

A DEM-based particle–force chain informatics framework for data-driven evaluation of pavement pre-compaction

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ABSTRACT

Pre-compaction beneath the paver screed strongly influences the mechanical response and durability of pavements, yet it cannot be measured directly in the field. This study develops a discrete element method (DEM)-based particle–force chain informatics framework for simulating screed device–particle interaction and for deriving interpretable, data-driven indicators of pavement pre-compaction quality. A Johnson–Kendall–Roberts (JKR)-based DEM model is formulated for a vibrating screed device acting on asphalt mixtures and is used to provide particle-to-particle contact and force chain descriptors. These heterogeneous descriptors are standardized by a QuantileTransformer (QT) and embedded into a low-dimensional latent space using a denoising variational autoencoder (DVAE), from which a Gaussian mixture model (GMM) yields data-driven labels and composite pre-compaction scores. Gradient-boosted decision trees (XGBoost) are then trained to predict these scores from the original descriptors, and Shapley-additive (SHAP) explanations quantify the contributions and interactions of individual micro-mechanical features. Numerical experiments on SMA-13, AC-13 and OGFC-13 mixtures, each with three gradation variants, show that the framework consistently captures the strengthening, elongation and orientation of load-bearing force chains, the reduction of weak chains, and the concentration of high stress particles as pre-compaction progresses. The resulting indicator set, together with the trained surrogate model, constitutes a reproducible and computationally efficient informatics route to assess, rank and compare pre-compaction conditions across mixtures and operating parameters, and demonstrates how DEM simulations can be systematically transformed into predictive, interpretable metrics for data-driven evaluation of pavement pre-compaction.

1. Introduction

Pre-compaction under the paver screed device is the asphalt layer's first encounter with externally imposed confinement and shear [1–3]. In this short window, the granular skeleton is born: particles rearrange, contacts are created and broken, and a percolating network of load paths begins to carry the screed pressure and vibration [4–6]. The state established at this stage will influence all subsequent processes. Roller compaction can reinforce or smooth the structure, but if the framework has not formed, the compaction process rarely solidifies it [7–9]. Field experience and manufacturer guidelines therefore emphasize screed settings [10,11]. Yet routine practice still tunes vibration, pressure, and paving speed largely by heuristics because the internal microstructure is inaccessible during paving [12–14]. Fig. 1 (a) and (b) show the field process and the screed device that governs this interaction. When pre-compaction is inadequate, traffic and environmental loads probe the weakest links of the skeleton, and the defects are familiar: cracks,

potholes, raveling, and shoving accumulate over service life (see Fig. 1 (c)).

A central yet insufficiently quantified determinant of pre-compaction quality is gradation [15–17]. Discontinuous, continuous, and open distributions do not merely change void content; they rewrite the statistics of contact formation and the topology of force chains [18–20]. As suggested in Fig. 1 (d), particles with different gradations evolve markedly different load-bearing networks under the same screed action: some rapidly develop strong, continuous force chains with high coordination, while others exhibit fragmented force chains, stress localization, and facile sliding. These mesoscale differences are precisely the features that surface proxies—layer thickness, texture, or vibration signatures—struggle to diagnose.

Current research faces three interrelated gaps. On site, sensing is predominantly surface-level and empirical, leaving the birth of the internal skeleton inferred rather than measured [21–23]. In modeling, continuum descriptions resolve global fields but homogenize the

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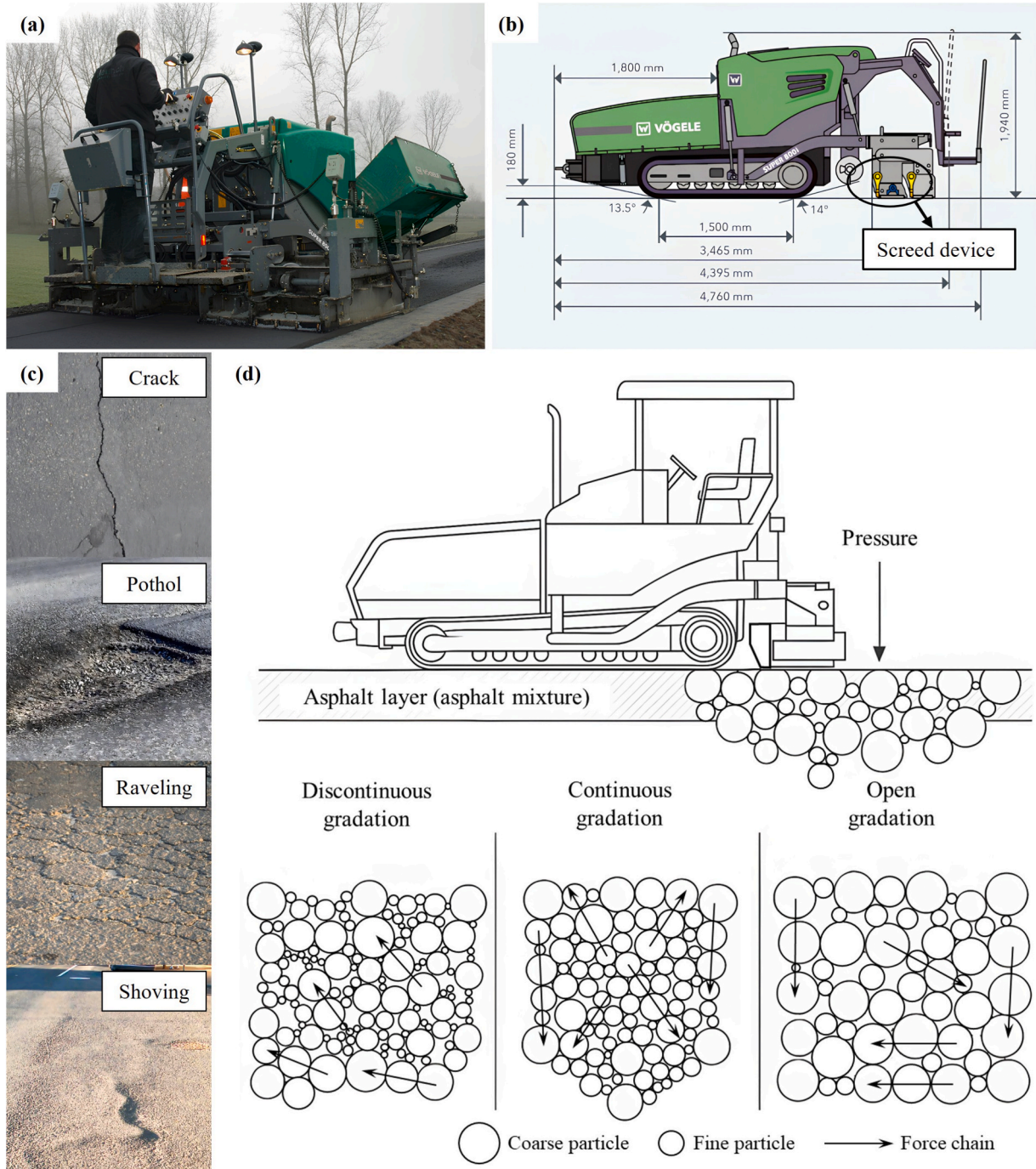


Fig. 1. Pre-compaction during paving: (a) on-site paving process, (b) geometric dimension of paver (VÖGELE SUPER 800i), (c) pavement defects caused by insufficient pre-compaction, (d) pre-compaction under different aggregate gradations.

mixture; constitutive models cannot represent the emergence, breakage, and persistence of discrete force chains or the statistics of high stress particles that signal marginal pre-compaction [24–26]. Even within discrete element method (DEM) studies, the community has focused more on roller compaction or on small coupons and single gradations [27–29]. Feature extraction is often manual, producing case-specific metrics that do not scale to broad parametric studies, cannot be evaluated automatically, and offer limited explainability for decision support [30,31].

To address these limitations, this study introduces an end-to-end, DEM-based particle–force chain informatics framework that targets the pre-compaction stage beneath the paver screed device and treats

gradation as the governing variable (see Fig. 1 (d)). The simulation employs the JKR contact model to describe the adhesive and frictional mechanical properties of asphalt particles, capturing normal and tangential compliance, microslip, and the transition between sticking and sliding that controls energy dissipation under screed vibration. From each simulation, two complementary data streams are exported by design: the particle distribution that encodes fabric, packing, and coordination, and the force chain network that captures load percolation, chain strength, and continuity. This separation disentangles structural effects (particle arrangement) from mechanical effects (force transmission) and attributes gradation sensitivity to the appropriate tier of the microstructure.

Table 1
Comparison of the proposed framework with representative state-of-the-art approaches.

Approach family	Methodology	Typical outputs	Validation/accuracy evidence	Computational efficiency	Interpretability
Proposed DEM + force-chain informatics (DVAE + clustering + XGBoost + SHAP)	DEM micro-mechanics + contact/force-chain descriptors + automated learning and attribution	Data-driven indicator set, latent-state grouping, indicator-importance ranking, and mechanism-oriented explanation	Internal consistency and mechanistic link from microstructure to evaluation	Moderate (multiple simulation runs; downstream learning is light)	High (structural descriptors + SHAP-based attribution)
FEM–DEM hybrid (coupled continuum–discrete) [15,32,33]	Continuum boundary/structure (FEM) + particle-scale mixture (DEM)	Dynamic response, aggregate motion, sometimes operating-parameter effects	Improves realism for equipment–material interaction; validated via targeted numerical/benchmark studies	Low (highest cost due to coupling and particle scale)	Medium (rich physics, but harder to automate feature attribution)
In situ sensing/intelligent compaction (ICMVs, paver/roller sensors) [34,35]	Field sensor signals (vibration/acceleration, machine kinematics, temperature)	Real-time compaction indicators and quality maps	Reported correlations with in-situ spot tests (density/stiffness), typically site- and mix-dependent	High (real-time capable)	Medium (signal-to-quality mapping can be opaque without physics/explainability)
Non-destructive evaluation (NDE) using ground-penetrating radar (GPR) for density/air-void estimation [36,37]	GPR dielectric response (often calibrated with cores/spot tests)	Continuous density/air-void profiles	Demonstrated feasibility for air-void/density estimation with calibration and careful processing	High (fast surveying)	Medium (physics-based EM link, but calibration/uncertainty management needed)
Sensing + machine learning (ML) density prediction [38,39]	Field/lab sensor features + ML regression/classification	Predicted density/compaction state, sometimes with field validation	Demonstrated prediction capability when trained on representative datasets	Moderate (inference is fast; training is moderate)	Medium (depends on model; explainability varies)

Building on these raw observables, algorithms are developed to automatically identify particle–particle and particle–screed device contacts, classify strong and weak force chains, and detect high and low stress particles. The resulting descriptors quantify contact orientation and anisotropy, coordination number and its heterogeneity, force chain length and persistence, stress assortativity, and the kinetics of contact mode transitions. Rather than relying on a fixed set of handcrafted indicators, the feature set is embedded in a data-analytics pipeline that normalizes measurements using QT, learns a compact latent representation with DVAE, and assigns data-driven labels using GMM. Supervised ranking with XGBoost links micro-level features to macroscopic pre-compaction adequacy, and SHAP-based attribution exposes the mechanisms—such as force chain continuity, contact fabric anisotropy, and the fraction of high stress particles—that dominate for a given gradation. In effect, the framework converts micro-scale DEM trajectories into interpretable, data-driven metrics that support quantitative evaluation and comparison of pavement pre-compaction conditions. To position the proposed framework relative to existing approaches, Table 1 summarizes representative simulation- and sensing-based methods in terms of validation evidence, computational efficiency, and interpretability.

The novelty is twofold. Methodologically, the work couples a physics-aware DEM model of aggregate–screed device interaction with a fully automated, explainable informatics stack that standardizes heterogeneous features, learns a compact latent space, assigns data-driven labels, and attributes model decisions. Scientifically, the study clarifies how pre-compaction reshapes the microstructure across gradations: strong force chains systematically intensify and become more continuous, directional anisotropy of the force chain field strengthens along the loading axis, and a larger share of particles participates in load-bearing subnetworks. The magnitude and localization of these changes are case-dependent rather than monotonic in gradation. For example, OGFC-13 often exhibits higher strong contact ratios and larger void decreases, SMA-13 tends to maintain higher coordination in some cases, and AC-13 commonly shows lower strong contact fractions, while force chain lengths increase modestly across all scenarios. By revealing these mechanisms in a quantitative and interpretable form, the framework addresses limitations of empirical tuning, continuum homogenization, and piecemeal DEM post-processing, and provides a feature-driven, explainable basis for data-driven evaluation of pavement pre-compaction.

2. Methodology

Fig. 2 illustrates the DEM-based particle–force chain informatics workflow used to transform discrete element simulations of the pavement pre-compaction stage into explainable, data-driven indicators for assessment. The process starts from a screed device–particle DEM model that resolves the pre-compaction region and employs the Johnson–Kendall–Roberts (JKR) contact model to capture adhesive and frictional particle interactions. Simulations are conducted for discontinuous, continuous, and open gradations to probe gradation sensitivity. The raw trajectories are post-processed along two coordinated data streams, namely a particle distribution stream and a force chain network stream. Automatic routines identify particle–particle and particle–screed contacts, detect strong and weak force chains, and separate high and low stress particles, with all outputs stored in a structured database. From these streams, a comprehensive set of features is extracted to describe both structure and mechanics, including average particle–particle and particle–screed device contact forces, mechanical coordination number, and related descriptors. The feature set is then standardized with a QuantileTransformer (QT), embedded into a compact latent space by a denoising variational autoencoder, labeled in a data-driven manner through a Gaussian mixture model (GMM), and evaluated by supervised learning with XGBoost. SHAP-based attribution finally provides a transparent mapping from features to pre-compaction adequacy. This informatics workflow separates fabric information from load-path information and enables consistent, gradation-aware evaluation of screed pre-compaction performance.

In engineering informatics terms, the proposed workflow is not merely a sequence of simulation and statistical analysis modules. Its core contribution is a structured knowledge extraction process that converts micro-scale DEM outputs into interpretable, decision-oriented information for pre-compaction evaluation. Rather than treating DEM results as generic high-dimensional data, the framework represents the evolving granular skeleton through the contact network and the force chain subnetwork, which encode connectivity, fabric anisotropy, and load path continuity associated with load-bearing structure formation beneath the screed. Based on this structure-aware representation, the learning and interpretation steps organize microstructural states and provide transparent indicator importance rankings and mechanism-oriented explanations, thereby yielding actionable knowledge on key signatures governing pre-compaction adequacy across gradations and

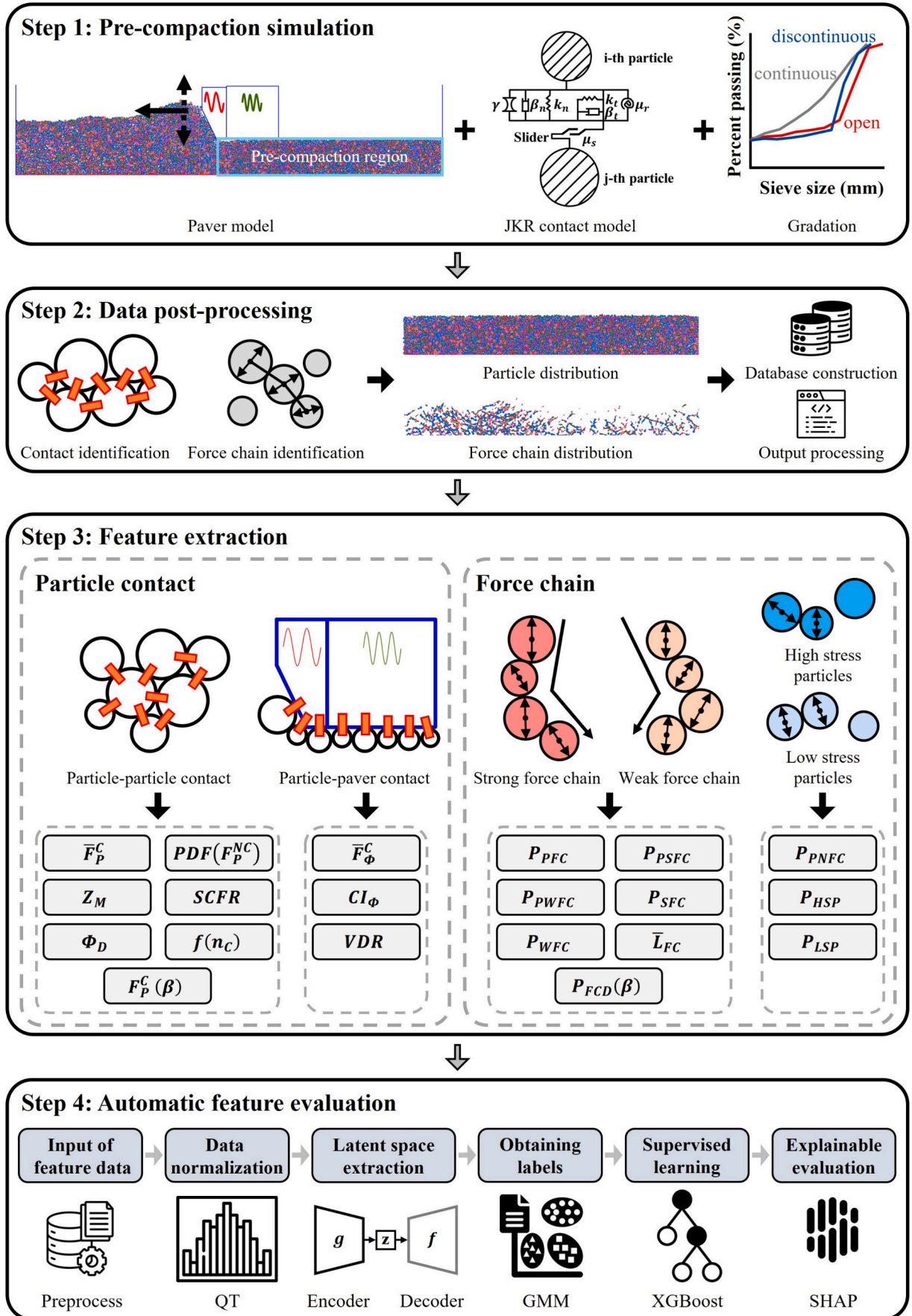


Fig. 2. Technical workflow.

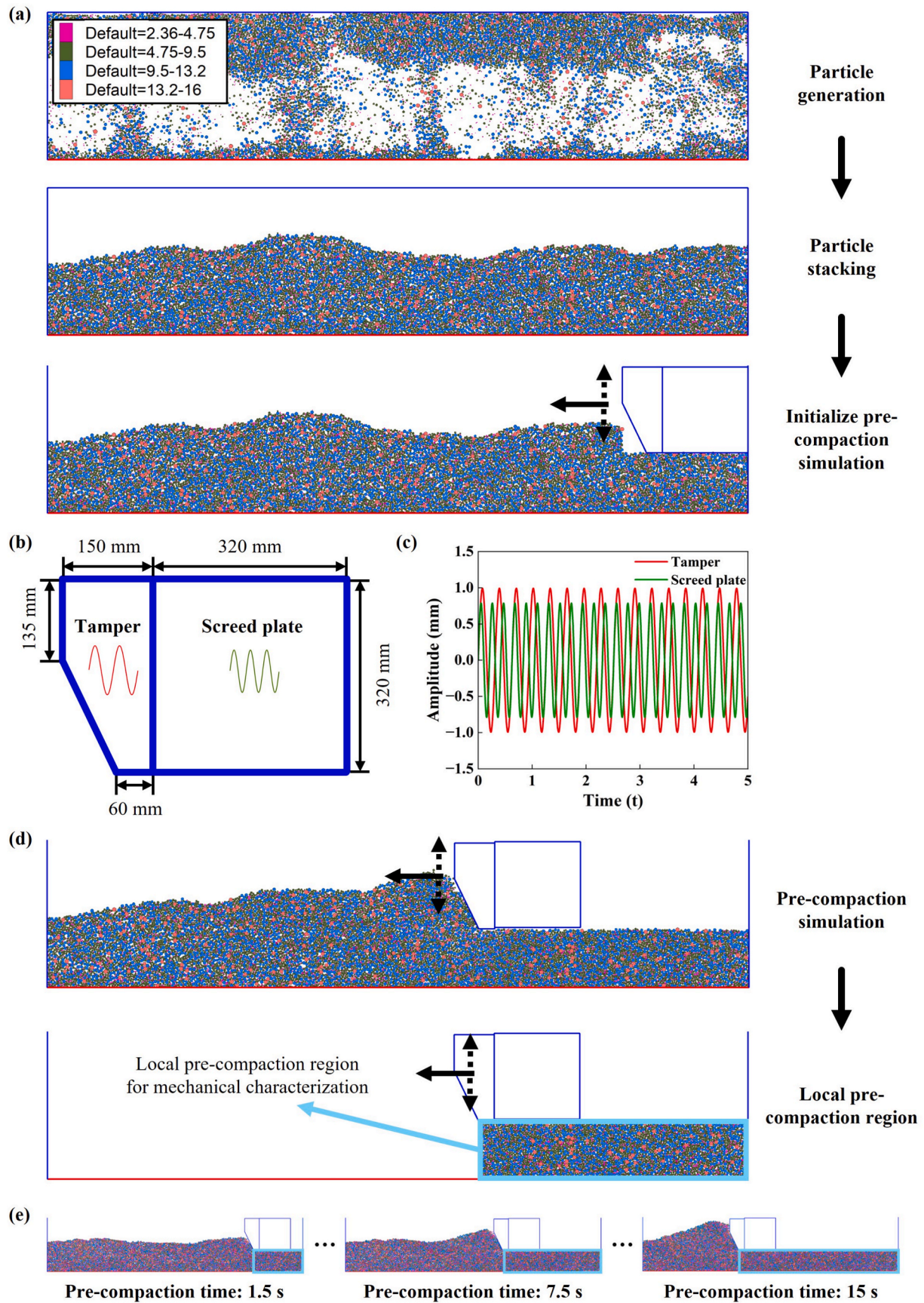


Fig. 3. Discrete element simulation of the pre-compaction process: (a) initialization of pre-compaction, (b) geometric dimensioning of screed device, (c) dynamic loading of tamper and screed plate, (d) extraction of the current pre-compaction region, (e) snapshots during the pre-compaction process.

