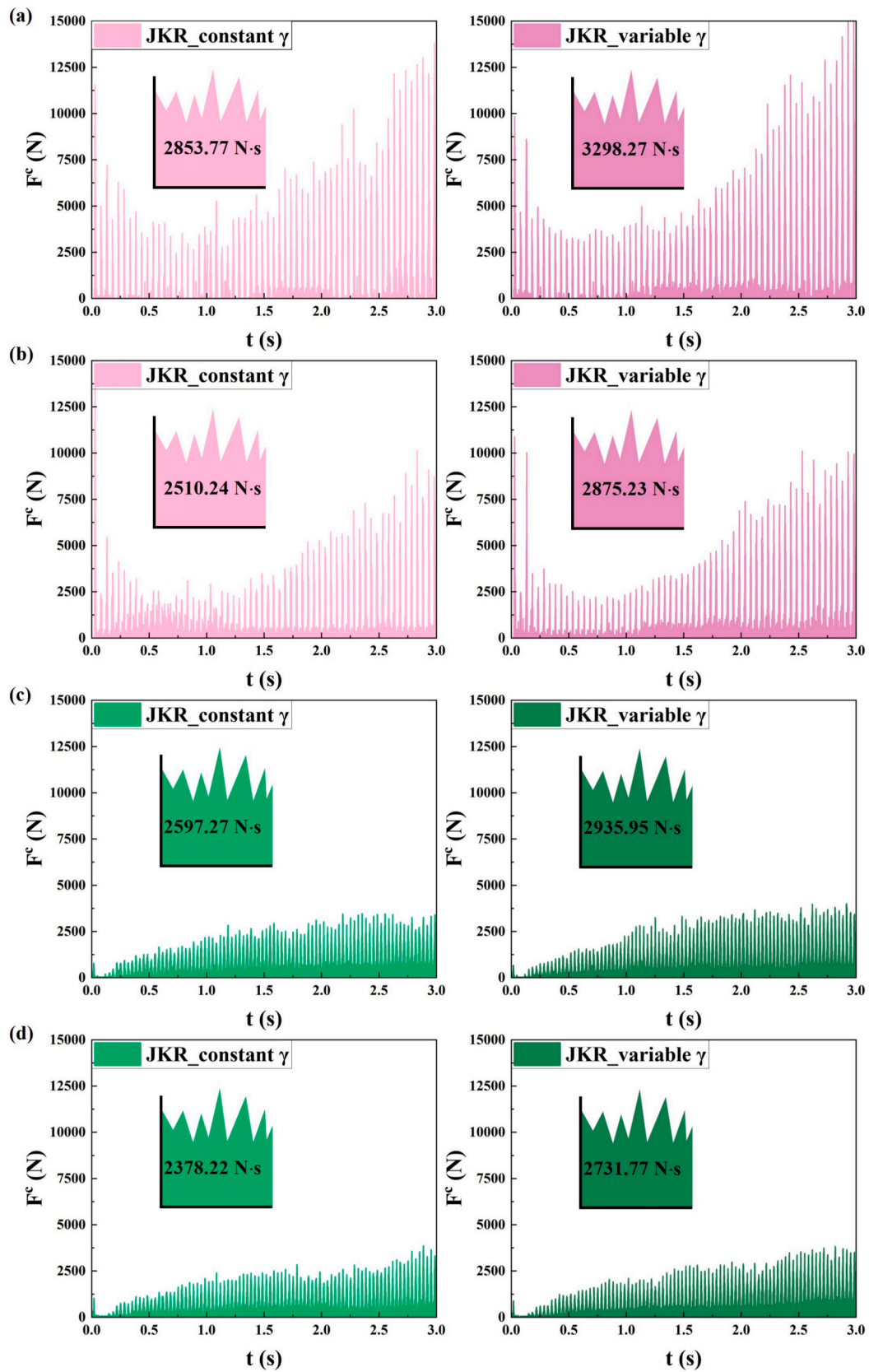
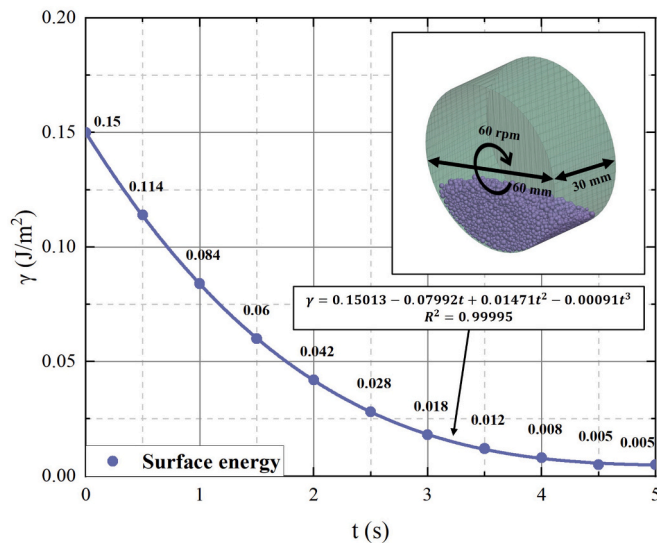


Fig. 15. Contact force between tamper and particles: (a) SMA-11, (b) AC-11; contact force between screed plate and particles: (c) SMA-11, (d) AC-11.