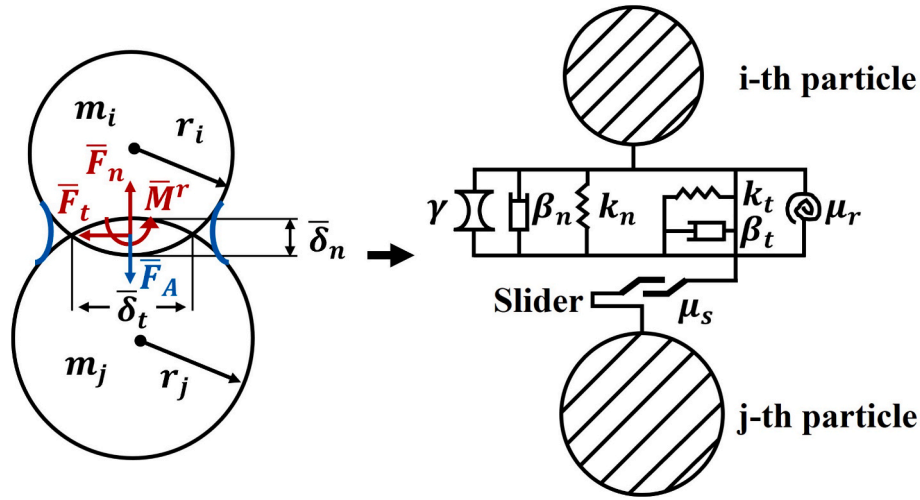


Fig. 4. Johnson-Kendall-Roberts (JKR) contact model.

Table 2
Simulation parameters for JKR contact model.

Young's modulus (Pa)	Density (kg/m ³)	Stiffness ratio	Poisson's ratio	Coefficient of restitution
5.5×10^{10}	2650	2.6	0.3	0.2
Particle-particle static friction coefficient	Particle-particle rolling friction coefficient	Particle-wall static friction coefficient	Particle-wall rolling friction coefficient	Surface energy (J/m ²)
0.5	0.65	0.3	0.35	0.155

operating conditions.

2.1. Pre-compaction simulation

To support the subsequent analysis, this subsection establishes the numerical foundation for the pre-compaction study. The methodology proceeds from model construction to contact model selection and calibration, and finally to the specification of representative gradations. Fig. 3 outlines the setup for the pre-compaction simulation. Considering the large volume of raw data required for this research, simulations were performed in two dimensions to accelerate data acquisition. Additionally, for the DEM simulation [40]—a particle-based numerical method that explicitly tracks the motion and contact forces of discrete particles and their interactions—this study employed the Particle Flow Code (PFC) 2D software for coding. Fig. 3 (a) shows the initial preparation: particles were generated according to their gradation, stacked under gravity to form a loose paving layer, and were then brought into contact with a virtual screed device to initiate pre-compaction. The screed device is the central component because it controls both material flow ahead of the screed and the early densification of the layer [41,42]. Its representation therefore followed the actual geometry of a VÖGELE SUPER 800i, and it was decomposed into two functional modules that acted sequentially on particles (see Fig. 3 (b)): the tamper, which primarily agitated and drove material under the screed, and the screed plate, which leveled and consolidated the layer. The tamper was assigned a sinusoidal motion with 1.0 mm amplitude at 20 Hz, and the screed plate vibrated with 0.8 mm amplitude at 30 Hz (see Fig. 3 (c)). Furthermore, to ensure consistency of results, all simulations were performed for 15 s. These boundary conditions govern the particle rearrangement immediately beneath the screed. Fig. 3 (d) presents the running pre-compaction simulation and highlights the local pre-compaction region that is extracted for subsequent mechanical

characterization. Representative snapshots at 1.5 s, 7.5 s, and 15 s illustrate the progressive smoothing of the surface and the evolution of internal packing under the combined action of the tamper and the vibrating screed plate (see Fig. 3 (e)).

In DEM, the contact model characterizes the mechanical behavior between particles. The Johnson-Kendall-Roberts (JKR) contact model (see Fig. 4) [43] was adopted in this study because pre-compaction of asphalt mixtures is governed not only by elastic repulsion and friction but also by binder-mediated adhesion at particle contacts. At paving temperatures, the aggregate surfaces are coated by a compliant, surface-active binder, which enlarges the real contact area and generates tensile forces during approach, hold, and separation. The JKR contact model explicitly couples the normal force to the contact area and surface energy, reproducing pull-off, loading and unloading hysteresis, and the stick-slip transitions that control energy dissipation under a vibrating screed, which models such as the Hertz-Mindlin [44] or the linear spring-dashpot without adhesion [40] cannot represent. Moreover, the model parameters—normal and tangential stiffness, surface energy, and friction—are physically interpretable and can be calibrated through relevant experiments (e.g., angle of repose tests, mixing tests). This makes the JKR contact model a suitable and tractable choice for capturing adhesion-sensitive contact mechanics during pre-compaction. The formulas for the JKR contact model are not repeated here and can be found in [43,45].

Based on previous literature [46–48], the parameters adopted for DEM simulation in this study are shown in Table 2. Although asphalt binder behavior is temperature- and rate-dependent, the present study adopts fixed JKR-related parameters as an effective representation of binder-mastic interaction under typical pre-compaction conditions. To support this assumption, the parameter set was checked using a Superpave gyratory compaction (SGC) simulation benchmark (see Fig. 5). The aggregate gradation used in the specimens was selected according to [49], as shown in Fig. 5 (a), where the coarse aggregate fraction with particle sizes greater than 2 mm was suitable for DEM simulation. The SGC kinematics and loading were set to standard values: a vertical stress of 600 kPa, a gyration speed of 30 rpm, and an internal angle of 0.82° (see Fig. 5 (b)). Loose asphalt mixture models were prepared by virtual compaction and preloading so that the particle size classes matched the target gradation (see Fig. 5 (c)). The SGC process was then simulated by confining the cylindrical specimen, applying the prescribed axial stress, and imposing the gyratory motion until a stable compacted state was obtained (see Fig. 5 (d)). The simulated height-gyration curves for three numerical replicates closely tracked the experimental reference from the literature [49], with small scatter among the replicates (see Fig. 5 (e)). This agreement indicated that the calibrated JKR parameters

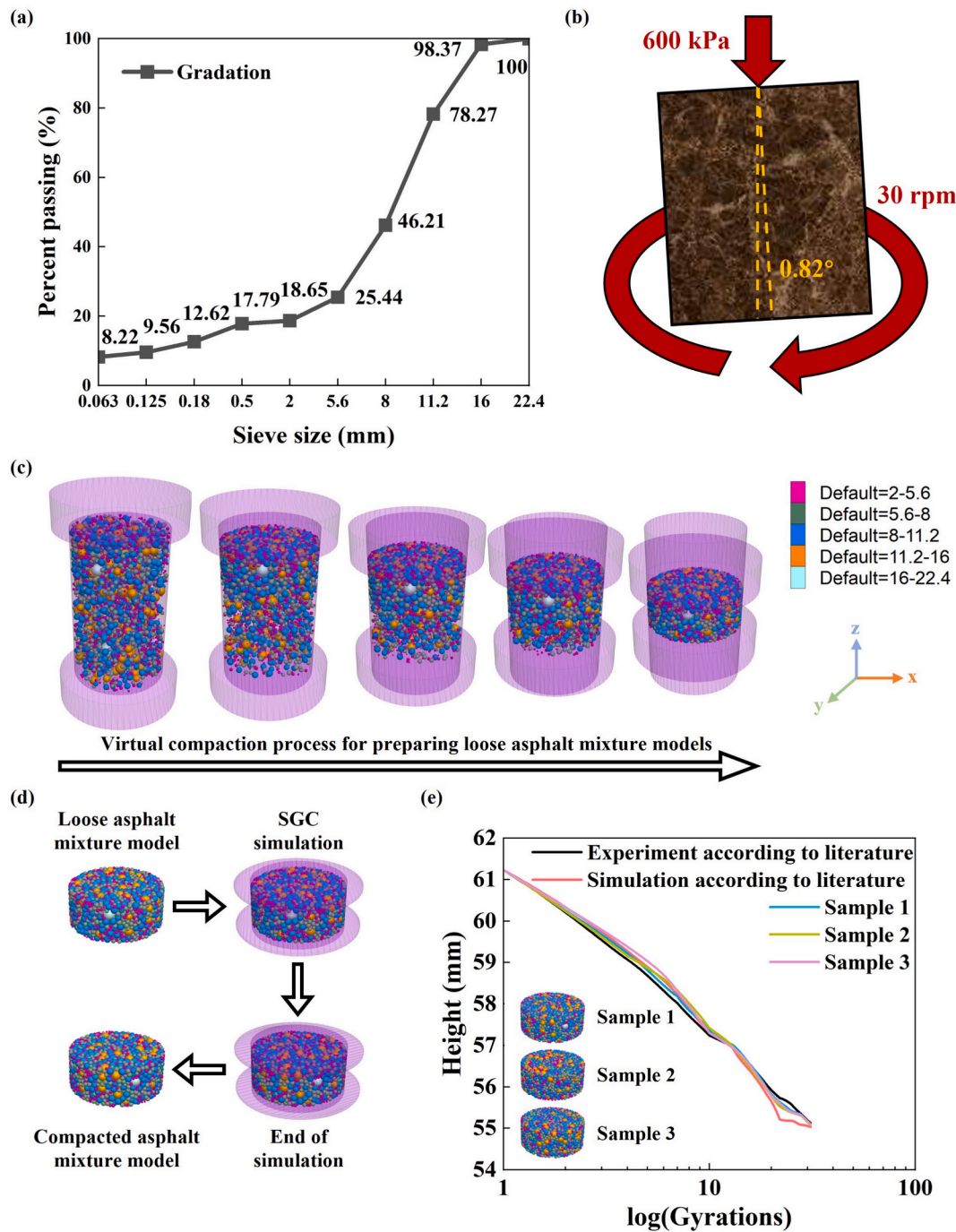


Fig. 5. Suprapave gyratory compaction (SGC) simulation: (a) selected gradation, (b) SGC parameter setting, (c) preparation of loose asphalt mixture model, (d) SGC simulation process, (e) SGC results.

reproduced the adhesion-friction mechanical properties relevant to SGC and were suitable for transfer to the subsequent 2D DEM simulations.

Three aggregate gradation families were considered to probe how particle size distribution governs pre-compaction: a discontinuous gradation (SMA-13), a continuous gradation (AC-13), and an open gradation (OGFC-13). For each family, three variants were defined with respect to the specification envelopes so that the DEM could isolate the role of relative fineness dominance. The first variant used the mid-point gradation obtained by taking the average between the upper and lower specification limits. The second variant shifted the distribution toward larger particles so that coarse fractions dominated while remaining within the allowable envelope. The third variant shifted the distribution

toward smaller particles so that fine fractions dominated. Additionally, to facilitate DEM simulation, only coarse aggregates with particle sizes greater than 2.36 mm were generated. This simplification is consistent with common asphalt-mixture terminology in which particles passing the 2.36 mm sieve are regarded as the fine fraction, and the binder together with fines is often treated as a mortar or mastic phase, while the primary load-bearing skeleton is dominated by coarse aggregate contacts [50]. Similar *meso-scale* modeling studies also focus on aggregates larger than 2.36 mm and incorporate smaller particles into the mortar phase for efficiency [51]. Accordingly, the present DEM model focuses on capturing the coarse aggregate contact network and force-chain transmission that dominate load transfer beneath the screed [52,53].

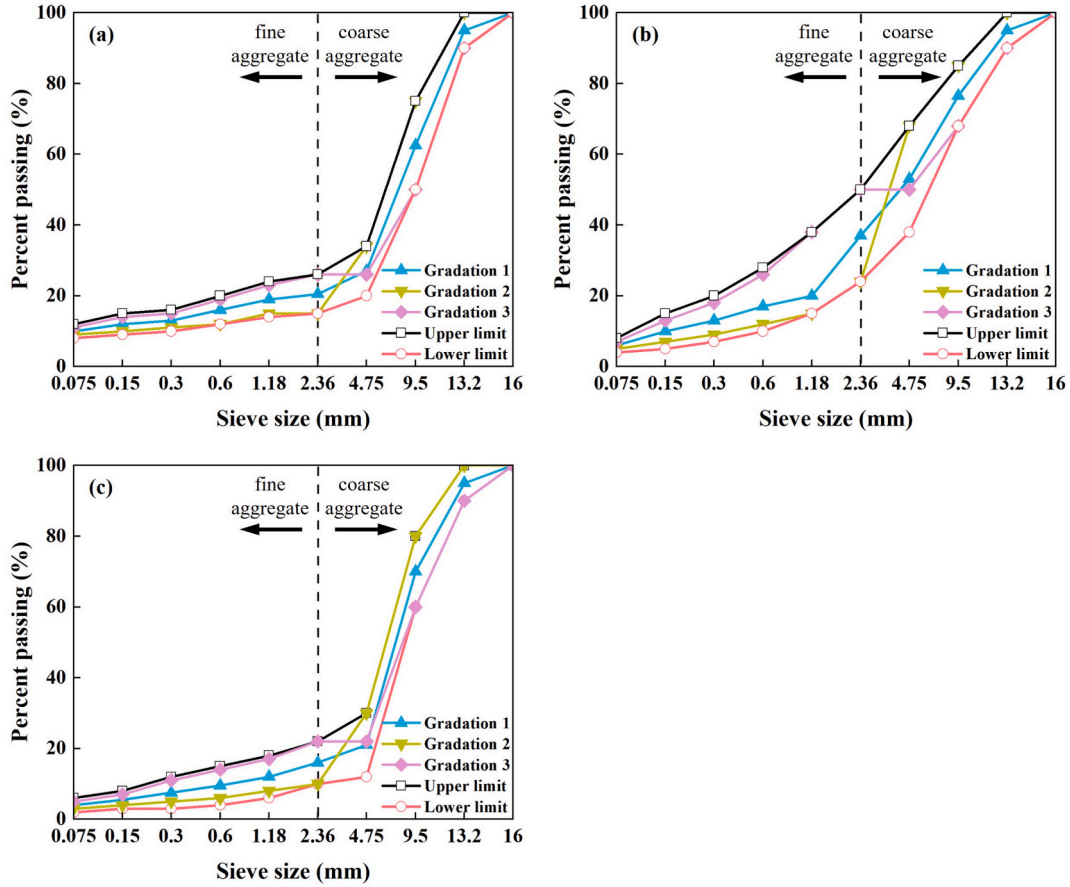


Fig. 6. Aggregate gradation curve for (a) discontinuous case (SMA-13), (b) continuous case (AC-13), (c) open case (OGFC-13).

Table 3

Aggregate gradation for pre-compaction simulation.

Sieve size (mm)			0.075	0.15	0.3	0.6	1.18	2.36	4.75	9.5	13.2	16
Gradation	SMA-13	Upper limit	12	15	16	20	24	26	34	75	100	100
		Lower limit	8	9	10	12	14	15	20	50	90	100
		Case 1	10	12	13	16	19	20.5	27	62.5	95	100
		Case 2	9	10	11	12	15	15	34	75	100	100
		Case 3	11	14	15	19	23	26	26	50	90	100
		Upper limit	8	15	20	28	38	50	68	85	100	100
	AC-13	Lower limit	4	5	7	10	15	24	38	68	90	100
		Case 1	6	10	13	17	20	37	53	76.5	95	100
		Case 2	5	7	9	12	15	24	68	85	100	100
		Case 3	7	13	18	26	38	50	50	68	90	100
		Upper limit	6	8	12	15	18	22	30	80	100	100
		Lower limit	2	3	3	4	6	10	12	60	90	100
	OGFC-13	Case 1	4	5.5	7.5	9.5	12	16	21	70	95	100
		Case 2	3	4	5	6	8	10	30	80	100	100
		Case 3	5	7	11	14	17	22	22	60	90	100

Fig. 6 illustrates the sieve-passing curves for all cases, while Table 3 lists the corresponding volumetric proportions for each size class.

2.2. Data post-processing

2.2.1. Contact identification

As shown in Fig. 7, contact identification at two interaction levels (particle-particle contact, particle-screed device contact) has been implemented in the DEM output. For particle-particle interactions, all neighboring particles in JKR contact were detected (see Fig. 7 (a)). The instantaneous contact force at the i -th contact is denoted f_i^C ; the particle-level contact intensity is defined as the scalar sum over all active

contacts:

$$F_p^C = \sum_{i=1}^{N_C} f_i^C = \sum_{i=1}^{N_C} (f_{n,i} n_i + f_{t,i} t_i) \quad (1)$$

where $f_{n,i}$ and $f_{t,i}$ are the components along the unit normal vector n_i and unit tangent vector t_i , respectively; N_C is the total number of particle contacts.

For particle-screed device interactions, contacts between particles and the tamper/screed plate boundaries were identified in the same manner (see Fig. 7 (b)). The instantaneous force transmitted to the screed device is:

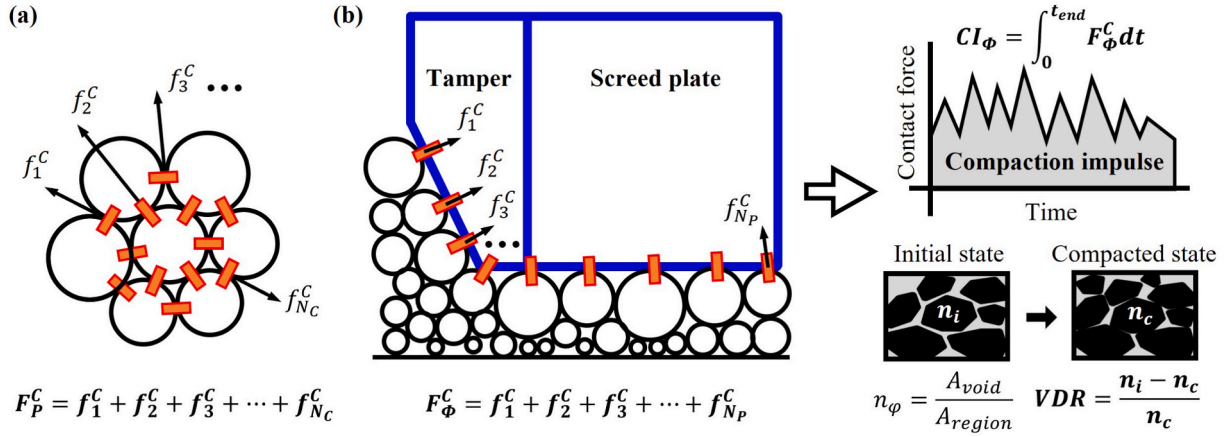


Fig. 7. Contact identification: (a) particle–particle contact, (b) particle-screed device contact and pre-compaction indicators.

$$F_{\Phi}^C = \sum_{j=1}^{N_p} f_j^C = \sum_{j=1}^{N_p} (f_{n_j} n_j + f_{t_j} t_j) \quad (2)$$

where Φ represents tamper or screed plate; N_p is the total number of contacts between the component (tamper or screed plate) and the particles.

The cumulative action delivered during the pre-compaction interval is measured by the compaction impulse (CI):

$$CI_{\Phi} = \int_0^{t_{end}} F_{\Phi}^C(t) dt \quad (3)$$

To relate contact force to local densification, a void index was computed over a moving window as the void area fraction:

$$n_{\varphi} = \frac{A_{void}}{A_{region}} \quad (4)$$

where φ represents any given moment, A_{void} denotes the void area, and A_{region} indicates the area of the measurement region.

The resulting densification was characterized by the void decrease ratio (VDR):

$$VDR = \frac{n_i - n_c}{n_c} \quad (5)$$

where n_i and n_c are the initial and compacted void indices, respectively. These above definitions establish a direct link between identified contacts, applied compaction effort, and microstructural densification.

2.2.2. Force chain identification

As a granular material, aggregate forms chain-like contact structures through compaction when subjected to external forces, enabling stress transfer. These structures are termed force chains. The intersection and fusion of force chains create a complex network that influences the macroscopic mechanical properties of asphalt layers [52,54,55]. Generally, for granular materials, force chains should satisfy three criteria: 1) contain at least three particles; 2) the principal stress on the particles exceeds the average contact stress; 3) the angle between the line connecting the centers of the contacting particles and the principal stress direction does not exceed the contact angle threshold α [56–59]. Following established granular-material practice, the separation between strong and weak force chains is commonly defined using a mean force (or mean stress) criterion, where contacts or particles carrying forces (or principal stresses) above the ensemble average are categorized as strong, and the remainder as weak [60]. For asphalt mixture force chain identification, prior DEM-based studies have likewise reported that using the average contact force as the threshold provides a stable and physically meaningful partition of strong versus weak force chains

across mixture types [61]. To maintain consistency and transparency, the same standards were applied in this study.

However, most existing studies focus on detecting strong force chains while neglecting the characterization of other contact points [53,62]. This view overlooks two elements that are equally consequential for pre-compaction. First, weak force chains form a surrounding scaffold that stabilizes strong paths, provide lateral support, and act as reservoirs for rearrangement and energy dissipation; their breakage or gradual strengthening often precedes force chain reorganization and macroscopic softening. Second, the spatial distribution of high stress and low stress particles governs where load is concentrated, where sliding initiates, and how percolating paths fragment or coalesce. Distinguishing these populations enables a more faithful description of the evolving load-bearing topology, including transitions between weak and strong force chains during vibration. Therefore, in addition to identifying strong force chains, this study explicitly detects weak force chains and classifies particles into high and low stress groups, allowing subsequent metrics to connect micro-level stress heterogeneity with the observed pre-compaction performance. Building upon the previous force chain identification process [53], this study further developed a force chain identification flowchart, as shown in Fig. 8.

(1) First, determine high/low stress particles:

$$\begin{cases} \sigma_1^k > \frac{1}{N_s} \sum_{t=1}^{N_s} |\sigma_1^t|, \text{ high stress particle} \\ \sigma_1^k < \frac{1}{N_s} \sum_{t=1}^{N_s} |\sigma_1^t|, \text{ low stress particle} \end{cases} \quad (6)$$

where N_s is defined as the number of particles in the sample; σ_1^t is the principal stress of particle:

$$\sigma_1^t = \frac{\sigma_{11}^t + \sigma_{33}^t}{2} + \sqrt{\left(\frac{\sigma_{11}^t - \sigma_{33}^t}{2}\right)^2 + (\sigma_{13}^t)^2}$$

$$\sigma_{ij}^t = \frac{1}{V} \sum_{c=1}^{N^C} f_i^c r_j^c \quad (7)$$

where N^C is the total number of contacts for particle t ; V is the volume of the particle; f_i^c is the i -th component of the force acting at contact C ; r_j^c represents the j -th component of the vector that extends from the centroid of the mass point to the contact point C .

(2) Select a high/low stress particle i and check whether its neighboring particles also exhibit high/low stress states. If no neighboring particle satisfies this condition, then $L = 1$. (L represents particles with high/low stress in the force chain.)

(3) When particle i has multiple high stress/low stress neighboring

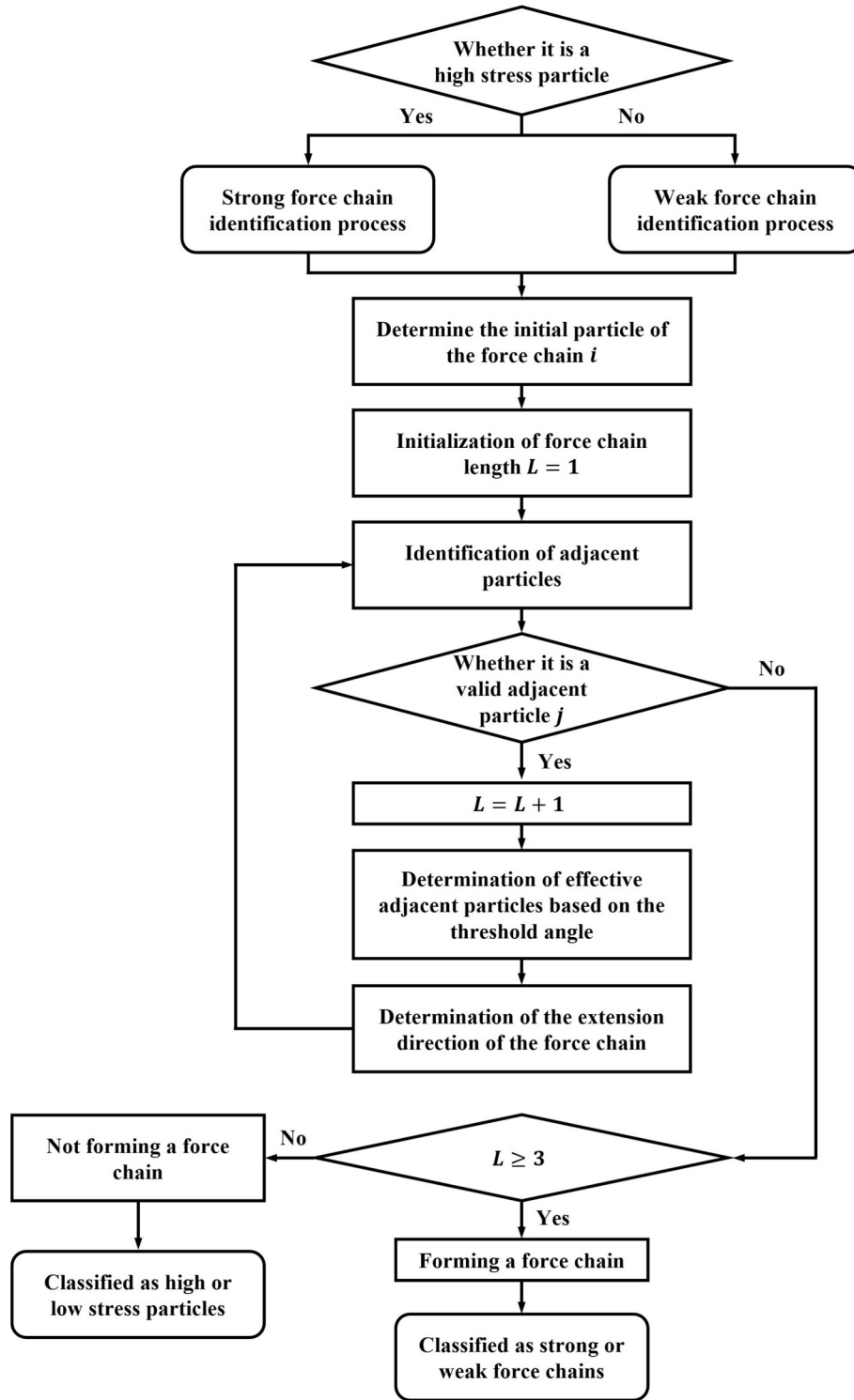


Fig. 8. Force chain identification flowchart.

particles, refer to the algorithm in [63] for further determination. Suppose particles j and k are both high stress/low stress neighbors of particle i (see Fig. 9 (a)). Taking i as the reference particle, if the angle θ between the line connecting the centroids of i and j and the principal stress direction satisfies Eq. (8), particle j is regarded as a valid neighbor of i , and the force chain length becomes $L = 2$; otherwise $L = 1$ and the chain terminates at i . The bidirectional arrows inside particles i and j in Fig. 9 (a) indicate the direction of σ_1 .

$$\cos\alpha < \theta = \frac{l_{ij}\sigma_1^i}{|l_{ij}||\sigma_1^i|} \leq 1 \quad (8)$$

where α is the angular threshold for effective adjacent particles. Previous studies indicate that when α is set to 45° , the results for the characteristic angle align with those obtained using the same threshold, while also exhibiting good robustness [63–65]. Therefore, this study adopted 45° as the reference value for different gradations. l_{ij} is the

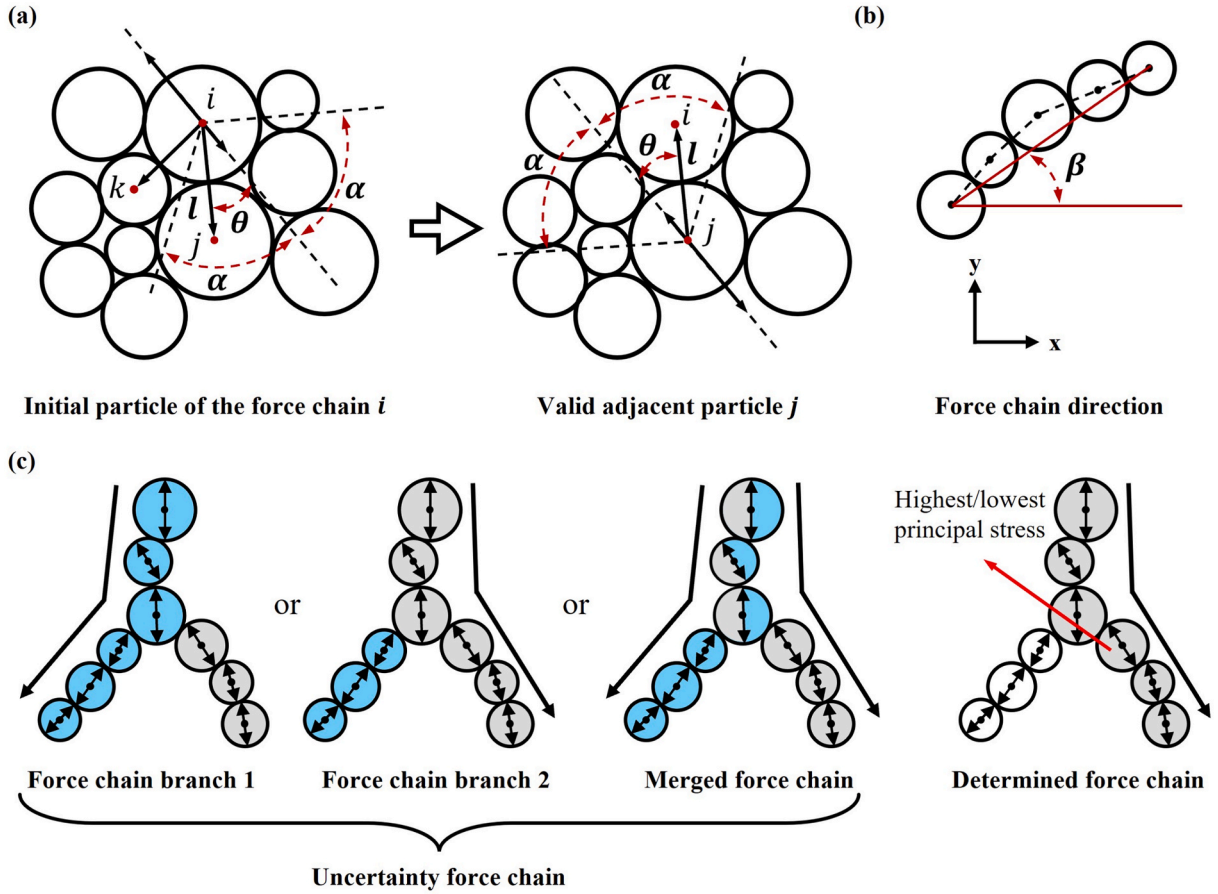


Fig. 9. Force chain identification: (a) adjacent particle detection process, (b) direction of the force chain, (c) branches of different force chains.

vector from the center of particle i to the center of particle j . Additionally, for a complete force chain, its direction was defined. The line connecting the centroids of the terminal particles in the connecting force chain was defined as the direction vector of the force chain. The angle between this vector and the x-axis was then defined as the direction angle θ of the force chain (see Fig. 9 (b)).

(4) When encountering branch points where multiple high/low stress skeleton particles may exist, different traversal sequences result in different force chain configurations, as shown in Fig. 9 (c). Furthermore, in more complex scenarios, force chains may merge. To eliminate these uncertainties, the algorithm in this study allowed only the particle with the highest/lowest principal stress to become the next particle in the force chain sequence.

(5) Repeat steps (3) and (4) to select eligible particles and add them to the force chain with a step size of $L = L + 1$ until the loop terminates. The final particle count L represents the force chain's length. Additionally, particles defined as high/low stress skeleton particles when $L < 3$ cannot form force chains.

2.3. Feature extraction

After data post-processing, relevant features need to be extracted to construct the original database. This study categorized features into two main types—particle contact and force chain—based on particle identification and force chain identification.

2.3.1. Particle contact

In this study, the features related to particle contact were categorized into particle–particle contact features and particle–screed device contact features (see Fig. 2). Firstly, the particle–particle contact features were

introduced.

The average contact force between particles $\bar{F}_p^C$ was defined as follows:

$$\bar{F}_p^C = \frac{F_p^C}{N_C} \quad (9)$$

where F_p^C is given by Eq. (1).

The mechanical coordination number Z_M [66,67], defined as the effective number of neighboring particles in contact with a given particle, serves as a crucial parameter for quantifying the internal structural characteristics of particle aggregates:

$$Z_M = \frac{2N_C - N_1}{N_P - N_0 - N_1} \quad (10)$$

where N_P , N_0 , and N_1 represent the total number of particles, the number of particles with no contact, and the number of particles with only one contact, respectively.

Given that particles interact at contact points, this study also focused on the anisotropy between particle orientation and the contact normal. As described in [68], the fabric tensor was employed to quantitatively investigate anisotropy variations. The general form of the fabric tensor, expressed in terms of the unit vector of particle orientation or the unit vector of the contact normal, is as follows [69]:

$$\Phi_{ij} = \frac{1}{N_C} \sum_{k=1}^{N_C} n_i^k n_j^k \text{ with } i, j \in \{1, 2\} \quad (11)$$

where n_i^k or n_j^k is the unit vector component (or contact normal vector) of the k -th particle in the i -th or j -th direction.

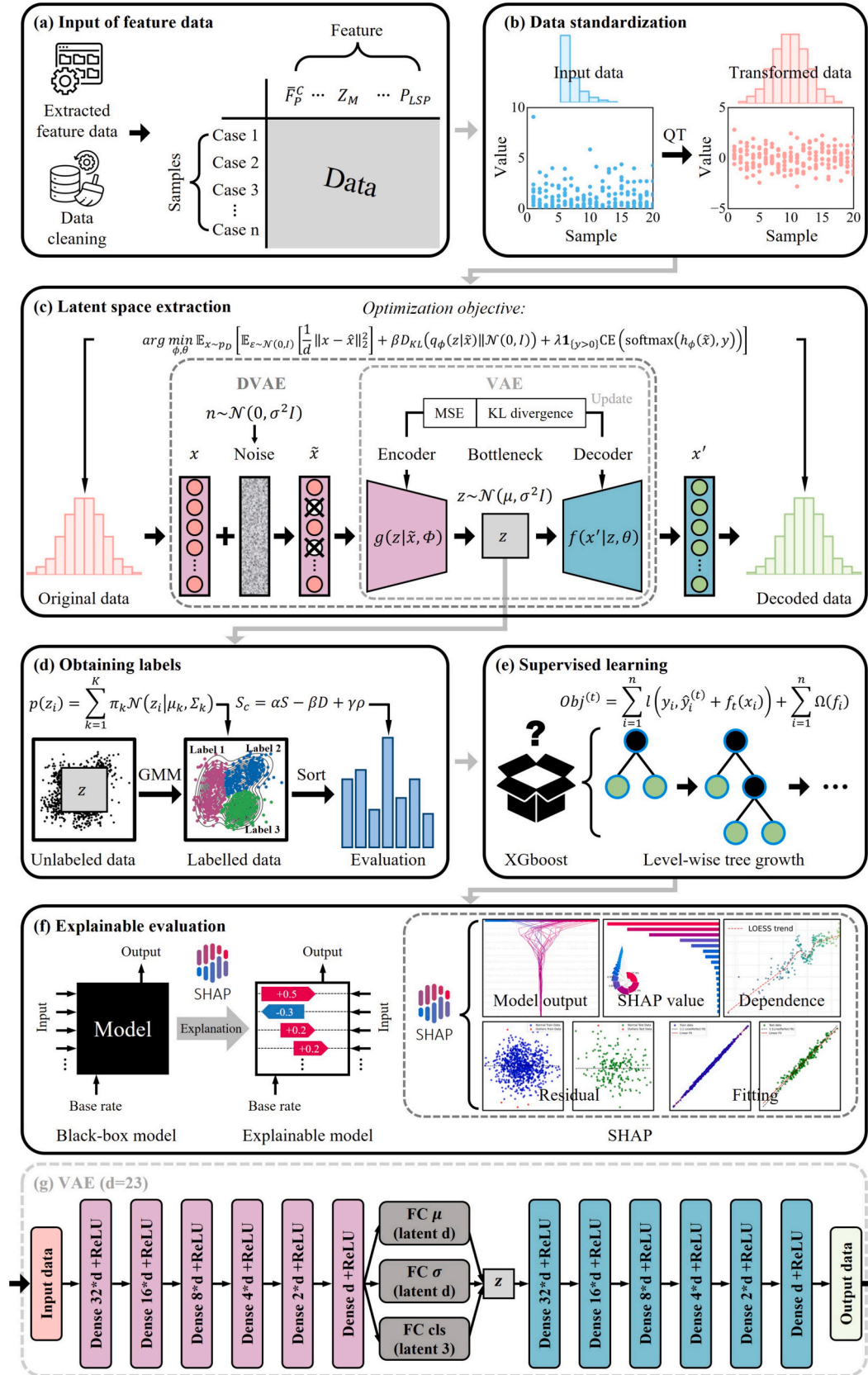


Fig. 10. Automatic feature evaluation framework: (a) input of feature data, (b) data standardization, (c) latent space extraction, (d) obtaining labels, (e) supervised learning, (f) explainable evaluation, (g) structure of variational autoencoder.

Then, this study employed deviatoric fabric to characterize the anisotropy between particles:

$$\Phi_D = 2\sqrt{\left(\frac{\Phi_{ii} - \Phi_{jj}}{2}\right)^2 + \Phi_{ij}^2} \quad (12)$$

This study further adopted the probability density function (PDF) of contact forces, which is an important and commonly used feature for investigating particle contacts. For the PDF of contact forces, as commonly observed in granular piles [70,71], the proportion of contacts with forces above the mean exhibits exponential decay, while the proportion of contacts below the mean $\langle F_p^C \rangle$ follows a power-law distribution:

$$PDF(F_p^C) = \begin{cases} \alpha_2(\eta)e^{-\alpha_1(\eta)(F_p^C/\langle F_p^C \rangle)}, & F_p^C > \langle F_p^C \rangle \\ \beta_2(\eta)\left(\frac{F_p^C}{\langle F_p^C \rangle}\right)^{\beta_1(\eta)}, & F_p^C < \langle F_p^C \rangle \end{cases}$$

$$F_p^{NC} = \frac{F_p^C}{\langle F_p^C \rangle} \quad (13)$$

where $\alpha_1(\eta)$, $\alpha_2(\eta)$, $\beta_1(\eta)$, and $\beta_2(\eta)$ are fitting parameters; F_p^{NC} is the normalized contact force.

Additionally, a strong contact force ratio (SCFR) was defined, representing the proportion of particle contact forces exceeding the average contact force:

$$SCFR = \frac{1}{N_p} \sum_{i=1}^{N_p} 1\{f_i^C > \bar{F}_p^C\} \quad (14)$$

where $1\{\cdot\}$ is the characteristic function, which takes the value 1 if the condition is true and 0 otherwise.

Then, the distribution frequency of the contact numbers for each particle was calculated:

$$f(n_c) = \frac{1}{N_p} \sum_{i=1}^{N_p} 1\{n_c^{(p)} = n_c\}, n_c = 0, 1, 2, \dots \quad (15)$$

where $n_c^{(p)}$ is the contact number of the p -th particle.

Furthermore, to investigate the distribution pattern of contact force directions, the contact force directions were divided into angular zones within the x-y plane. Then, fitting was performed according to the following formula [72]:

$$F_p^C(\beta) = \bar{F}_p^C \left[1 + a_n \sin\left(\pi \frac{\beta - \beta_n}{T/2}\right) \right] \quad (16)$$

where a_n is the Fourier coefficient, whose value characterizes the anisotropy coefficient of force chain intensity; T is the minimum positive period; β_n is the principal direction of contact force distribution.

Finally, the contact features of the particle-screed device were presented. The average contact force between particles and screed device was defined as follows:

$$\bar{F}_\Phi^C = \frac{F_\Phi^C}{N_p} \quad (17)$$

Additionally, this study employed CI and VDR to characterize the contact properties between particles and the screed device. These two features have been discussed previously and will not be repeated here (see Eq. (3) and Eq. (5)).

2.3.2. Force chain

In this study, features related to force chains were categorized into strong/weak force chain features and strong/weak particle stress features (see Fig. 2).

First, the features related to force chains were considered. Since not

all contact particles lie on force chains, it is necessary to first clearly distinguish the proportion of particles located on force chains (P_{PFC}):

$$P_{PFC} = \frac{N_{PFC}}{N_p} \quad (18)$$

where N_{PFC} is the number of particles on the force chain.

Furthermore, it can be categorized into two scenarios: proportion of particles on the strong force chain (P_{PSFC}) and particles on the weak force chain (P_{PWFC}):

$$P_{PSFC} = \frac{N_{PSFC}}{N_p}$$

$$P_{PWFC} = \frac{N_{PWFC}}{N_p} \quad (19)$$

where N_{PSFC} and N_{PWFC} are the numbers of particles on the strong force chain and weak force chain, respectively.

Then, the proportion of strong force chains (P_{SFC}) and weak force chains (P_{WFC}) was considered:

$$P_{SFC} = \frac{N_{SFC}}{N_{TFC}}$$

$$P_{WFC} = \frac{N_{WFC}}{N_{TFC}} \quad (20)$$

where N_{SFC} , N_{WFC} , and N_{TFC} represent the number of strong force chains, the number of weak force chains, and the total number of force chains, respectively.

Then, the average force chain length ($\bar{L}_{FC}$) was defined:

$$\bar{L}_{FC} = \frac{1}{N_\Phi} \sum_{j=1}^{N_\Phi} L_j \quad (21)$$

where N_Φ represents the number of strong or weak force chains; and the length of the j -th force chain is denoted as $L_j \in \{1, 2, 3, \dots\}$.

Additionally, to investigate the distribution pattern of force chain directions, the force chain directions were divided into angular regions within the x-y plane (see Fig. 9 (b)). Then, fitting was performed according to the following formula:

$$P_{FCD}(\beta) = \frac{1}{2\pi} \left[1 + a_n \sin\left(\pi \frac{\beta - \beta_n}{T/2}\right) \right] \quad (22)$$

Then, features related to particle stress were considered. Since only particles not on force chains could be used for further statistics, the proportion of particles not on force chains (P_{PNFC}) was calculated:

$$P_{PNFC} = \frac{N_{PNFC}}{N_p} = 1 - P_{PFC} \quad (23)$$

where N_{PNFC} is the number of particles not on the force chain.

Subsequently, the ratio of high stress particles (P_{HSP}) and low stress particles (P_{LSP}) was calculated:

$$P_{HSP} = \frac{N_{HSP}}{N_{PNFC}}$$

$$P_{LSP} = \frac{N_{LSP}}{N_{TFC}} \quad (24)$$

where N_{HSP} and N_{LSP} represent the number of particles under strong stress and weak stress, respectively.

2.4. Automatic feature evaluation

After extracting all relevant features, an automatic feature evaluation procedure was applied to organize them into a coherent, data-driven assessment of pre-compaction behavior. Fig. 10 summarizes the

Table 4
Extracted features.