**Table 3**  
Simulation parameters for wet and dewatered particles.

| Young's modulus [Pa] | Density [kg/m <sup>3</sup> ]               | Stiffness ratio                            | Poisson's ratio                          | Coefficient of restitution               |
|----------------------|--------------------------------------------|--------------------------------------------|------------------------------------------|------------------------------------------|
| $1.5 \times 10^{10}$ | 1800                                       | 2.3                                        | 0.15                                     | 0.2                                      |
| Local damping        | Coefficient of static friction (ball-ball) | Coefficient of static friction (wall-ball) | Rolling friction coefficient (ball-ball) | Rolling friction coefficient (wall-ball) |
| 0                    | 0.5                                        | 0.75                                       | 0.05                                     | 0.08                                     |



**Fig. 16.** Surface energy-time relationship for particles dewatering.

compaction in terms of energy. The results of this study were consistent with [27] in terms of conclusions. Compared to the compaction impulses between the screed plate and particles, the compaction impulses between the tamper and particles were larger. This indicated that the tamper contributed more to the pavement leveling in pre-compaction. Compared to the original JKR contact model, the modified JKR contact model can reflect the increase in surface energy with time, i.e., the adhesion increases with time. Before 1.5 s, the difference between the values in the green curve and the values in the red curve was relatively small; this was attributed to the relatively small change in surface energy during the early stage of pre-compaction. After 1.5 s, the difference between the values in the green curve and the values in the red curve became gradually larger; this was attributed to the gradually increasing surface energy. Using the original JKR contact model as the benchmark, the percentage differences in values using the two different models were 15.57 %, 14.54 %, 13.04 %, and 14.87 %, respectively. The above differences can reflect the expected relationship between temperature and adhesion. Therefore, the modified JKR contact model shows adaptability for simulating the increase in surface energy of granular materials over time.

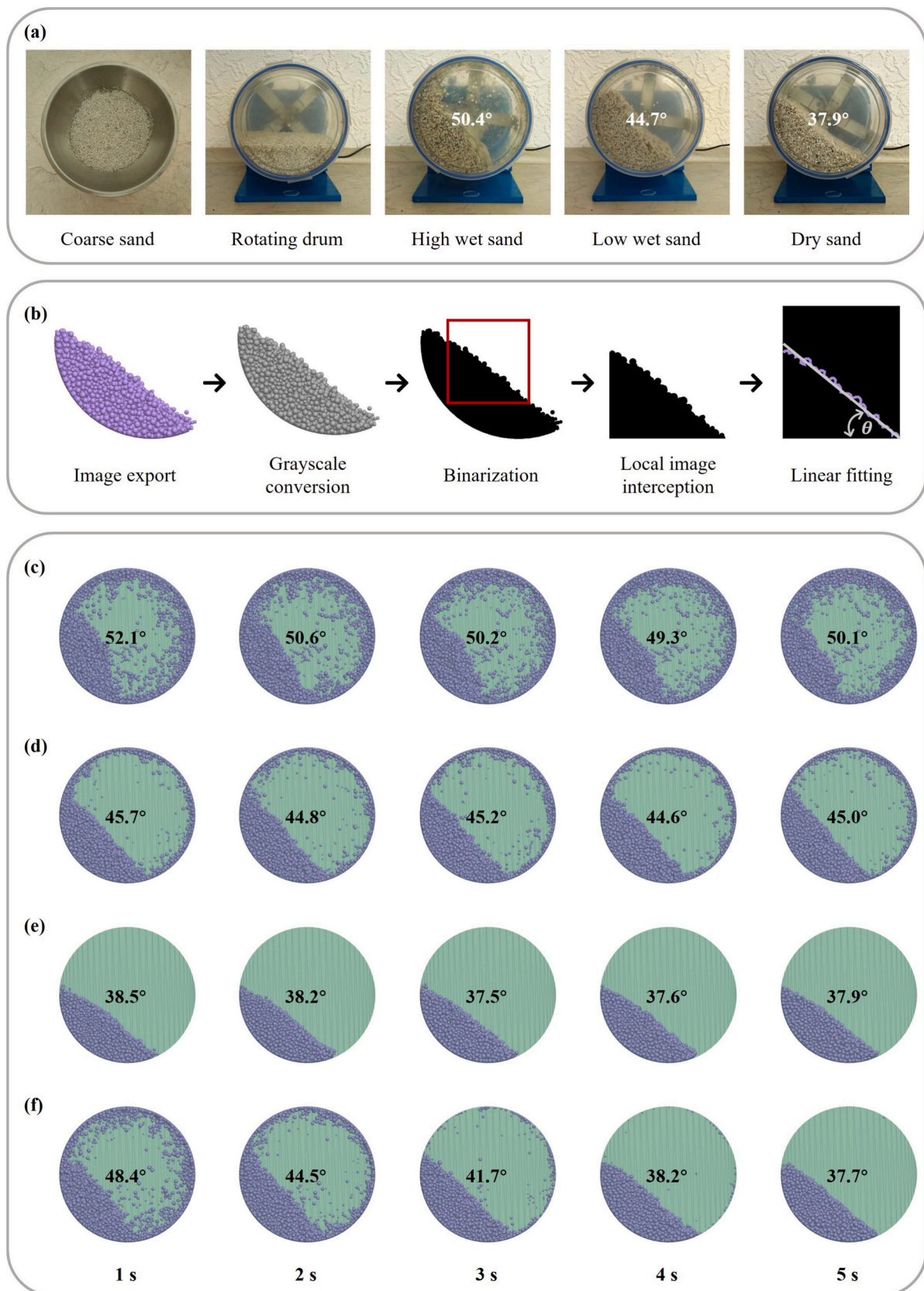
#### 4.2. Simulation of wet and dewatered particles