Feature ID	Symbol for effective features	Meaning	Identifier
1	$\bar{F}_P^C$	Average contact force between particles	F_PC
2	$\bar{F}_P^{NC}$	Normalized average contact force between particles	F_PNC
3	Z_M	Mechanical coordination number	Z_M
4	$SCFR$	Strong contact force ratio	SCFR
5	Φ_D	Deviatoric fabric	Phi_D
6	$\bar{n}_C$	Average particle contact number	f_nc
7	a_n	Fourier coefficient for contact force directions	F_PCβ
8	$\bar{F}_T^C$	Average contact force of particle-tamper	F_TC
9	$\bar{F}_{SP}^C$	Average contact force of particle-screed plate	F_SPC
10	CI_T	Compaction impulse of tamper	CI_TC
11	CI_{SP}	Compaction impulse of screed plate	CI_SPC
12	VDR	Void decrease ratio	VDR
13	P_{SFC}	Proportion of strong force chains	P_SFC
14	P_{WFC}	Proportion of strong force chains	P_WFC
15	P_{PFC}	Proportion of weak force chains	P_PFC
16	P_{PSFC}	Proportion of particles on the strong force chain	P_PSFC
17	P_{PWFC}	Proportion of particles on the weak force chain	P_PWFC
18	P_{PNFC}	Proportion of particles not on force chains	P_PNFC
19	P_{HSP}	Ratio of high stress particles	P_HSP
20	P_{LSP}	Ratio of low stress particles	P_LSP
21	$\bar{L}_{FC}^S$	Average strong force chain length	L_FC_S
22	$\bar{L}_{FC}^W$	Average weak force chain length	L_FC_W
23	a_n	Fourier coefficient for force chain directions	P_FCDβ

corresponding workflow. First, the simulated-case features were collected, cleaned, and assembled into an input matrix (see Fig. 10 (a)). Data standardization via a QuantileTransformer (QT) was then performed so that heterogeneous feature distributions were mapped to comparable scales (see Fig. 10 (b)). Latent-space extraction with a denoising variational autoencoder (DVAE) compressed the standardized features into a low-dimensional vector z while reconstructing the inputs (see Fig. 10 (c)). Data-driven labels were obtained by clustering the latent vectors using a Gaussian mixture model (GMM), and a composite score was computed for ranking and evaluation (see Fig. 10 (d)). Supervised learning with XGBoost was subsequently conducted to relate the original features to the obtained labels and to build a predictive surrogate model (see Fig. 10 (e)). Explainable evaluation using SHAP was carried out to attribute model outputs to specific features and to visualize effects, residuals, and dependence trends (see Fig. 10 (f)). The representative network architecture used for the VAE, including encoder, latent layer, and decoder configurations, is provided for completeness (see Fig. 10 (g)). Taken together, these steps convert raw feature sets into labeled, predictive, and interpretable informatics descriptors of pavement pre-compaction.

2.4.1. Input of feature data

After the DEM simulations concluded, feature extraction was performed based on the content mentioned in Section 2.3. In this study, a total of 23 relevant features were considered, with their detailed symbols for effective features, meanings, and identifiers shown in Table 4. In addition, all feature input data corresponded to values at the end of the pre-compaction moment ($t = 15s$).

Subsequently, data cleaning was performed on the extracted features. The objective of this step was to provide a clean, scalar feature matrix ready for direct analysis, ensuring subsequent processes—

standardization, representation learning, and classification—remained unaffected by data quality issues. Because all features were scalar summaries, the influence of atypical values could bias downstream standardization and learning. Therefore, only outliers were considered at this stage. A robust z-score based on the median and the median absolute deviation (MAD) was used. For feature j with observations $x_{1j}, \dots, x_{nj}$, the statistics were computed as [73]:

$$m_j = \text{median}_i(x_{ij}) \quad (25)$$

and the robust score for sample i was:

$$r_{ij} = \frac{x_{ij} - m_j}{1.4826 \cdot \text{MAD}_j} \quad (26)$$

Observations with $|r_{ij}| > \tau$ (typically $\tau \in [3, 4]$, set to 3.5 in this study) were flagged as outliers. Flagged values were then winsorized at the feature-wise p and $1 - p$ quantiles (e.g., $p = 0.01$ in this study):

$$\tilde{x}_{ij} = \min\left(\max(x_{ij}, Q_j^p), Q_j^{1-p}\right) \quad (27)$$

which preserved sample size while limiting undue leverage from extreme measurements. This procedure yielded a stable, analysis-ready matrix of scalar features.

2.4.2. Data standardization

After data cleaning, each scalar feature was standardized with the QT [74,75] so that heterogeneous marginal distributions became comparable for downstream learning. The transform was applied feature-wise and preserves rank information while reducing the influence of extreme values.

To ensure transparency and reproducibility, the QT was implemented feature-wise with a fixed target distribution and explicit control of the quantile grid. For a given feature j with observations $x_{1j}, \dots, x_{nj}$, the empirical cumulative distribution function (ECDF) was computed as:

$$\hat{F}_j(x) = \frac{1}{n} \sum_{i=1}^n \mathbf{1}\{x_{ij} \leq x\} \quad (28)$$

Each observation was first mapped to its empirical quantile:

$$u_{ij} = \hat{F}_j(x_{ij}) \approx \frac{\text{rank}(x_{ij}) - 0.5}{n} \quad (29)$$

Linear interpolation was employed on the ECDF nodes, with extrapolation permitted at the tails when necessary. To stabilize the inverse CDF step, the mapped quantiles were truncated at the endpoints:

$$\tilde{u}_{ij} = \min(\max(u_{ij}, \varepsilon), 1 - \varepsilon) \text{ with } \varepsilon = 10^{-7} \text{ in this study} \quad (30)$$

The standardized values were then obtained by pushing $\tilde{u}_{ij}$ through the inverse CDF of the target distribution G :

$$z_{ij} = G^{-1}(\tilde{u}_{ij}) \quad (31)$$

where G is the standard normal ($G = \Phi$) in this study.

So that each feature acquired approximately Gaussian marginals with mean zero and unit scale while preserving rank order. (When a uniform target was required, the mapping reduced to $z_{ij} = \tilde{u}_{ij}$.)

Because the raw ECDF can contain a large number of nodes, a bounded quantile grid was enforced to make the fitted transform portable. Let $n_q = \min(1000, \max(2, n))$ denote the maximum number of CDF nodes retained per feature. The original ECDF nodes $\{(x, u)\}$ were thinned onto equally spaced probabilities:

$$u_g = \frac{k - 0.5}{n_q} \text{ with } k = 1, \dots, n_q \quad (32)$$

and the corresponding abscissae x_g were obtained by linear interpola-

tion on (x, u) . The fitted pair $\{(x_g, u_g)\}$ was stored and reused for out-of-sample transformation, ensuring that the same monotone map $x \mapsto z$ was applied across datasets. Features with fewer than two finite samples were left unchanged and flagged, preserving the sample set while avoiding ill-posed fits. Through these settings—target $G = \Phi$, endpoint clip $\varepsilon = 10^{-7}$, and quantile grid size n_q —the transform produced stable, order-preserving standardization suitable for the subsequent representation learning and classification.

2.4.3. Latent space extraction

A variational autoencoder (VAE) [76] was employed to compress the standardized feature vector $x \in \mathbb{R}^d$ ($d = 23$) into a latent representation $z \in \mathbb{R}^l$ ($l = 23$) (see Fig. 10 (c)). To improve robustness, a denoising variant (DVAE) [77] was optionally used: the encoder received a corrupted input $\tilde{x}$ while the decoder reconstructed the clean target x . Additive Gaussian noise was employed:

$$\tilde{x} = x + \sigma_n \epsilon \in (\mathcal{N}(0, I)) \quad (33)$$

where σ_n is 0.15 in this study, I is the identity covariance matrix (isotropic Gaussian noise).

The encoder defined the approximate posterior:

$$q_\phi(z|\tilde{x}) = \mathcal{N}\left(\mu_\phi(\tilde{x}), \text{diag}\left(\sigma_\phi^2(\tilde{x})\right)\right) \quad (34)$$

$$z = \mu_\phi(\tilde{x}) + \sigma_\phi(\tilde{x}) \odot \epsilon \text{ with } \epsilon \in \mathcal{N}(0, I)$$

where $\odot$ is Hadamard product.

This was followed by a decoder $p_\theta(x|z)$, which generated $\hat{x} = f_\theta(z)$. Training minimized a composite objective consisting of reconstruction fidelity, a β -weighted Kullback–Leibler (KL) regularizer to the unit Gaussian prior $p(z) = \mathcal{N}(0, I)$, and a masked cross-entropy term that shaped the latent space using available class labels $y \in \{1, 2, 3\}$ (SMA-13, AC-13, OGFC-13).

The training objective can be formulated as a single expectation minimization problem for the parameters of the encoder, decoder, and classifier (ϕ, θ) . The model is fitted on samples $x \sim p_D$ drawn from the standardized feature dataset. For DVAE training a corrupted input $\tilde{x}$ is provided to the encoder, while the clean x is the reconstruction target. Latent sampling uses the reparameterization as shown in Eq. (34). The objective combines (i) the expected squared reconstruction error normalized by the feature dimension d , (ii) a KL regularizer that encourages the approximate posterior $q_\phi(z|\tilde{x})$ to match the unit Gaussian prior, and (iii) a supervised cross-entropy on the encoder's classifier head $h_\phi(\tilde{x})$, applied only when a label y is available. Formally:

$$\begin{aligned} \argmin_{\phi, \theta} \mathbb{E}_{x \sim p_D} \left[\mathbb{E}_{\epsilon \sim \mathcal{N}(0, I)} \left[\frac{1}{d} \|x - \hat{x}\|_2^2 \right] + \beta D_{KL}(q_\phi(z|\tilde{x}) \| \mathcal{N}(0, I)) \right. \\ \left. + \lambda 1_{\{y>0\}} CE(\text{softmax}(h_\phi(\tilde{x}), y)) \right] \end{aligned} \quad (35)$$

where β and λ weight the KL and supervised terms, $1_{\{y>0\}}$ masks unlabeled samples. This expression makes explicit that the model jointly learns a reconstruction-friendly, prior-regularized latent space that is aligned with class information when labels are present.

Then, the loss function denoted as:

$$\begin{aligned} \mathcal{L}(\phi, \theta) = \frac{1}{d} \|x - \hat{x}\|_2^2 + \beta D_{KL}(q_\phi(z|\tilde{x}) \| \mathcal{N}(0, I)) \\ + \lambda 1_{\{y>0\}} CE(\text{softmax}(h_\phi(\tilde{x}), y)) \end{aligned} \quad (36)$$

The structure of the VAE is shown in Fig. 10 (g), which employs a fully connected ReLU network. The encoder mapped $\mathbb{R}^d \mapsto \mathbb{R}^l$ through hidden widths $[32d, 16d, 8d, 4d, 2d, d]$ and produced three heads: $\mu \in \mathbb{R}^l$, $\log \sigma^2 \in \mathbb{R}^l$, and class logits in $\mathbb{R}^3$. The decoder symmetrically mapped

$\mathbb{R}^l \mapsto \mathbb{R}^d$ with widths $[d, 2d, 4d, 8d, 16d, 32d]$ and a linear output layer. Data were split into 70% training and 30% validation with a random seed. Optimization used Adam with learning rate 2×10^{-5} , $\beta_1 = 0.9$, $\beta_2 = 0.999$, minibatch size 20, and 300 epochs. Hyperparameters were set to $\beta = 1.0$ (KL weight) and $\lambda = 1.0$ (cross-entropy weight).

Through the above process, a compact and structured latent space was generated. In this study, a VAE-type encoder–decoder is used as a nonlinear, parametric mapping from the standardized indicator space to a latent space, which is convenient for subsequent clustering and predictive modeling. This differs from principal component analysis (PCA), which is inherently linear and may not capture the nonlinear coupling among microstructural descriptors [78]. It also differs from t-SNE, which is primarily designed for visualization and typically requires re-optimization when embedding new samples, making it less suitable as a stable representation in an automated pipeline [79]. The denoising training strategy further encourages the encoder to learn noise-invariant factors by reconstructing the clean target from a perturbed input, a mechanism that has been shown to improve robustness in representation learning [77,80]. In addition, the prior regularization inherent to VAEs promotes a smoother and more structured latent space, and related VAE variants have been widely used to encourage more interpretable latent factors, which supports the mechanism-oriented interpretation pursued in this work [81,82].

2.4.4. Obtaining labels

Labels were obtained in the learned latent space z (see Fig. 10 (d)) by fitting a Gaussian mixture model (GMM) [83,84] with $K = 3$ components corresponding to the three gradation families (SMA-13, AC-13, OGFC-13). Let $Z = \{z_i\}_{i=1}^n$ denote the latent means produced by Section 2.4.3. The mixture density is:

$$p(z_i) = \sum_{k=1}^K \pi_k \mathcal{N}(z_i | \mu_k, \Sigma_k) \text{ with } \pi_k \geq 0, \sum_k \pi_k = 1 \quad (37)$$

where $\{\pi_k, \mu_k, \Sigma_k\}_{k=1}^K$ were estimated by Expectation–Maximization (EM).

Initialization used k-means centroids with full empirical covariances, followed by ridge regularization to ensure numerical stability and invertibility. The algorithm alternated expectation and maximization steps until the log-likelihood converged under a stringent relative improvement criterion, and full covariances were retained to capture anisotropy in the latent geometry. Posterior responsibilities then provided both hard labels and confidence scores for subsequent evaluation:

$$\Sigma_k \leftarrow \Sigma_k + \varepsilon I$$

$$\frac{\mathcal{L}^{(t)} - \mathcal{L}^{(t-1)}}{|\mathcal{L}^{(t-1)}|} < 10^{-6}$$

$$\hat{y}_i = \argmax_k \gamma_{ik}$$

$$c_i = \max_k \gamma_{ik} \quad (38)$$

where I is the identity matrix of size equal to the latent dimension, $\varepsilon = 10^{-4}$ is a small ridge parameter for covariance regularization, $\mathcal{L}^{(t)}$ denotes the data log-likelihood at EM iteration t , γ_{ik} is the posterior responsibility of component k for sample i , $\hat{y}_i$ is the resulting pseudo label (maximum a posteriori assignment), and c_i is the associated confidence (maximum posterior probability).

Then, to evaluate and rank the nine cases, three complementarity indicators were computed in the latent space:

1 Silhouette indicator (S) [85] (larger is better):

For sample i , let $a(i)$ be the mean distance from i to points in its own cluster and $b(i)$ the smallest mean distance from i to any other cluster. The silhouette value is:

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}} \in [-1, 1]$$

$$S = \frac{1}{n} \sum_{i=1}^n s(i) \quad (39)$$

2 Davies–Bouldin indicator (D) [86] (smaller is better):

Let d_k denote the average within-cluster dispersion for cluster k , and m_{kj} the distance between centroids k and j . Define:

$$R_{kj} = \frac{d_k + d_j}{m_{kj}}$$

$$D = \frac{1}{K} \sum_{k=1}^K \max_{j \neq k} R_{kj} \quad (40)$$

3 Density indicator (ρ) (larger is better):

Using the GMM posteriors, the dataset-level confidence is:

$$\rho = \frac{1}{n} \sum_{i=1}^n \max_k \gamma_{ik} \in [0, 1] \quad (41)$$

Then, a composite score was formed to rank the scenarios:

$$S_c = \alpha S - \beta D + \gamma \rho \text{ with } \alpha, \beta, \gamma \geq 0 \quad (42)$$

and scenarios were sorted in descending order of S_c . In this study, equal weights were used ($\alpha = \beta = \gamma = 1$), which balanced separation quality (S), compactness vs. separation (D), and probabilistic concentration (ρ).

2.4.5. Supervised learning

After preprocessing and latent space extraction, a labeled dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$ with $x_i \in \mathbb{R}^{23}$ (standardized features) and $y_i \in \{1, \dots, 9\}$ (“case_true”) was obtained. To retain the ordinal structure of the labels while exploiting tree ensembles, prediction was formulated as scalar regression on y_i .

Features were standardized using statistics from the training partition only:

$$z_{ij} = \frac{x_{ij} - \mu_j}{\sigma_j}$$

$$\mu_j = \frac{1}{n_{\text{train}}} \sum_{i \in \text{train}} x_{ij}$$

$$\sigma_j = \sqrt{\frac{1}{n_{\text{train}}} \sum_{i \in \text{train}} (x_{ij} - \mu_j)^2 + \varepsilon} \text{ with } \varepsilon = 10^{-4} \quad (43)$$

Data were split into training and test sets with an 80/20 ratio. The fitted scaler was then applied to the test set.

Gradient-boosted decision trees (XGBoost) [87] with mean squared error as the objective function were adopted (see Fig. 10 (e)). Let $F^{(t)}$ denote the additive predictor after t boosting rounds. At round t , a tree $f_t \in \mathcal{F}$ was added with learning rate η :

$$\hat{y}_i^{(t)} = F^{(t-1)}(x_i) + \eta f_t(x_i) \quad (44)$$

The stagewise objective combined a second-order Taylor approximation of the loss with a structure penalty:

$$Obj^{(t)} = \sum_{i=1}^n l(y_i, \hat{y}_i^{(t-1)} + \eta f_t(x_i)) + \Omega(f_t)$$

$$l(y, \hat{y}) = \frac{1}{2} (y - \hat{y})^2$$

$$\Omega(f_t) = \gamma T + \frac{1}{2} \lambda \sum_{j=1}^T w_j^2 \quad (45)$$

where T is the number of leaves and w_j is the weight of leaf j . γ and λ denote the structure penalty per leaf and the L_2 regularization on leaf weights $\{w_j\}$, respectively. Both γ and λ used the default values 0 and 1.

The optimal leaf weight and split gain were:

$$w_j^* = - \frac{\sum_{i \in I_j} g_i}{\sum_{i \in I_j} h_i + \lambda}$$

$$Gain = \left[-\frac{1}{2} \frac{(\sum_{i \in I_L} g_i)^2}{\sum_{i \in I_L} h_i + \lambda} - \frac{1}{2} \frac{(\sum_{i \in I_R} g_i)^2}{\sum_{i \in I_R} h_i + \lambda} + \frac{1}{2} \frac{(\sum_{i \in I} g_i)^2}{\sum_{i \in I} h_i + \lambda} \right] - \gamma$$

$$g_i = \partial_y l(y_i, \hat{y})|_{\hat{y}=\hat{y}_i^{(t-1)}} = \hat{y}_i^{(t-1)} - y_i$$

$$h_i = \partial_y^2 l(y_i, \hat{y})|_{\hat{y}=\hat{y}_i^{(t-1)}} = 1 \quad (46)$$

where I_L and I_R are the sample sets assigned to the left child node and right child node, respectively.

Model selection was performed by grid search with 5-fold cross-validation on the training split. The grid configuration for this study was:

$$n_estimators \in \{100, 200, 300\}$$

$$max_depth \in \{3, 5, 7\}$$

$$learning_rate \in \{0.01, 0.05, 0.10\}$$

$$subsample \in \{0.7, 1.0\}$$

$$colsample_bytree \in \{0.6, 1.0\} \quad (47)$$

The selection metric was the mean cross-validated coefficient of determination R^2 . The best configuration was refit on the full training data to obtain the final predictor $\hat{F}$. Predictive performance was reported on both training and test sets using:

$$R^2 = 1 - \frac{\sum_{i=1}^m (y_i - \hat{y}_i)^2}{\sum_{i=1}^m (y_i - \bar{y})^2}$$

$$MSE = \frac{1}{m} \sum_{i=1}^m (y_i - \hat{y}_i)^2$$

$$RMSE = \sqrt{MSE}$$

$$MAE = \frac{1}{m} \sum_{i=1}^m (y_i - \bar{y})^2 \quad (48)$$

where m is the number of evaluated samples and $\bar{y}$ is the empirical mean of y .

2.4.6. Explainable evaluation

As shown in Fig. 10 (f), this study further adopted a Shapley (SHAP)-value-based framework [88,89] to interpret the results obtained using XGBoost in Fig. 10 (e). Explanations were computed on the standardized feature space (23 variables) using the SHAP, and were summarized at both global and local levels.

Let $f(x) : \mathbb{R}^d \rightarrow \mathbb{R}$ denote the trained model and $x \in \mathbb{R}^d$ ($d = 23$) a sample. The SHAP represents the prediction as a sum of a baseline and feature contributions:

$$f(x) = \phi_0 + \sum_{j=1}^d \phi_j(x) \quad (49)$$

where $\phi_0 = \mathbb{E}_X[f(X)]$ is the expected model output over a background distribution and $\phi_j(x)$ is the Shapley value of feature j at x . For any



Fig. 11. Distribution of particles and force chains before pre-compaction: (a) simulation initialization, (b) distribution of strong force chains, (c) distribution of high stress particles, (d) distribution of weak force chains, (e) distribution of low stress particles.

feature subset $S \subseteq \{1, \dots, d\} \setminus \{j\}$, the Shapley value is calculated as:

$$\phi_j(x) = \sum_S \frac{|S|!(d - |S| - 1)!}{d!} \left[f_{S \cup \{j\}}(x) - f_S(x_S) \right] \quad (50)$$

where f_S is the model that marginalizes features outside the feature subset S . These attributions satisfy efficiency $\sum_j \phi_j(x) = f(x) - \phi_0$, symmetry, dummy, and additivity, ensuring a unique, game-theoretic allocation of contributions.

Global importance for feature j was quantified by the expected absolute attribution:

$$I_j = \mathbb{E}_x[|\phi_j(x)|] \approx \frac{1}{n} \sum_{i=1}^n |\phi_j(x^{(i)})| \quad (51)$$

The expectation terms were estimated by empirical averages over the evaluation set. For univariate effects ($|S| = 1$), individual conditional expectation (ICE) curves were computed for each observation i as:

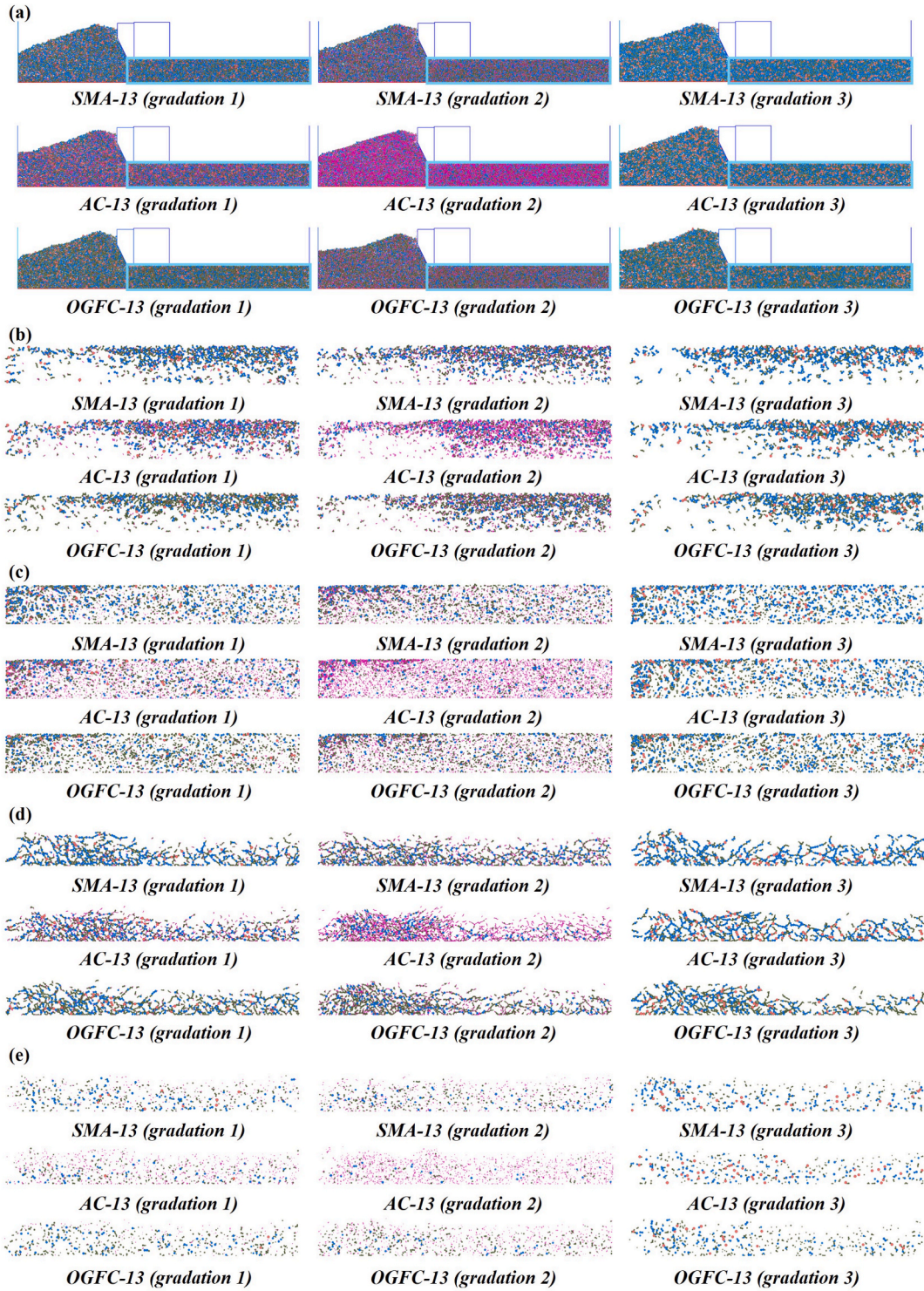


Fig. 12. Distribution of particles and force chains after pre-compaction: (a) simulation initialization, (b) distribution of strong force chains, (c) distribution of high stress particles, (d) distribution of weak force chains, (e) distribution of low stress particles.

$$ICE_i(x_j) = f(x_j, x_{-j}^{(i)}) \quad (52)$$

where $x_{-j}^{(i)}$ denotes the observed values of all features except x_j for instance i . And the partial dependence (PD) function was obtained as the cross-sectional average of the ICE curves:

$$PD(x_j) = \frac{1}{n} \sum_{i=1}^n ICE_i(x_j) \quad (53)$$

yielding an empirical approximation of $\mathbb{E}_{x_{-j}}[f(x_j, X_{-j})]$. ICE trajectories and PD trends can be visualized synchronously. Additionally, to summarize the central trend of the ICE cloud cluster, this study overlaid a LOESS smoother (using span = 0.3). This smoother serves solely as a descriptive auxiliary tool and does not alter the underlying model or estimates.

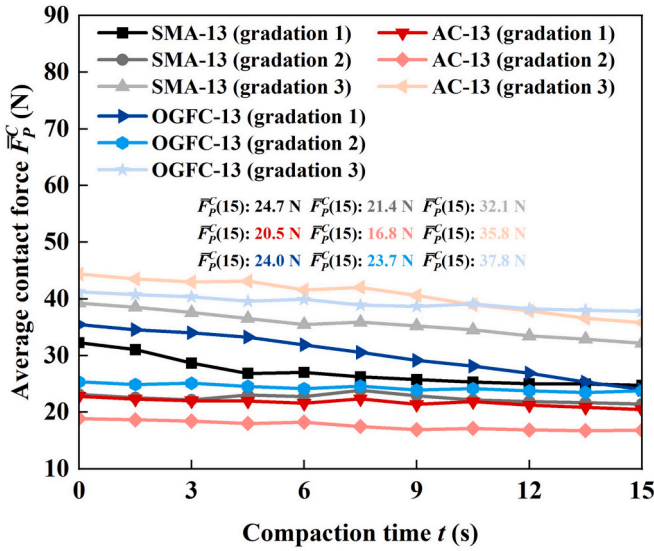


Fig. 13. Average contact forces between particles ($\bar{F}_p^C$) for different gradations.

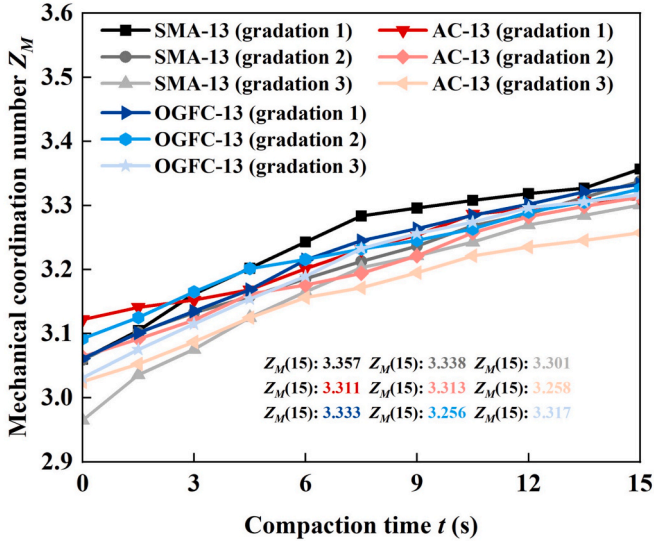


Fig. 14. Mechanical coordination number (Z_M) for different gradations.

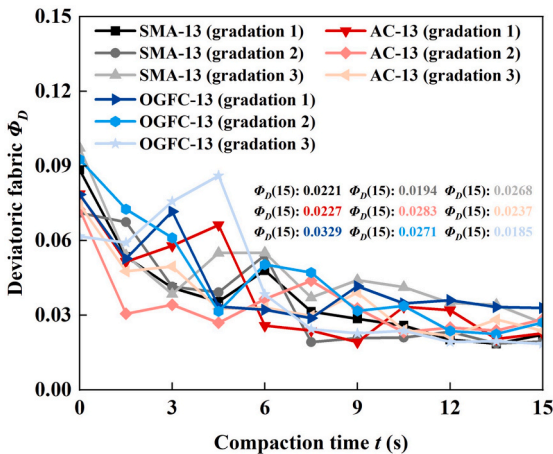


Fig. 15. Deviatoric fabric (Φ_D) for different gradations.

3. Results and discussion

The study employed PFC 2D to simulate the pre-compaction process (see Section 2.1). For each gradation shown in Fig. 6 (SMA-13, AC-13, and OGFC-13) and for each corresponding case, 50 simulations were conducted using different random seeds, yielding 450 simulations in total. This indicates that the study includes nine nominal condition combinations (i.e., 3 gradations $\times$ 3 corresponding cases). Each condition was simulated with 50 independent random seeds, resulting in 450 final-state samples. The feature extraction (see Section 2.2 and 2.3) was implemented in PFC via FISH scripting, and the automatic feature evaluation (see Section 2.4) was carried out jointly using MATLAB and Python.

As an additional consideration in interpreting the findings, the study employed a two-dimensional DEM representation to enable controlled, repeatable exploration of micro-mechanical descriptors and to support large-scale simulation–analytics coupling. Prior experimental and computational evidence has shown that 2D granular systems reproduce key phenomenology of force networks (heterogeneous load partitioning, intermittent strong/weak chains, stress-induced fabric), making them suitable for mechanism discovery and comparative analysis under consistent boundary conditions [90,91]. Nevertheless, direct numerical equivalence to three-dimensional pavements should not be presumed. In 3D, network connectivity and loop structure differ, anisotropy can redistribute over additional orientations, and coordination and force-chain length metrics may shift due to out-of-plane contacts [92,93]. Furthermore, modeling aggregates as disks underrepresents angular interlock and surface roughness, potentially biasing contact orientation and chain continuity relative to assemblies of angular 3D particles (e.g., clumps, polyhedra, superquadrics) [94,95]. Accordingly, the present 2D results are most reliable for relative comparisons across gradations and pre-compaction settings within the defined framework, whereas absolute values of 3D-dependent indicators warrant cautious interpretation.

3.1. Pre-compaction simulation

After simulating each case, typical results before and after pre-compaction simulation were visualized, as shown in Fig. 11 and Fig. 12. Prior to pre-compaction (see Fig. 11), the particle assemblies were loosely arranged and exhibited a high void ratio. Strong force chains were sparse, short, and spatially fragmented, indicating limited load-bearing continuity. Weak force chains dominated the contact network and were widely dispersed. High stress particles and low stress particles occurred only intermittently and were scattered without forming stable clusters. Overall, the contact graph showed low connectivity and weak anisotropy, consistent with an unconsolidated granular skeleton.

After pre-compaction (see Fig. 12), the packing density increased markedly and the microstructure reorganized into a more coherent skeleton. Strong force chains became more numerous and formed extended, nearly continuous paths that connected the loading boundary to the base, evidencing clear load transfer corridors. The network anisotropy increased, with force chains displaying a clearer preferential alignment toward the principal compression direction. High stress particles concentrated along these strong force chain corridors and at constraint zones (e.g., near boundaries), whereas weak force chains and low stress particles retreated to interstitial regions between the load-bearing columns. The reduction of weak force chain prevalence and the emergence of longer, thicker strong force chains signaled an increase in contact coordination and mechanical interlock.

Across the three gradations (SMA-13, AC-13, OGFC-13) and the three cases examined within each gradation (gradations 1–3), pre-compaction consistently increased packing density, extended portions of strong force chains, and concentrated high stress particles along force chain corridors. Nevertheless, the geometry and localization of these changes were case-dependent rather than monotonic across gradations. Within the

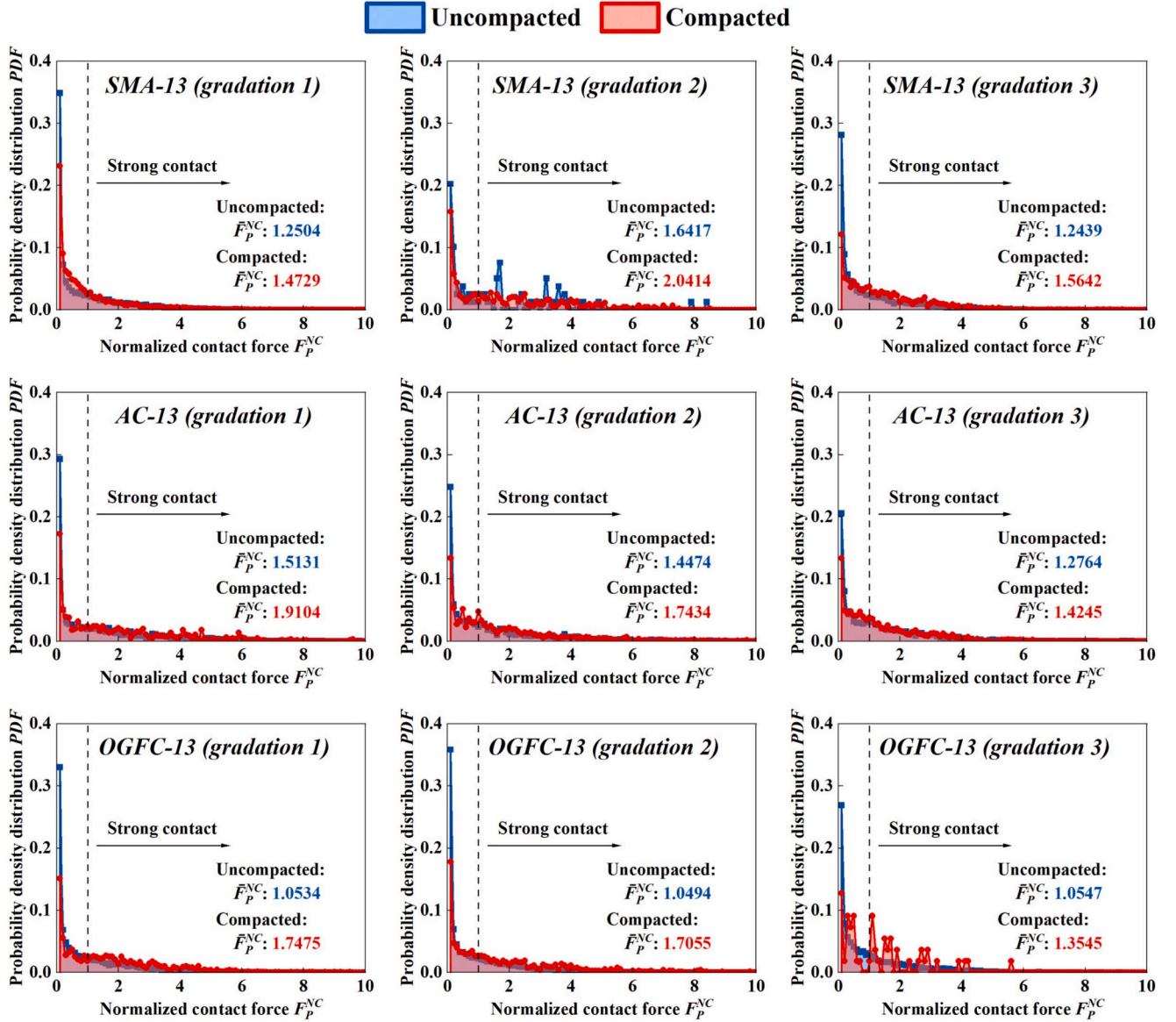


Fig. 16. Probability density function of contact forces ($PDF(F_p^{NC})$) for different gradations.

SMA-13 range, the compacted force chain field exhibited a systematic trend of anisotropy enhancement, while the dominant orientation varied depending on specific conditions. In some cases, force chains preferentially connected the loading zone to the substrate; in others, they formed several shorter force chain bands interspersed with regions of weak force. In AC-13, strengthening was evident but remained spatially heterogeneous across the three cases, with moderate depth clusters of high stress particles forming in some cases and more dispersed branch-like force chains in others. For OGFC-13, strong force chains intensified mainly near support boundaries and the base in all three cases, yet frequent interruptions persisted; the degree of continuity and the breadth of weak force chain fields varied across its three cases.

In summary, pre-compaction produced more continuous strong force pathways and a more anisotropic contact force field, with orientations tending toward the compression direction, but the magnitude and spatial pattern of these changes were case- and gradation-specific rather than monotonic across SMA-13, AC-13, and OGFC-13.

3.2. Pre-compaction quality evaluation based on feature extraction

In this section, all related features extracted in Section 2.3 were statistically analyzed to evaluate the pre-compaction quality across different gradations from both quantitative and qualitative perspectives. The evaluation provided a prior baseline for comparison with the results produced later by the automated evaluation framework. At each sampling location, outcomes from 50 simulations per case were averaged to obtain representative values. The section was organized around two feature families: (i) particle contact features (see Section 2.3.1) and (ii) force chain features (see Section 2.3.2).

3.2.1. Particle contact

Fig. 13 depicts the evolution of the average particle–particle contact force $\bar{F}_p^C$ with pre-compaction time for the three gradation types (SMA-13, AC-13, OGFC-13), each evaluated under three cases. For all curves, $\bar{F}_p^C$ decreased monotonically during the 0–15 s window, approximately linearly at first and then approaching a plateau after about 12–15 s, indicating stress relaxation and redistribution of inter-particle contacts during pre-compaction. At $t = 15$ s, the strongest residual contacts were

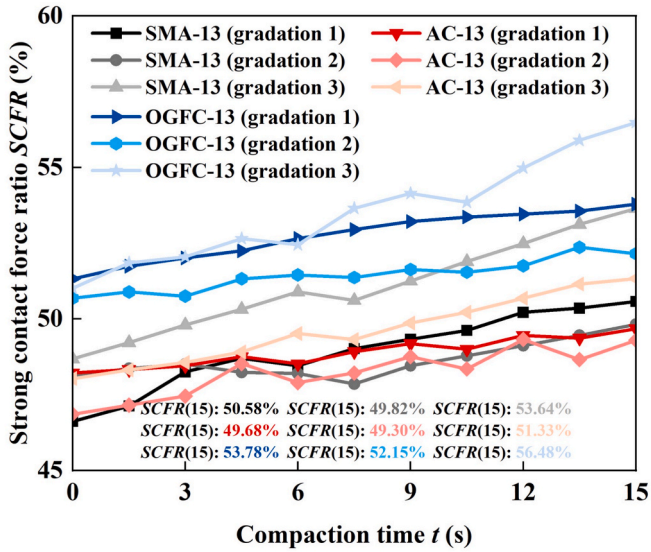


Fig. 17. Strong contact force ratio (SCFR) for different gradations.

observed for the “gradation-3” cases within each gradation: SMA-13-3 reached about 32.1 N, AC-13-3 about 35.8 N, and OGFC-13-3 about 37.8 N. In contrast, AC-13-2 yielded the weakest terminal level ($\bar{F}_p^C = 16.8$ N), while several mid/low curves converged to a narrow band near 23–25 N, e.g., SMA-13-1 ($\bar{F}_p^C = 24.7$ N), OGFC-13-1 ($\bar{F}_p^C = 24.0$ N), and OGFC-13-2 ($\bar{F}_p^C = 23.7$ N). Taken together, gradation-3 configurations generally preserved stronger particle contacts after pre-compaction, whereas AC-13-2 exhibited the weakest particle contact.

Fig. 14 shows the evolution of the mechanical coordination number Z_M during pre-compaction for the three gradations (SMA-13, AC-13, OGFC-13) under their three different cases. Across all curves, Z_M increased monotonically from roughly 3.0–3.1 at $t = 0$ to about 3.25–3.36 at $t = 15$ s, with a gradually diminishing slope, indicating progressive formation and stabilization of inter-particle contacts. At the end of pre-compaction, SMA-13 exhibited the highest coordination: SMA-13 (gradation-1) reached $Z_M(15) = 3.357$ and SMA-13 (gradation-2) reached $Z_M(15) = 3.338$, followed by OGFC-13 (gradation-1) at $Z_M(15) = 3.333$. Intermediate terminal levels were observed for OGFC-13 (gradation-3 with $Z_M(15) = 3.317$) and AC-13 (gradation-2 with $Z_M(15) = 3.313$ and gradation-1 with $Z_M(15) = 3.311$). The lowest coordination occurred in AC-13 (gradation-3 with $Z_M(15) = 3.258$) and OGFC-13 (gradation-2 with $Z_M(15) = 3.256$). Differences among cases were moderate, but the ordering indicated that SMA-13 configurations, particularly gradation-1, formed slightly denser and more connected contact networks by the end of pre-compaction, whereas AC-13 (gradation-3) and OGFC-13 (gradation-2) retained the sparsest contact topology.

Fig. 15 shows the evolution of the deviatoric fabric Φ_D over pre-compaction time for all gradation-case combinations. The deviatoric fabric Φ_D generally decreased over pre-compaction time, showing a rapid drop during the first 0–6 s followed by a gradual approach to a low plateau. By $t = 15$ s, the SMA-13 cases converged to similar residual anisotropy, with $\Phi_D(15) = 0.0221$ (gradation-1), $\Phi_D(15) = 0.0194$ (gradation-2), and $\Phi_D(15) = 0.0268$ (gradation-3). The AC-13 series ended at $\Phi_D(15) = 0.0227$ (gradation-1), $\Phi_D(15) = 0.0283$ (gradation-2), and $\Phi_D(15) = 0.0237$ (gradation-3), while OGFC-13 retained the broadest spread, with $\Phi_D(15) = 0.0329$ (gradation-1), $\Phi_D(15) = 0.0271$ (gradation-2), and $\Phi_D(15) = 0.0185$ (gradation-3). Early oscillatory behavior was observed across all curves, consistent with particle rearrangements during the formation and breakage of force chains, whereas late-time behavior stabilized near $\Phi_D \in (0.018, 0.033)$ depending on gradation.

Fig. 16 shows the probability density functions (PDF) of the normalized contact force F_p^{NC} for all gradation-case combinations, comparing the uncompacted (blue) and compacted (red) states. The distributions within each subgraph were right-skewed with a high peak near zero and a heavy tail. This indicates that contact forces between particles are concentrated in regions of weak contact ($F_p^{NC} < 1$; dashed line). From before to after pre-compaction, the densities systematically shifted to the right, indicating a reduced proportion of weak contacts and an increased fraction of strong contacts ($F_p^{NC} \geq 1$). The distribution tails also extended farther toward large forces after pre-compaction, reflecting the emergence of higher stress particles. The shift was corroborated by the mean normalized force $\bar{F}_p^{NC}$, which increased from 1.0494 to 1.6417 before pre-compaction to 1.3545 – 2.0414 after pre-compaction across all cases. Within SMA-13, gradation-2 exhibited the highest average values ($\bar{F}_p^{NC} = 2.0414$) after pre-compaction, while gradation-1 and gradation-3 rose to 1.4729 and 1.5642, respectively. The AC-13 series showed moderate growth, with average values ranging from 1.4245 (gradation-3) to 1.9104 (gradation-1) after pre-compaction. OGFC-13 started from the lowest pre-compaction means (1.0494) but displayed the largest relative gains in gradation-1 and gradation-2 (to 1.7475 and 1.7055), whereas gradation-3 increased more modestly (to 1.3545). Collectively, these PDFs evidenced that pre-compaction redistributed contact forces toward stronger interactions and stress networks, with the magnitude of the shift dependent on gradation.

Fig. 17 illustrates the evolution of the strong contact force ratio (SCFR) during pre-compaction for all gradation-case combinations. Across gradations, SCFR increased approximately monotonically with time, indicating a progressive conversion of weak contacts into strong ones as densification proceeded. At the end of pre-compaction ($t = 15$ s), OGFC-13 exhibited the highest levels: gradation-3 reached 56.48%, followed by gradation-1 at 53.78% and gradation-2 at 52.15%. SMA-13 achieved intermediate values, with gradation-3 at 53.64%, gradation-1 at 50.58%, and gradation-2 at 49.82%. AC-13 remained the lowest overall, ending at 51.33% (gradation-3), 49.68% (gradation-1), and 49.30% (gradation-2). Overall, OGFC-13 (particularly under gradation-3 conditions) exhibited the largest fraction of strong contacts throughout the pre-compaction process, while AC-13 maintained the smallest fractions. Within each case, gradation-3 consistently delivered the greatest SCFR, suggesting that this gradation favored the formation of robust force chains under the imposed pre-compaction.