In this case study, wet and dewatered particle simulations in a rotating drum were used to investigate the effect of different contact models on the results. Table 3 shows the parameters used in the rotating drum simulation for wet and dewatered particles. The parameters were selected by combining previous literature [19,48,49] and practical situations. According to ISO 14688 [50], the fraction of coarse sand (grain size between 0.63 and 2.0 mm) was selected for use in the simulation; the amount of coarse sand was distributed based on the normal distribution. Referring to [19], the surface energy of the high wet sand was assumed to be 0.15 J/m<sup>2</sup> in this study; then, surface energies of 0.05 J/

m<sup>2</sup> and 0.005 J/m<sup>2</sup> were assumed for low wet and dry sand to be used for comparison tests. In the PFC, the setting of the surface energy must be greater than 0 J/m<sup>2</sup>; therefore, a lower surface energy of 0.005 J/m<sup>2</sup> was selected to represent the state of the dry sand. The above constant surface energy settings were used for the original JKR contact model. Fig. 16 shows the decrease in surface energy as a function of time to reflect the dewatering process of the sand. The simulation continued for a total of 5 s and ran using the modified JKR contact model. The surface energy was 0.15 J/m<sup>2</sup> at the beginning of the simulation and decreased to 0.005 J/m<sup>2</sup> at the end of the simulation. The geometry of the rotating drum was shown in Fig. 16; the sand was modeled using the ball as the model object to simplify numerical computations; the rotating drum was rotated at 60 rpm; the simulation was performed using PFC 3D.

To ensure the comparability of the simulation results, a particle dewatering experiment was first conducted, as shown in Fig. 17 (a). Coarse sand with a dry mass of 512 g was selected for the experiment in a rotating drum. Moisture contents of 0 %, 1 %, and 3 % were considered to represent dry sand, low wet sand, and high wet sand, respectively. The rotational speed was set to 60 rpm. To quantitatively characterize the degree of adhesion between particles, the angle of repose (AOR) of the particles in the rotating drum was measured. The AOR of granular material is defined as the steepest slope that the unconfined material can achieve without collapsing [51]. For each case, the AOR was measured at four positions along the slope, and the average value was taken. The AORs corresponding to high wet sand, low wet sand, and dry sand were 50.4°, 44.7°, and 37.9°, respectively. This indicates that higher moisture content enhances the cohesive forces between particles, making the sand pile less prone to collapse and thus maintaining a higher AOR. As the moisture content decreases, the interparticle cohesion is significantly weakened, leading to a corresponding reduction in AOR. These physical observations form the basis for applying the modified JKR contact model to simulate particle dewatering.