Fig. 18 presents the probability distributions of the particle contact number $f(n_c)$ before and after pre-compaction for all gradation-case combinations (blue: uncompacted; red: compacted). For every gradation, the compacted curves shifted to the right, indicating an increase in contacts per particle. The mean contact number $\bar{n}_c$ rose from 2.9543 to 3.0160 (gradation-1 for SMA-13), 2.9492 to 2.9826 (gradation-2 for SMA-13), and 2.9421 to 3.0910 (gradation-3 for SMA-13); from 2.9643 to 2.9912 (gradation-1 for AC-13), 2.9602 to 3.0523 (gradation-2 for AC-13), and 2.9659 to 2.9915 (gradation-3 for AC-13); and from 2.9526 to 3.0256 (gradation-1 for OGFC-13), 2.9694 to 2.9930 (gradation-2 for OGFC-13), and 2.9731 to 3.0369 (gradation-3 for OGFC-13). Across all compacted cases, SMA-13 (gradation-3) achieved the highest mean ($\bar{n}_c = 3.0910$), followed by AC-13 (gradation-2) and OGFC-13 (gradation-3) ($\bar{n}_c = 3.0523$ and $\bar{n}_c = 3.0369$, respectively), whereas SMA-13 (gradation-2) remained the lowest $\bar{n}_c = 2.9826$. The distributions were unimodal and right-skewed; pre-compaction predominantly increased the probability mass in the $n_c \in [4, 8]$ range, reflecting denser and more connected particle assemblies after pre-compaction.

Fig. 19 depicts polar (rose) diagrams of contact force directions $F_p^C(\beta)$ for each gradation-case combination before (blue) and after (red) pre-compaction, together with three fitted descriptors in each subplot: the mean contact force $\bar{F}_p^C$, the Fourier coefficient a_n , and the principal orientation β_n . Across almost all gradations, pre-compaction produced a

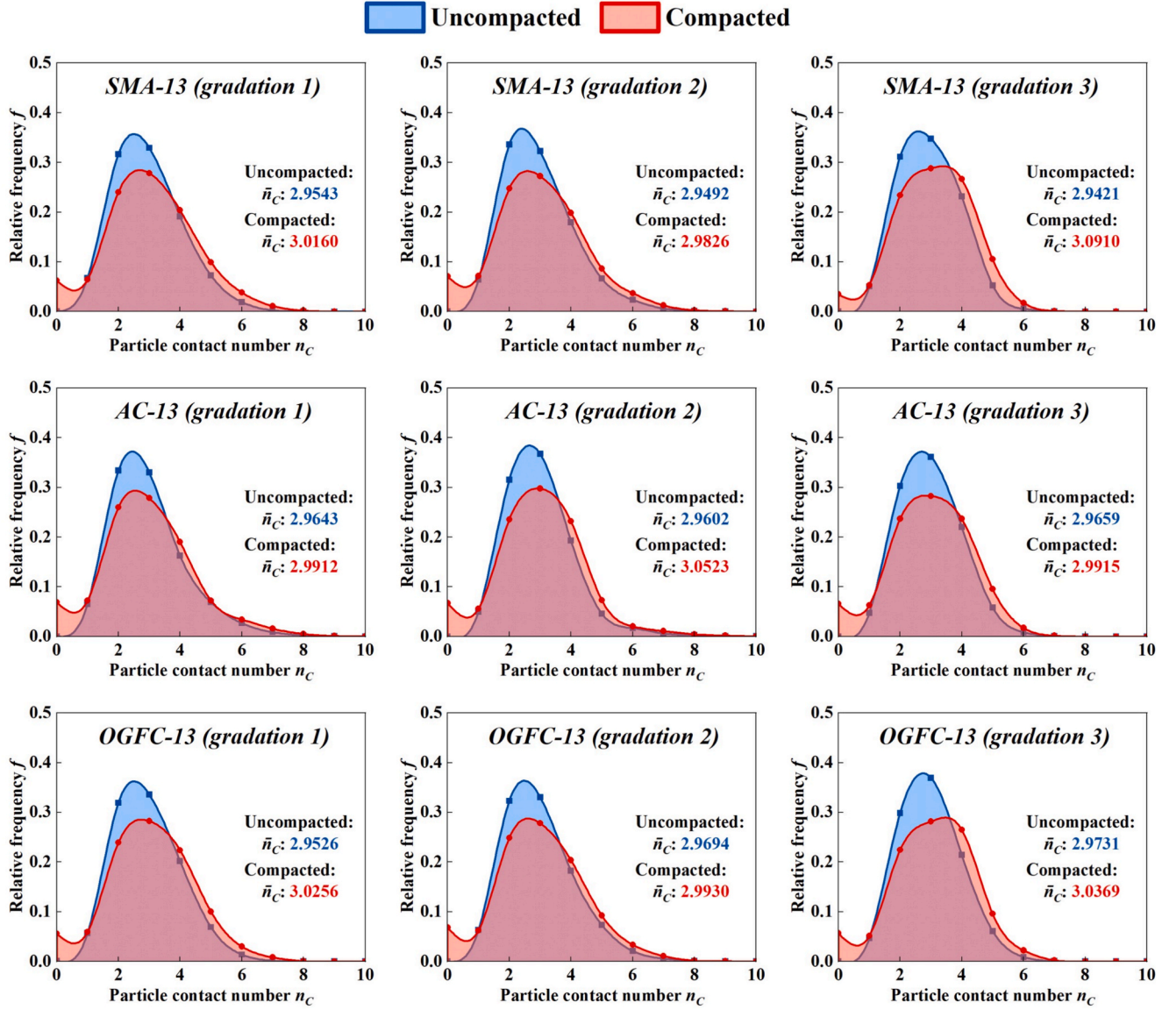


Fig. 18. Distribution frequency of the contact numbers ($f(n_c)$) for different gradations.

reduction in $\bar{F}_p^C$ and a weakening of directional anisotropy (smaller $|a_n|$), yielding more isotropic lobes in the rose plots. The decrease in $\bar{F}_p^C$ ranged from about 1.7–11.4 N, with the strongest drops observed for OGFC-13 (gradation-1) and SMA-13 (gradation-1 and gradation-3), and the smallest changes for SMA-13 (gradation-2) and OGFC-13 (gradation-2). The anisotropy magnitude $|a_n|$ generally shrank—for example, SMA-13 changed from -0.226 to 0.151 (gradation-1), -0.266 to 0.215 (gradation-2), and -0.261 to 0.120 (gradation-3); AC-13 from -0.222 to 0.155 (gradation-1), -0.207 to 0.112 (gradation-2), and -0.172 to 0.180 (gradation-3); OGFC-13 from -0.253 to 0.143 (gradation-1), -0.252 to 0.103 (gradation-2), and -0.203 to 0.106 (gradation-3). The fitted principal angle β_n rotated by approximately 8 – 35° toward the pre-compaction axis in most cases (e.g., from -1.16° to -23.71° for SMA-13 (gradation-1) and from 1.24° to -30.19° for OGFC-13 (gradation-3)), indicating a reorientation of force chains consistent with the pre-compaction loading direction. Overall, the rose diagrams evidenced a redistribution of contact forces into a denser, more isotropic network with orientations aligned more closely to the imposed pre-compaction direction.

Fig. 20 reports the evolution of the average normal contact force at

the tamper–particle interface $\bar{F}_t^C$ (left) and at the screed plate–particle interface $\bar{F}_{sp}^C$ (right) during pre-compaction for all nine gradation–case combinations. Across cases, both interface forces increased gradually with time, indicating that load transfer between the screed device and aggregate progressively strengthened as pre-compaction progressed. At $t = 15s$, the tamper interface consistently carried larger forces than the screed plate interface for the same gradation, e.g., SMA-13 (gradation-1) 28.5 N vs. 25.8 N, SMA-13 (gradation-2) 26.1 N vs. 23.9 N, SMA-13 (gradation-3) 35.6 N vs. 34.4 N; AC-13 (gradation-1) 23.5 N vs. 22.4 N, AC-13 (gradation-2) 19.4 N vs. 16.9 N, AC-13 (gradation-3) 43.5 N vs. 42.9 N; OGFC-13 (gradation-1) 33.5 N vs. 29.1 N, OGFC-13 (gradation-2) 38.4 N vs. 34.1 N, OGFC-13 (gradation-3) 40.9 N vs. 36.7 N. Ranking at the end of pre-compaction was therefore led by AC-13 (gradation-3), followed by OGFC-13 (gradation-3 and gradation-2) and SMA-13 (gradation-3); intermediate magnitudes were observed for OGFC-13 (gradation-1) and SMA-13 (gradation-1), whereas the lowest levels occurred in AC-13 (gradation-2). The screed plate–contact curves exhibited mild oscillations superposed on the overall increase, while the tamper–contact curves were smoother, consistent with the more direct transmission of compaction energy through the tamper.

Fig. 21 depicts the time histories of the screed device–aggregate

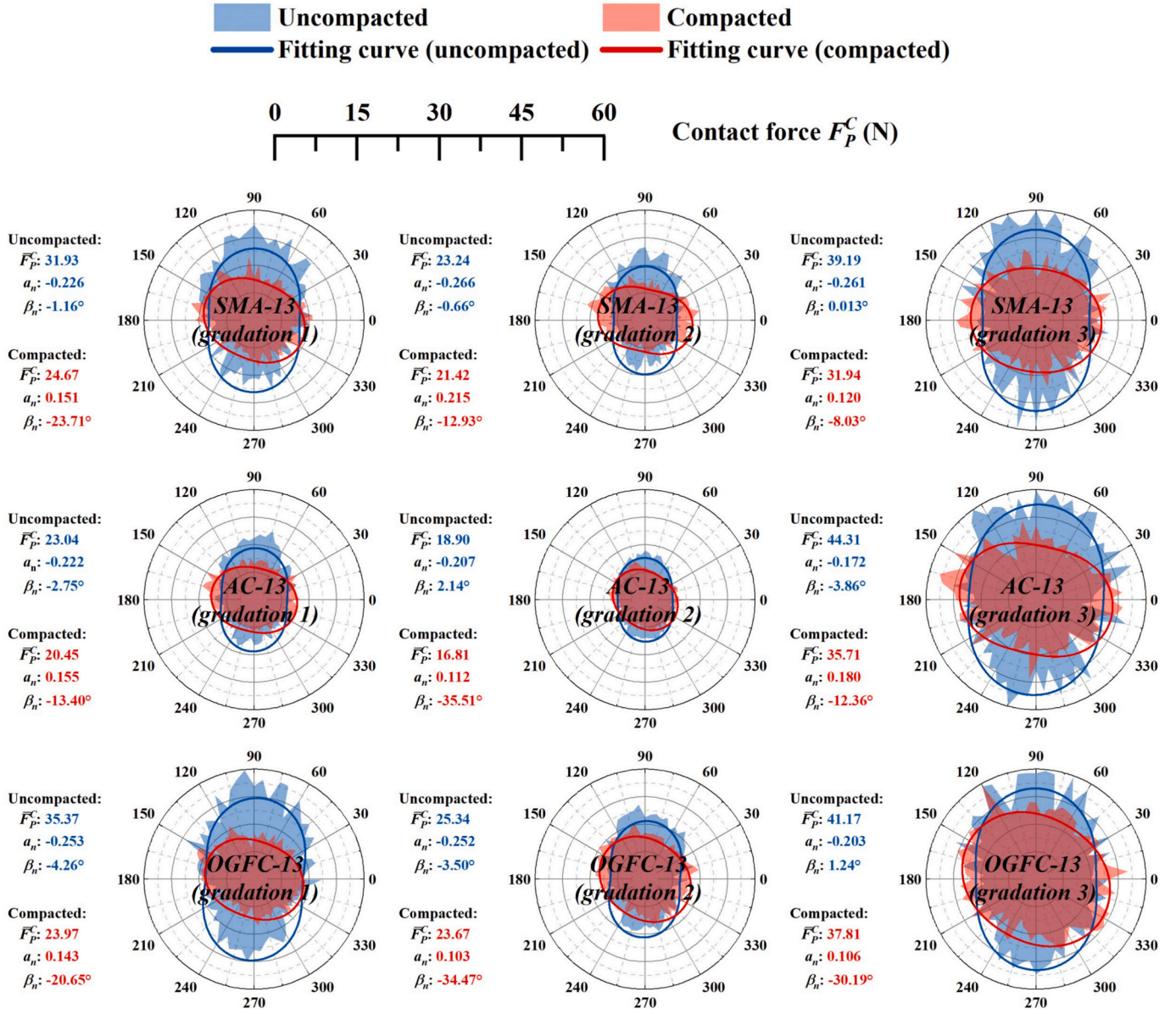


Fig. 19. Rose diagram of contact force direction (F_p^C) for different gradations.

contact forces (F_p^C) and the corresponding compaction impulses (CI_Φ)—defined as the time integral of contact force over the 15 s window—at the tamper–particle interface (CI_T) and the screed plate–particle interface (CI_{SP}). Across all nine gradation–case combinations, CI_T consistently exceeded CI_{SP} , reflecting the more direct transmission of compaction impulses through the tamper. The impulses also exhibited bursty time series with intermittent high peaks, whereas the screed signals were relatively smoother and of smaller amplitude. Quantitatively, CI_T ranged from about 1.30×10^4 Ns to 2.06×10^4 Ns and CI_{SP} from about 1.14×10^4 Ns to 1.77×10^4 Ns. The largest impulses occurred in SMA-13 (gradation-2) ($CI_T = 20621.32$ Ns, $CI_{SP} = 17708.40$ Ns), followed by AC-13 (gradation-2) ($CI_T = 18025.14$ Ns, $CI_{SP} = 15861.55$ Ns). At the other end, the smallest impulses were observed in OGFC-13 (gradation-3) ($CI_T = 12995.63$ Ns, $CI_{SP} = 11435.24$ Ns) and AC-13 (gradation-3) ($CI_T = 14012.50$ Ns, $CI_{SP} = 12132.72$ Ns). Within each gradation, the ordering was consistent: gradation-2 > gradation-1 > gradation-3 for both interfaces. These results indicated that the gradation-2 configurations stored and transmitted the greatest compaction impulse to the aggregate skeleton, whereas gradation-3 configurations transmitted the least.

Fig. 22 shows the evolution of the void decrease ratio (VDR) during the 15 s pre-compaction window for all nine gradation–case combinations. For every curve, VDR increased monotonically with time while the growth rate gradually diminished, indicating progressive densification with a tendency to approach a plateau. Clear between-group differences were observed at $t = 15$ s: OGFC-13 (gradation-3) attained the largest reduction $VDR(15) = 8.1\%$, followed by OGFC-13 (gradation-1) at 6.2% and AC-13 (gradation-3) at 6.0%. Moderate responses were recorded for SMA-13 (gradation-3) (4.4%), AC-13 (gradation-1) (4.5%), and OGFC-13 (gradation-2) (4.2%). The smallest reductions occurred in SMA-13 (gradation-1) (2.8%) and SMA-13 (gradation-2) (2.3%), with AC-13 (gradation-2) also remaining relatively low at 3.6%. Overall, within a fixed compaction time, pre-compaction using OGFC-13 gradation demonstrated the greatest reduction in void ratio, while SMA-13 gradation (particularly gradation-2) exhibited the smallest reduction in void ratio.

3.2.2. Force chain

Fig. 23 tracks the following results for each gradation and case: the temporal proportions of particles on force chains (P_{PFC}), on strong and

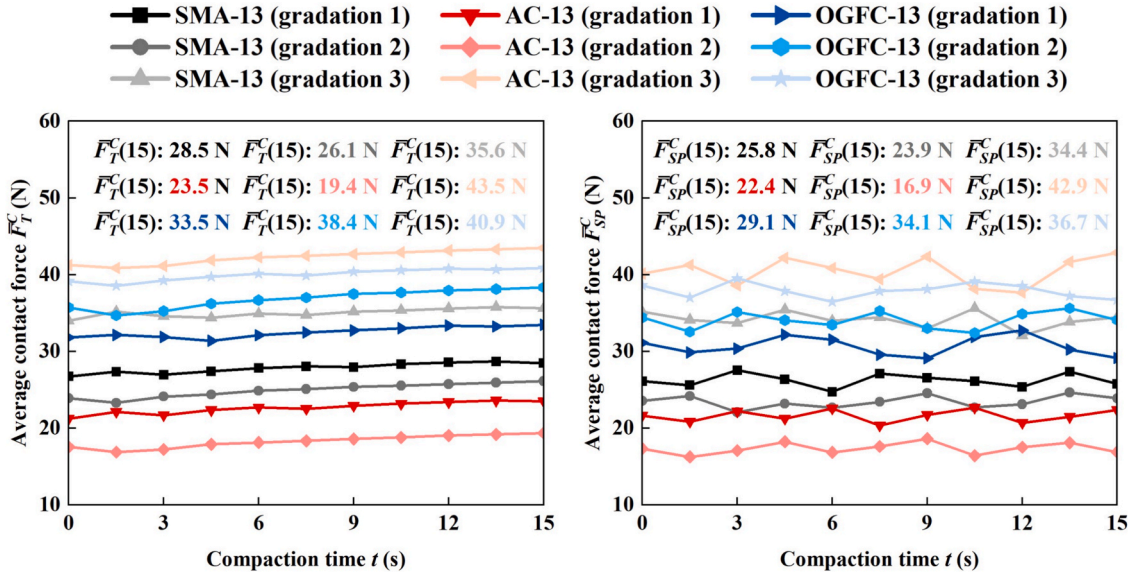


Fig. 20. Average contact force between particles and tamper ($\bar{F}_T^C$) and average contact force between particles and screed plate ($\bar{F}_{SP}^C$) for different gradations.

weak subsets (P_{PSFC} , P_{PWFC}), particles not on force chains (P_{PNFC}), as well as the sheet-level shares of strong/weak force chains (P_{SFC} , P_{WFC}) and the fractions of high and low stress particles (P_{HSP} , P_{LSP}) during pre-compaction. Across all nine scenarios, P_{PFC} exhibited a gradual rise with compaction time, accompanied by a systematic increase in P_{PSFC} and a concomitant decline in P_{PWFC} . Consistently, the proportion of strong force chains P_{SFC} increased while that of weak force chains P_{WFC} decreased, indicating a progressive consolidation of load-bearing pathways. The proportion of particles not on force chains P_{PNFC} showed a decreasing trend, reflecting the incorporation of particles previously outside force chains into the subnetwork of force chains. Stress stratification followed the same direction: P_{HSP} rose moderately as more particles aligned with strong force chains, whereas P_{LSP} decreased. Although numerical values varied across different gradations/cases, the qualitative pattern of increased participation in strong force chains alongside reduced participation in weak force chains or non-force chain groups remained consistent throughout.

Fig. 24 summarizes the net changes before versus after pre-compaction for the same quantities, where N_p represents the total number of particles in the current region. In every gradation and case, the compacted state showed a higher P_{PFC} than the uncompacted state, driven primarily by an increase in P_{PSFC} and a decrease in P_{PWFC} . The fraction of particles outside force chains P_{PNFC} consistently dropped after pre-compaction, confirming the time series trends in Fig. 23. The stress-based partitions corroborated these shifts: P_{HSP} increased, while P_{LSP} decreased after pre-compaction, indicating that stress became more concentrated along the strengthened force chains. Taken together, Fig. 23 and Fig. 24 demonstrated that pre-compaction systematically transforms the microstructure from a weakly connected network dominated by non-force chain/weak force chain particles into a more integrated skeletal structure characterized by a higher proportion of strong force chains and a greater percentage of high stress particles.

Fig. 25 presents force chain statistics categorized by length L and type (strong force chain P_{SFC} and weak force chain P_{WFC}) across all classifications and scenarios before and after pre-compaction. Across all nine scenarios, the length distributions were right-skewed: short force chains ($L = 3-4$) dominated and the frequency decayed rapidly with increasing L , leaving a thin long force chain tail. Pre-compaction shifted the distributions upward for strong force chains and downward for weak force chains, most visibly at small L , indicating the conversion of many short weak branches into load-bearing links. The total number of force chains N_{TFC} generally increased after pre-compaction, with the increase

primarily attributable to strong force chains N_{SFC} ; by contrast, the number of weak force chains N_{WFC} decreased or changed only marginally. Consistent with these count changes, the proportion of strong force chains P_{SFC} rose by several percentage points (typically 2–7%), whereas the proportion of weak force chains P_{WFC} declined in every gradation and case. These observations were in agreement with Fig. 23, which tracked the temporal growth of P_{SFC} and the shrinkage of P_{WFC} . The strength enhancement of force chain length primarily occurred in the short force chain segment (where the highest count values were recorded), while the tail end of long force chains maintained moderate extension. This indicates a slight improvement in force chain segment continuity rather than the emergence of extremely long force chain segments. Differences among gradations were quantitative rather than qualitative. AC-13 cases tended to exhibit larger absolute force chain counts, whereas OGFC-13 retained comparatively more weak links prior to pre-compaction. However, across all gradations and cases, the force chains exhibited identical reorganization patterns after pre-compaction: trimming weak short force chains and strengthening short-to-medium force chains into robust force chain trunks. This consistently increased P_{SFC} and decreased P_{WFC} across all scenarios.

Fig. 26 shows the evolution of mean force chain length ($\bar{L}_{FC}$) during pre-compaction. In all gradations and cases, weak force chains remained longer than strong ones ($\bar{L}_{WFC} > \bar{L}_{SFC}$) and both increased slightly with time. Strong force chain length rose from about 3.66–3.74 at $t = 0$ to roughly 3.79–3.97 at $t = 15$ s; weak force chain length increased from 4.02 to 4.43 to 4.39–4.80. The magnitude of growth varied moderately across cases (e.g., larger in AC-13/OGFC-13 gradation-2, smaller in SMA-13 gradation-2 and gradation-3), but the qualitative pattern was consistent: pre-compaction lengthened chains modestly without altering the ordering between weak and strong branches.

Fig. 27 depicts rose diagrams of force chain orientation ($P_{FC}(\beta)$) before and after pre-compaction for all gradations and cases. Pre-compaction generally increased directional anisotropy, as indicated by a larger fitted amplitude $|a_n|$ and a clearer elliptical outline of the distributions. For example, a_n changed from negative, near-isotropic values in the uncompacted states (e.g., SMA-13 gradation-1: $a_n = -0.137$; OGFC-13 gradation-1: $a_n = -0.118$) to positive and distinctly larger magnitudes after pre-compaction (SMA-13 gradation-1: $a_n = 0.231$; OGFC-13 gradation-1: $a_n = 0.233$). The increase was case-dependent rather than monotonic across gradations; the smallest gain appeared in SMA-13 gradation-3 (a_n from -0.134 to 0.110), whereas the largest gains occurred in SMA-13 and OGFC-13 gradation-1. The fitted principal

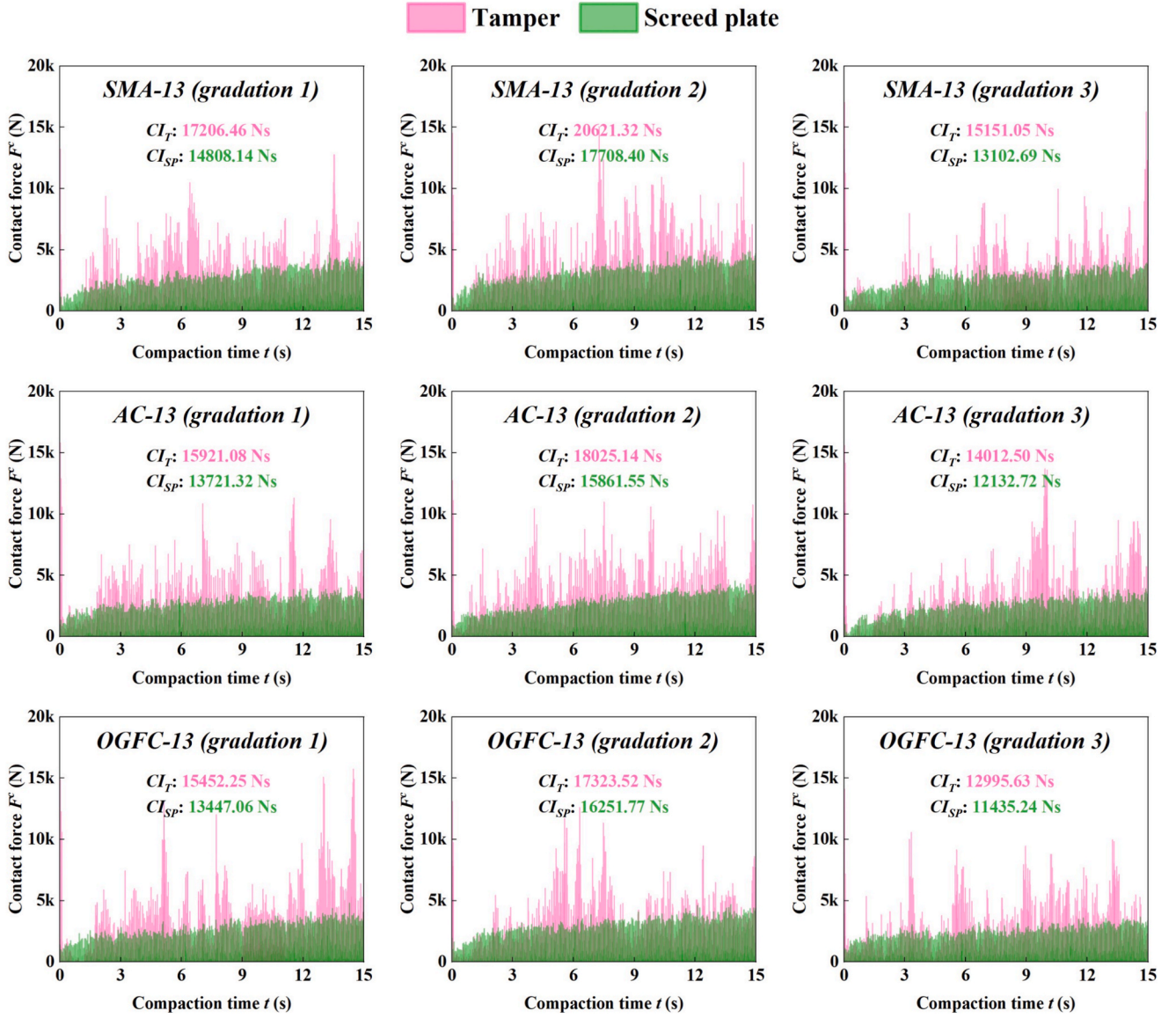


Fig. 21. Compaction impulse between particles and tamper (CI_T) and compaction impulse between particles and screed plate (CI_{SP}) for different gradations.

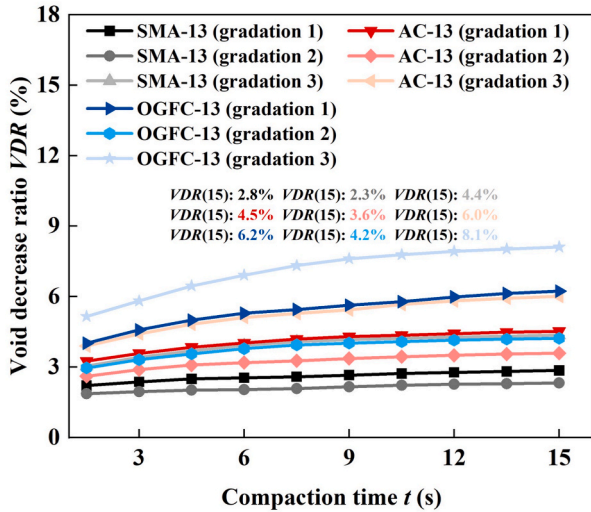


Fig. 22. Void decrease ratio (VDR) for different gradations.

directions β_n remained close to the pre-compaction axis in all scenarios, shifting only modestly from near-zero values before pre-compaction to approximately 4° – 10° after pre-compaction (e.g., SMA-13 gradation-2: from $\beta_n = -1.55^\circ$ to $\beta_n = 6.60^\circ$; AC-13 gradation-3: from $\beta_n = 5.69^\circ$ to $\beta_n = 9.91^\circ$). These small angles indicate that the preferred force chain orientation aligned with the imposed loading direction, with limited rotation across cases. Overall, pre-compaction produced more pronounced, loading-aligned orientation patterns of force chains, while the strength of anisotropy varied moderately among gradations and their three cases.

3.3. Automatic feature evaluation

In the previous section, all relevant features extracted in Section 2.3 were subjected to statistical analysis. Building on that foundation, this section employed the proposed automated workflow (see Section 2.4) to transform the micro-mechanical descriptors (see Table 4) from Section 2.4.1 into quantitative, reproducible evaluations of pre-compaction quality.

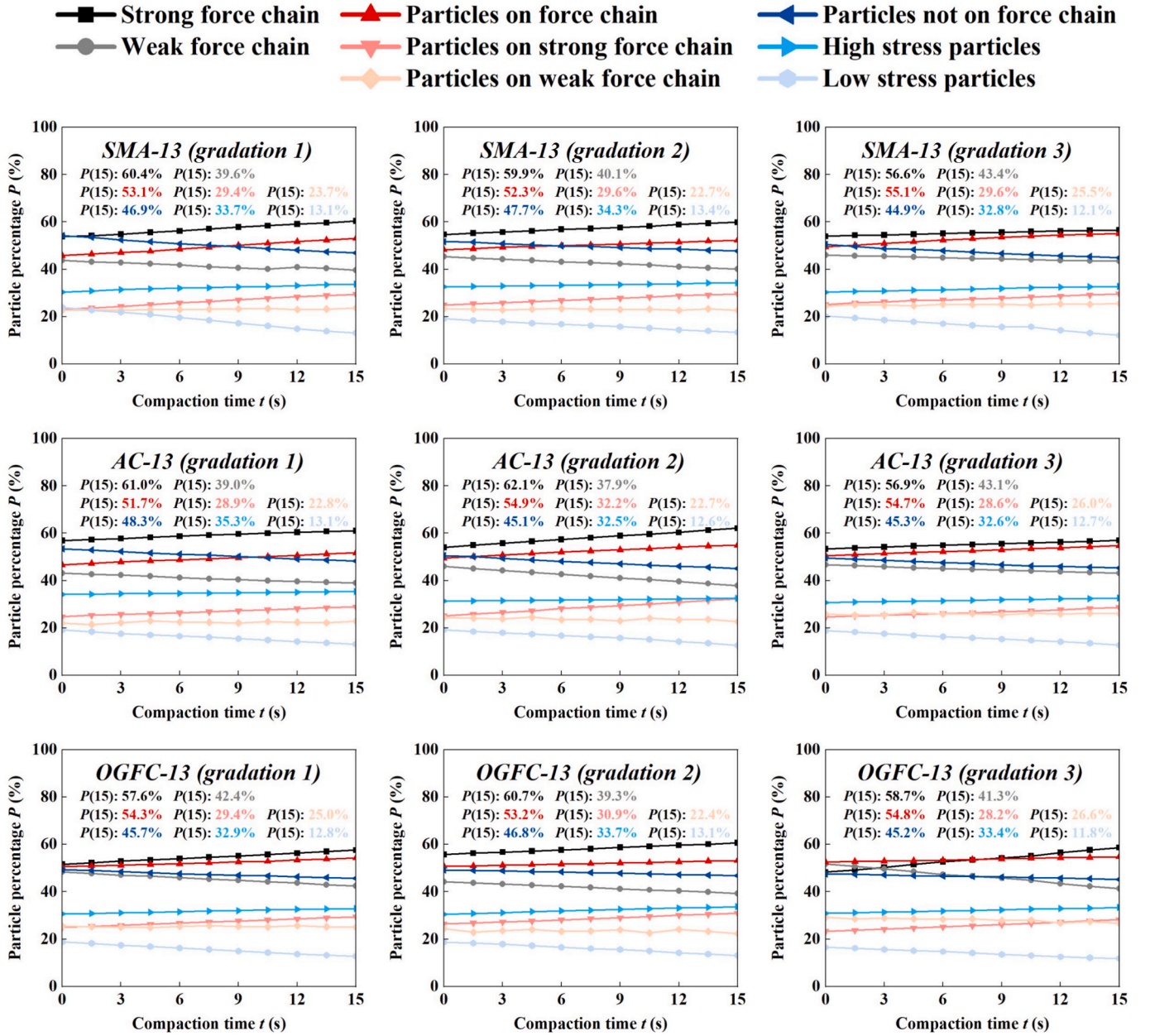


Fig. 23. Ratio of force chain and non-force chain particles during pre-compaction for different gradations: particles located on force chains (P_{PFC}), particles on the strong force chain (P_{PSFC}), particles on the weak force chain (P_{PWFC}), strong force chains (P_{SFC}), weak force chains (P_{WFC}), particles not on force chains (P_{PNFC}), high stress particles (P_{HSP}), low stress particles (P_{LSP}) for different gradations.

3.3.1. Data standardization

QT produced a stable marginal distribution approximating a Gaussian distribution for each variable. In Fig. 28 (a), the post-QT histograms for the 23 features are approximately unimodal and symmetric, with means close to zero and comparable dispersion. Features that originally exhibited strong skewness or bounded support (e.g., proportions such as P_{SFC} , P_{WSFC} , P_{PFC} , P_{PNFC} , P_{HSP} , P_{LSP} ; ratios such as VDR ; and contact force metrics such as CI_T and CI_{Sp}) show markedly reduced tail heaviness after transformation. The pooled inset confirms that the transformed values overlay a standard normal distribution pattern, indicating that extreme values were compressed and central mass slightly spread, yielding a more regular distribution across features.

Fig. 28 (b) provides distributional diagnostics that are consistent with the histograms. The transformed ECDFs for all features closely track a standard-normal CDF, with smooth S-shaped curves and minimal step-like jumps, suggesting that discreteness and clustering present

before standardization were alleviated. The quantile–quantile (QQ) comparison against $N(0,1)$ is nearly linear over the central 80–90% quantile range, demonstrating good alignment in both location and scale. Small, systematic deviations persist only at the extreme tails, which is expected for finite samples and for variables whose original domains are strictly bounded (0–1 or non-negative); these residual departures do not affect the overall normalization.

Taken together, the figure indicates that QT homogenized scales across heterogeneous features, dampened the influence of outliers while preserving rank order, and rendered the marginals broadly comparable and close to standard normal. This standardization benefits subsequent steps in the automatic evaluation pipeline by reducing distribution-driven artifacts, facilitating cross-feature comparison, improving the stability of cross-validation, and enhancing the reliability of interpretability plots, thereby placing all predictors on a common, robust scale.

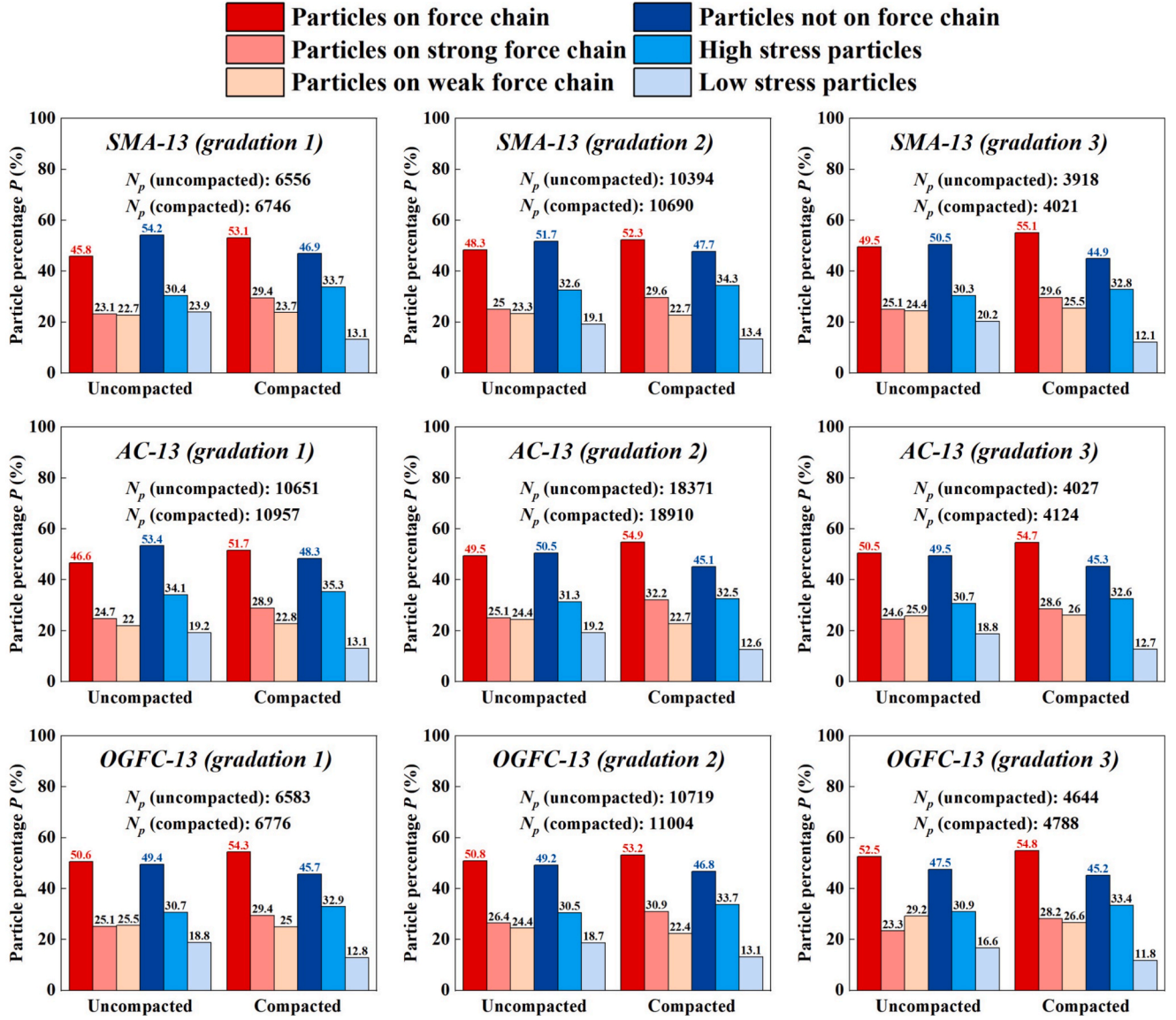


Fig. 24. Ratio of force chain and non-force chain particles before and after pre-compaction for different gradations: particles located on force chains (P_{PFC}), particles on the strong force chain (P_{PSFC}), particles on the weak force chain (P_{PWFC}), particles not on force chains (P_{PNFC}), high stress particles (P_{HSP}), low stress particles (P_{LSP}) for different gradations.

3.3.2. Latent space extraction

Fig. 29 shows DVAE-based latent space diagnostics for $d = 23$, summarizing optimization behavior, geometry of the learned manifold, feature-latent associations, and reconstruction fidelity.

Training dynamics were stable (see Fig. 29 (a)). The raw loss decreased rapidly during early iterations and then tapered gradually; the moving average curve smoothed this trajectory and approached a plateau without secondary rises or oscillatory drift. This pattern indicates that the encoder-decoder settled into a well-behaved minimum with no signs of overfitting late in training.

The latent embeddings were compact and structured (see Fig. 29 (b) and (c)). When colored by superclass (see Fig. 29 (b)), three partially separated clusters emerged, with small overlap at their margins; their centroids were close to the origin, consistent with a regularized (nearly Gaussian) latent prior. When the same embedding was colored by the nine cases (see Fig. 29 (c)), each superclass split into finer subclusters, suggesting that the DVAE preserved intra-class variability relevant to case differences while still enforcing global cohesion. The clouds were roughly elliptical and showed mild elongation along one axis, implying a

dominant direction of variation coupled with secondary, orthogonal variability.

Feature-latent associations were distributed and complementary rather than concentrated (see Fig. 29 (d)). The top-10 absolute correlations between micro-mechanical features and latent coordinates exhibited a mosaic pattern across dimensions from z_1 to z_{23} . Contact descriptors and force chain statistics loaded on different subsets of latent axes, and no single coordinate dominated all features. This dispersion implies that the DVAE captured multiple, partially independent generative factors: some dimensions align more with contact force and coordination, others with force chain intensity or directional structure. Such multi-axis encoding is desirable for downstream tasks because it avoids collapsing heterogeneous physics into a single latent direction.

Reconstruction accuracy was consistent across samples (see Fig. 29 (e)). The histogram of sample-wise RMSE was unimodal and narrow, with the bulk of observations clustered near the mode and only a modest right tail. This indicates that most microstate reconstructions were of comparable quality and that high error cases were infrequent. The absence of a heavy tail suggests limited sensitivity to rare or extreme

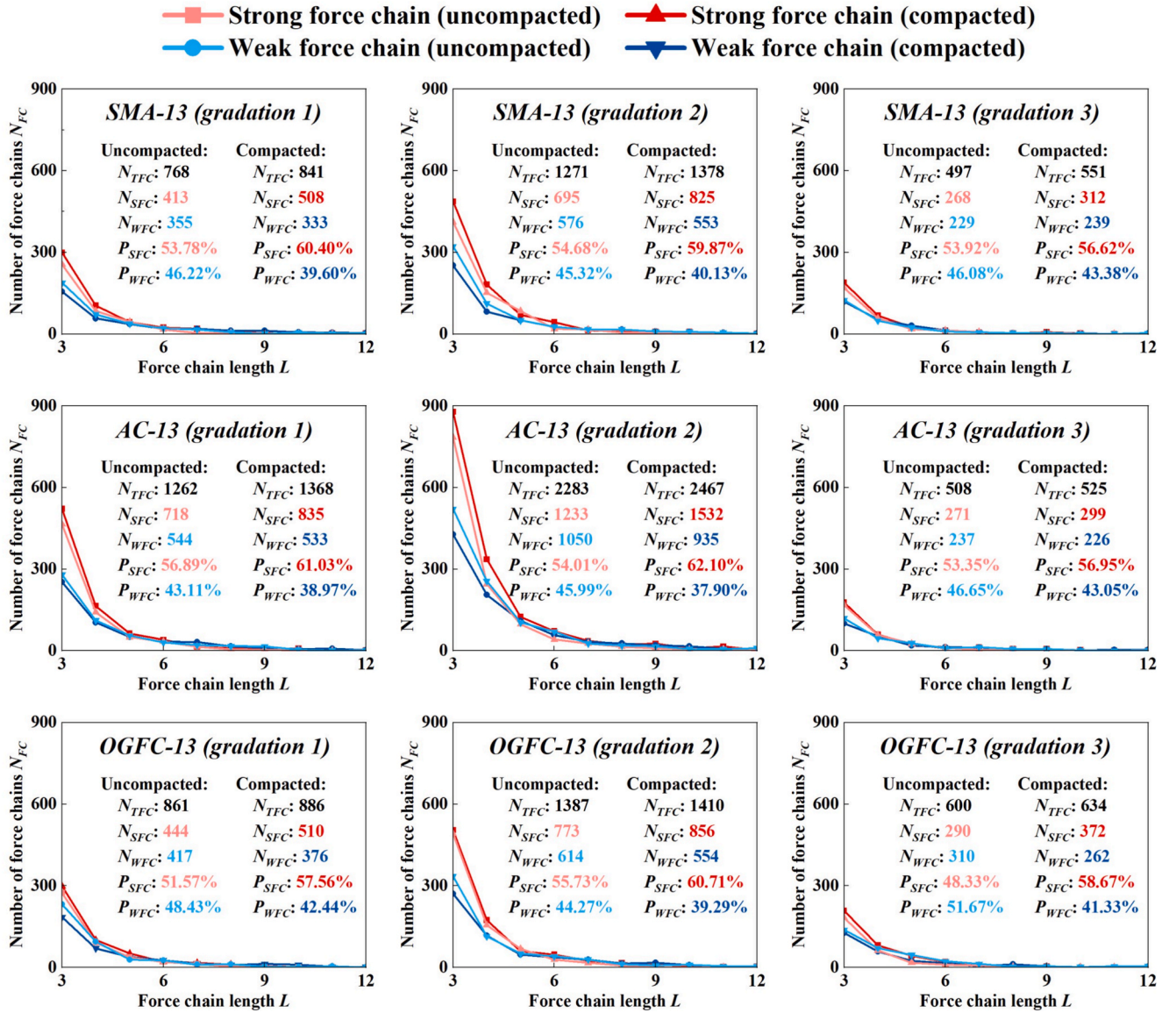


Fig. 25. Ratio of strong force chains (P_{SFC}) and weak force chains (P_{WFC}) for different gradations.

configurations after training.