Fig. 17 (b) shows the measurement method of the AOR: first, a color image of the simulation result was exported; then, a grayscale conversion was performed on the color image; after that, the full domain of the image was searched to binarize the image; next, the binarized image was locally intercepted to facilitate the edge extraction of the pile slope; finally, linear fitting was performed on the discrete points to obtain the AOR. Fig. 17 (c) shows the simulation results for the high wet particles ( $\gamma = 0.15$  J/m<sup>2</sup>). At different times, the differences between the individual AORs were insignificant, and the maximum variance between the different AORs did not exceed 3°. Due to the high surface energy, some particles adhered to the top and side of the rotating drum. This is attributed to the fact that the adhesion of the particles to the wall (or particles) is greater than their gravity; thus, they cannot fall freely. Fig. 17 (d) shows the simulation results for the low wet particles ( $\gamma = 0.05$  J/m<sup>2</sup>). At different times, the maximum variance between the different AORs did not exceed 1.5°. Compared to the high wet particles, the low wet particles had a lower AOR, and the number of particles adhering to the top and side of the rotating drum was also lower. This is because the lower surface energy reduces the adhesion between the particles and the wall (or particles). Fig. 17 (e) shows the simulation results for the dry particles ( $\gamma = 0.005$  J/m<sup>2</sup>). At different times, the maximum variance between the different AORs did not exceed 1°. For dry particles, the extremely low surface energy made the adhesion between particles essentially negligible. The AOR is only a result of the



**Fig. 17.** Particle dewatering: (a) Dewatering experiment, (b) calculation of angle of repose, (c) simulation for high wet particles, (d) simulation for low wet particles, (e) simulation for dry particles, (f) simulation for particle dewatering.



natural stacking and is independent of the adhesion. This resulted in the lowest AOR and no particles adhering to the wall. Fig. 17 (f) shows the simulation results for the dewatering process of the particles according to the relationship in Fig. 16. The surface energy gradually decreased with time, i.e., the adhesion gradually decreased. This was intuitively reflected in the continuous decrease of the AOR and the decrease of particles adhering to the top and side of the rotating drum. At 1 s, the result of AOR was between the AOR results of high and low wet particles; at 2 s, the result of AOR was close to the AOR result of low wet particles; at 3 s, the result of AOR was between the AOR results of low wet and dry particles; and, at 4 s and 5 s, the result of AOR was close to the AOR result of dry particles. The above results are consistent with the expected relationship between the dewatering process and AOR, and they align well with the actual experimental observations. The relationship between moisture content and adhesion can be reflected. Therefore, the modified JKR contact model can effectively simulate the process of particle dewatering, demonstrating significant advantages in capturing the transition of particles from wet to dry states.

## 5. Conclusions and outlook

In this study, a modified JKR contact model with time-dependent surface energy was proposed to overcome the limitation of the original model, which assumes constant surface energy. Both theoretical analyses and application-oriented simulations were conducted, and the main findings are summarized as follows.

- In the ball-ball pull-off test, the adhesive peeling work increased from  $0.936F_{p0}\delta_{t0}$  (original) to  $1.778F_{p0}\delta_{t0}$  in Case 1 (surface energy doubling) and decreased to  $0.379F_{p0}\delta_{t0}$  in Case 2 (halving). Similarly, in the gravitational loading test, Case 1 exhibited increasing maximum load and contact energy with cycles exceeding four, while Case 2 showed decreasing trends with fewer cycles, whereas the original model remained constant. Importantly, all cases satisfied energy conservation, confirming that the modified model not only reflects adhesion changes induced by environmental effects but also maintains physical consistency, thereby validating its theoretical soundness and robustness.
- The pre-compaction simulation using the modified JKR model, which accounts for surface energy increasing with temperature, showed that compaction impulses between tamper and particles increased by 15.57 % (SMA-11) and 14.54 % (AC-11), while those between screed plate and particles increased by 13.04 % (SMA-11) and 14.87 % (AC-11), respectively, compared to the original model. These results demonstrate the modified model's ability to capture previously underestimated compaction work and its strong adaptability in simulating pre-compaction dynamics.
- In the dewatering simulation, the modified model described surface energy decreasing with moisture content. Using a rotating drum test, the angle of repose (AOR) of wet coarse sands decreased from  $48.4^\circ$  to  $37.7^\circ$  over 5 s, reflecting improved flowability. This confirms the model fills the gap in traditional JKR applications by capturing flowability changes during wet-to-dry transitions.

Overall, the modified JKR contact model is feasible for DEM simulations of particulate materials with evolving adhesion properties. Potential applications include temperature-dependent asphalt fracture, soil flow, and tire rut simulations. To enhance the realism and accuracy of engineering simulations, future studies should focus on incorporating the effects of irregular particle shapes into the model. Considering particle shape heterogeneity is expected to significantly impact contact mechanics and adhesion behavior, thereby improving model precision. Further development and validation in this area will broaden the applicability and robustness of the modified JKR contact model in complex real-world scenarios.

## CRedit authorship contribution statement

**Dong Feng:** Writing – original draft, Visualization, Data curation, Conceptualization. **Chaoliang Fu:** Writing – review & editing, Validation, Supervision, Formal analysis. **Pengfei Liu:** Writing – review & editing, Supervision, Project administration, Funding acquisition.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this study.

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## Data availability

Data will be made available on request.

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