Latent capacity usage was selective (see Fig. 29 (f)). The KL divergence contributions across dimensions show a heterogeneous distribution: several coordinates contributed materially, whereas a non-trivial subset contributed only weakly. This pattern implies an effective latent dimensionality smaller than the nominal 23, consistent with automatic pruning of redundant directions and suppression of noise. In combination with the compact, clustered embeddings and stable loss trajectory, these diagnostics indicate that the DVAE learned a parsimonious perceptual manifold that preserves case separability and the most informative micro-mechanical variations, thereby providing a robust basis for subsequent labeling and supervised evaluation.

3.3.3. Obtaining labels

Label acquisition in latent space via the Gaussian mixture model (GMM) is illustrated in Fig. 30. The figure verifies that the supervised clustering stage produced labels that were both coherent in the latent space and usable for subsequent supervised learning.

In Fig. 30 (a), the row-normalized confusion matrix (overall accuracy: 89.3%) indicates that most samples belonging to SMA-13, AC-13, and OGFC-13 were assigned to their intended class. The diagonal entries

were all dominant, which means that the GMM components captured the core structure of the three gradations. Misclassifications mainly appeared between SMA-13 and OGFC-13, not between AC-13 and the other two. This pattern implies that SMA-13 and OGFC-13 shared partially overlapping latent characteristics (e.g., similar force chain proportions or contact force levels in some cases), whereas AC-13 preserved a more distinctive latent signature.

Fig. 30 (b) shows the 2D latent embedding with class hulls and their geometric centers. The three superclasses occupied contiguous but separable regions. AC-13 formed the most compact cluster with a well-defined centroid, which is consistent with its high per-class scores later in Fig. 30 (d). SMA-13 and OGFC-13 were more spread, and the interpenetration of their convex hulls explains the off-diagonal elements in Fig. 30 (a). Even so, both clusters still exhibited a clear orientation in latent space, which indicates that the DVAE had already disentangled the gradation-specific micro-mechanical information before the GMM step.

The posterior confidence distribution in Fig. 30 (c) further assesses the reliability of the labeling. The maximum posterior for each sample was narrowly concentrated, without a long tail toward regions of low confidence. This means that, for the vast majority of samples, one GMM

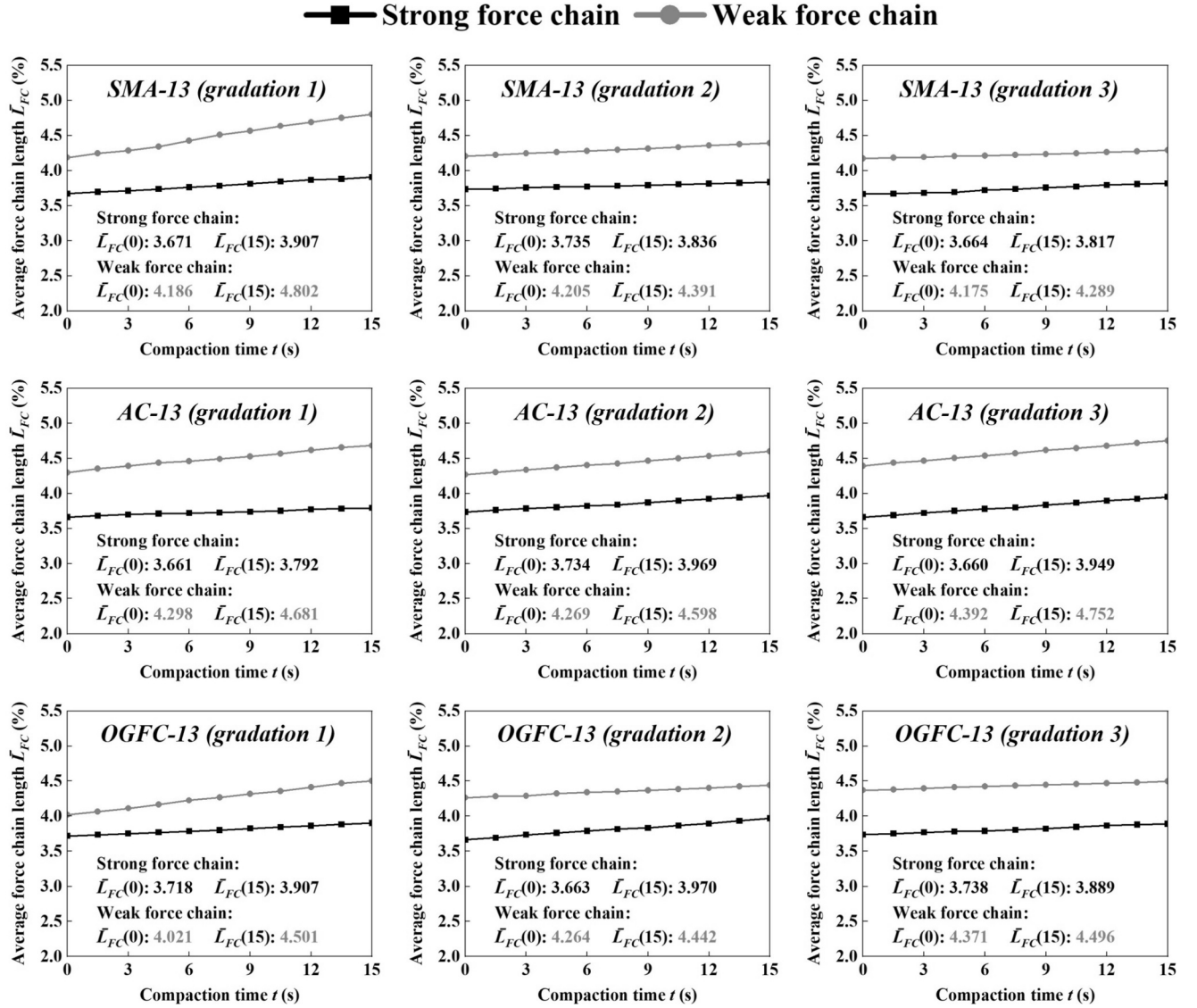


Fig. 26. Average force chain length ($\overline{L_{FC}}$) for different gradations.

component was clearly preferred over the others. The absence of a secondary mode suggests that there was no large ambiguous subgroup; only a small fraction of points lay close to class boundaries in Fig. 30 (b), which is typical for mixtures fitted to partially overlapping states.

Fig. 30 (d) summarizes the precision, recall, and F1 score across classes. All three metrics were high and well balanced across the three gradations, showing that the GMM did not favor one class at the expense of the others. AC-13 achieved the most even triplet of scores, which is consistent with its compact latent geometry. OGFC-13 showed a slightly lower precision, reflecting occasional leakage from SMA-13 in Fig. 30 (a), but its recall remained high, so OGFC-13 samples were rarely left unlabeled. This balance indicates that the automatically obtained labels were suitable for training the subsequent XGBoost model without the need for manual relabeling.

Fig. 30 (e) ranks the clusters by overall positive rating. The highest-ranked groups (such as SMA13-1 and AC13-4) corresponded to the densest parts of the latent space and can be regarded as prototypical realizations of their gradations. Lower-ranked groups matched the edge zones of Fig. 30 (b), where latent variables of different gradations started to intermingle. This ranking is useful because it identifies which simulations or sampling conditions produced the most typical microstructural response and which ones should be treated as marginal or

transition states. To strengthen the physical grounding of this ranking, the cluster-wise ratings can be interpreted alongside macroscopic densification proxies available from the DEM states (e.g., bulk packing density/void ratio): higher-rated clusters generally align with more compacted states, whereas cases with comparable densification but different ranks mainly reflect differences in particle arrangement, contact connectivity, and force-chain persistence. Notably, the cluster-level ranking also shows a trend that is consistent with reported engineering observations. Several SMA groups appear among the higher-rated clusters, whereas a larger portion of AC clusters fall into mid- to lower-ranked regions, reflecting a comparatively less consolidated microstructural response under the same modeling and boundary conditions. This pattern agrees with prior pavement studies that generally report superior field performance of SMA relative to conventional dense-graded AC, which is commonly attributed to a more stable stone-on-stone skeleton and improved resistance to deformation [5,96].

Fig. 30 (f) shows one-vs-rest precision-recall (PR) curves for the three latent classes, with average precision (AP) values of about 0.93, 0.94, and 0.92. The PR curves stayed high over a wide recall range, meaning that, even when more samples were retrieved, the precision did not collapse. This confirms that the latent clusters were not an artifact of overfitting in Fig. 30 (a), but reflected real separability in the encoded

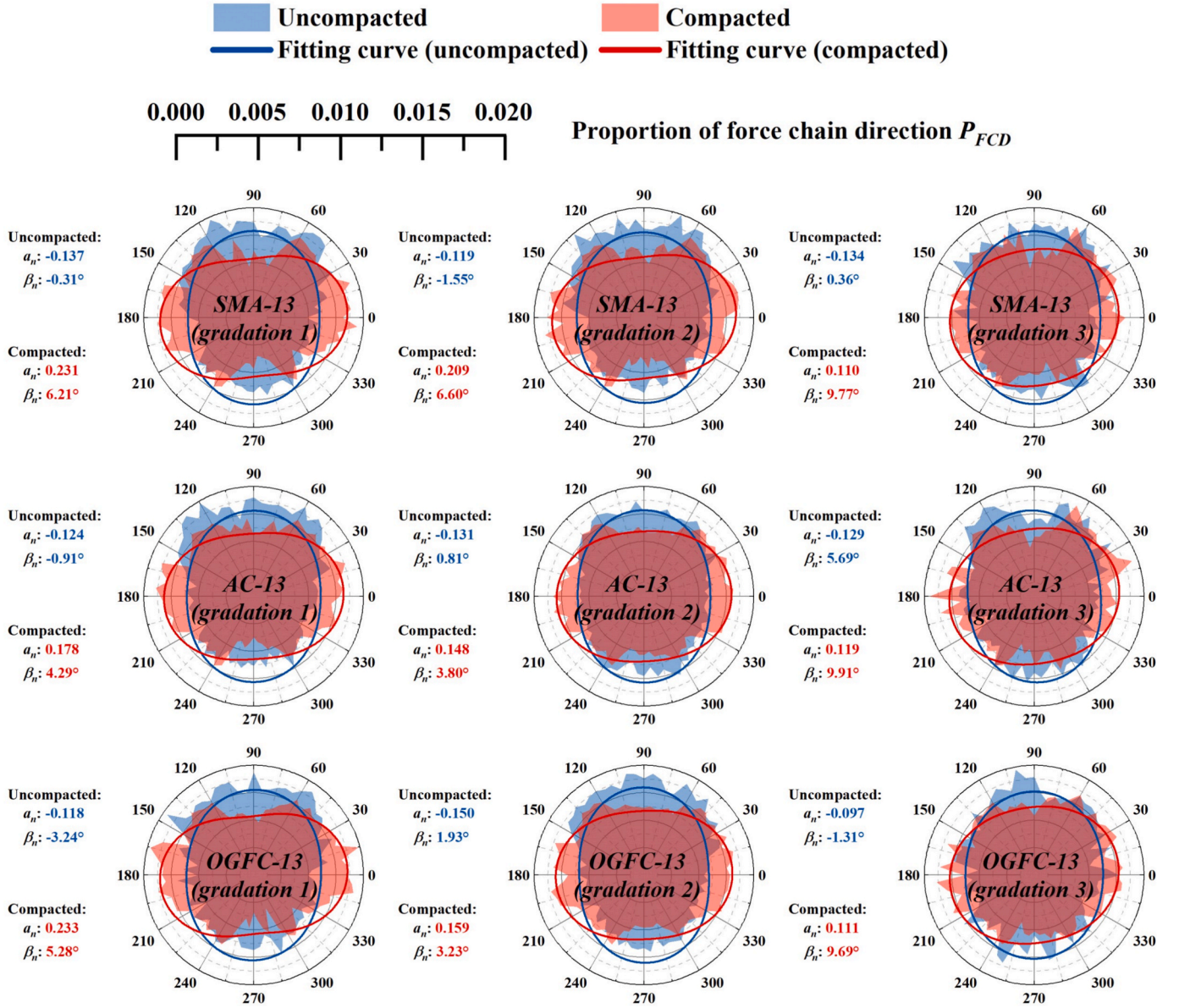


Fig. 27. Rose diagram of force chain directions ($P_{FCD}(\beta)$) for different gradations.

micro-mechanical patterns. Together, Fig. 30 demonstrates that the proposed GMM-based procedure yielded stable, high-quality labels that preserved the three gradation structures and were adequate for driving the subsequent supervised evaluation stage.

Fig. 31 further examines the necessity of two upstream components by removing QT and/or DVAE and re-running the same supervised stage. Overall, the three confusion matrices (see Fig. 31 (a)) exhibit highly consistent error patterns, and the overall accuracy remains in a narrow range (about 82.7%–84.4%). This indicates that the class prediction is not overly sensitive to whether QT or DVAE is enabled, and that the separability of the three gradation classes is already strongly supported by the underlying micro-mechanical descriptors. Across all three settings, SMA-13 and OGFC-13 are classified with relatively high recall, whereas AC-13 shows the largest confusion, mainly being misidentified as SMA13 and, to a lesser extent, as OGFC-13. This is consistent with AC-13 occupying a more intermediate structural regime, where its latent responses partly overlap with the other gradations.

Complementing Fig. 31 (a), Fig. 31 (b) shows the mean accuracies over 20 random initializations. The full framework (QT + DVAE) achieves $88.3\% \pm 1.4\%$, exceeding “No QT (DVAE on)” ($82.5\% \pm 2.5\%$),

“No DVAE (VAE only, QT on)” ($81.4\% \pm 2.3\%$), and “No QT + No DVAE” ($81.9\% \pm 3.1\%$). The narrower error bars for the full framework indicate improved stability across runs. This variance reduction suggests that QT and DVAE complement each other: QT standardizes heterogeneous feature scales, while DVAE provides a smoother latent representation, together yielding a more consistent decision boundary under different seeds and data splits.

Importantly, the ablation results suggest that QT and DVAE primarily play a stabilizing and regularizing role, rather than being the sole drivers of classification accuracy. In other words, even without these components, the pipeline still preserves the dominant decision boundary implied by the microstructural features, which supports the robustness of the overall framework.

3.3.4. Supervised learning

Fig. 32 summarizes the regression diagnostics for the XGBoost model. In the residual–prediction plots (see Fig. 32 (a)), training residuals were tightly centered around zero with a narrow spread and only a few flagged outliers, indicating that the fitted function captured the dominant signal with little systematic bias on the training set. Test

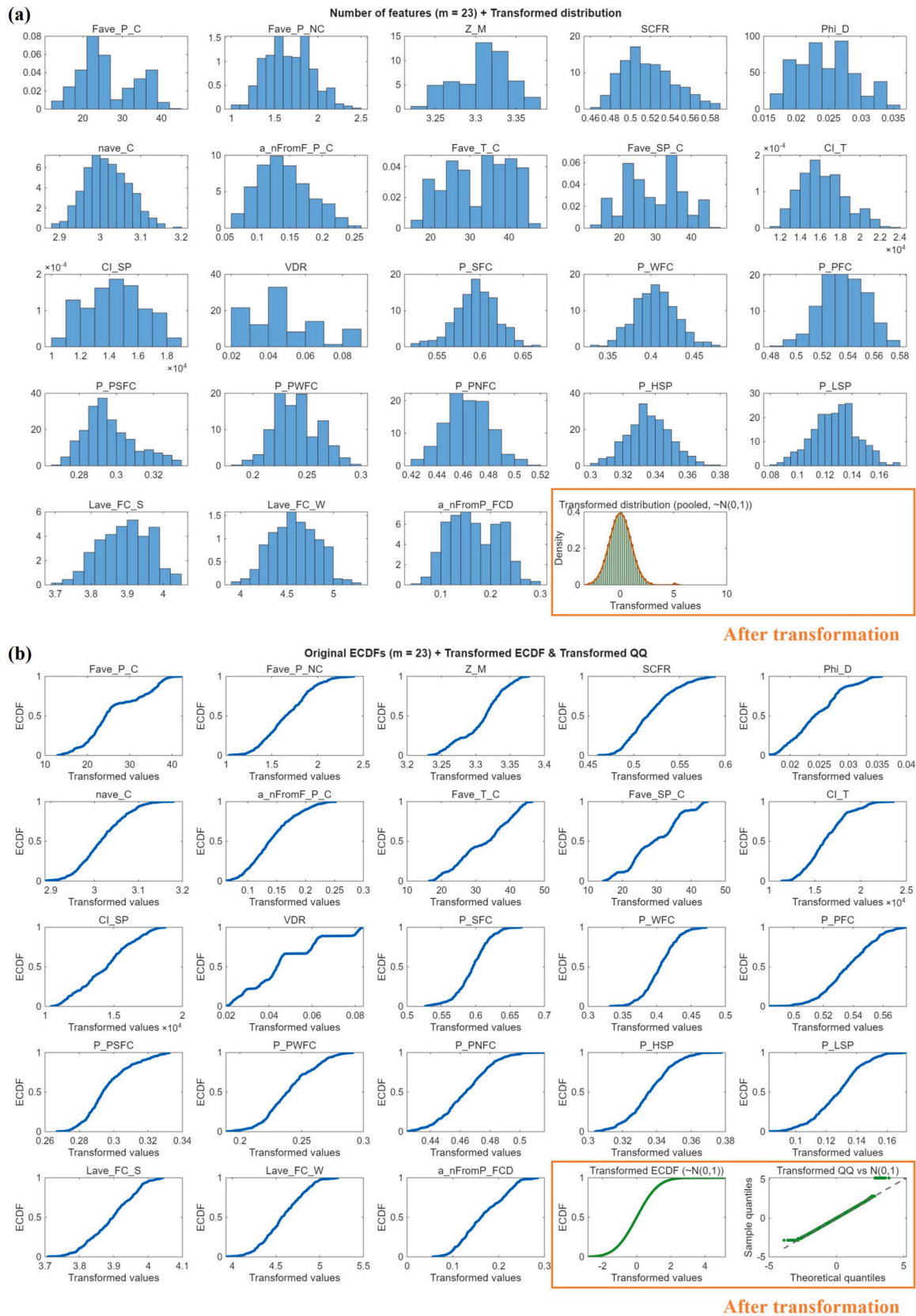


Fig. 28. Data standardization by QuantileTransformer (QT) for 23 features: (a) transformed histograms, (b) empirical cumulative distribution functions (ECDFs) and quantile–quantile (QQ) plot against $N(0, 1)$.

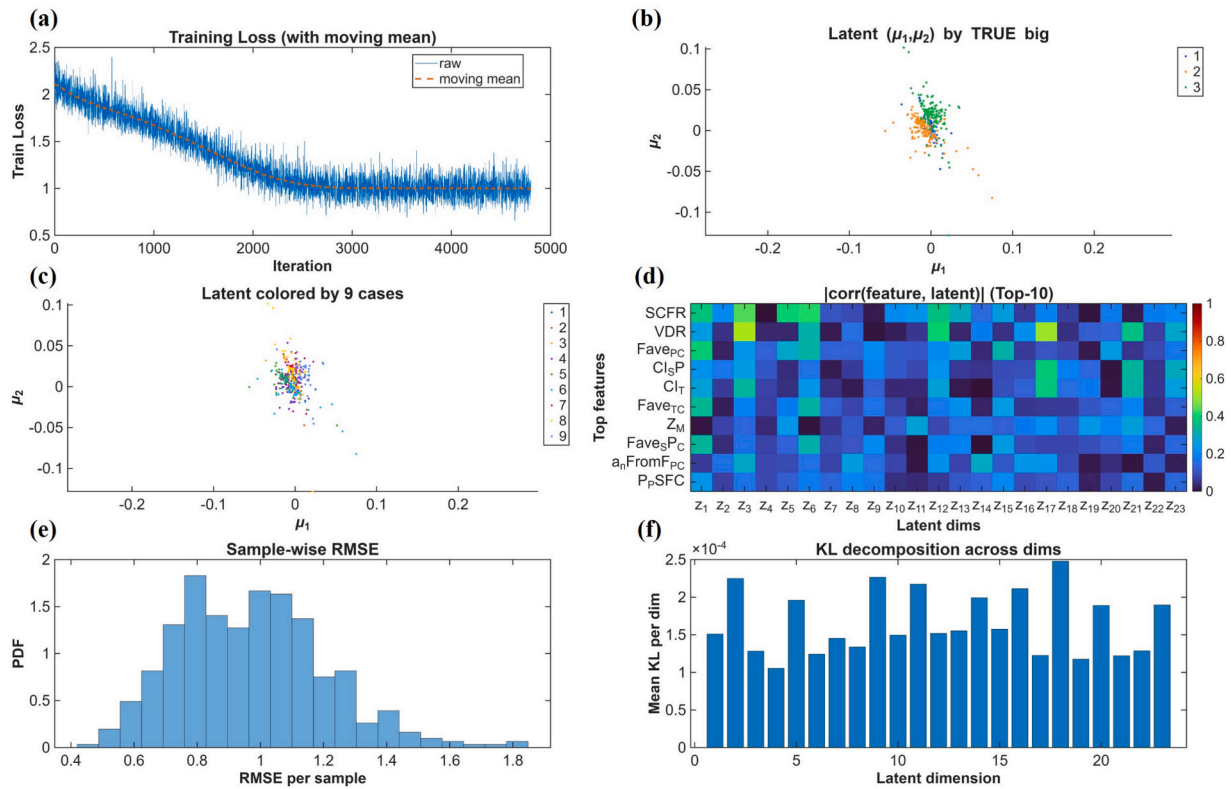


Fig. 29. DVAE-based latent space diagnostics ($d = 23$): (a) training loss, (b–c) 2D latent embeddings by super-class and by 9 cases, (d) top-10 absolute feature–latent correlations, (e) sample-wise RMSE distribution, and (f) per-dimension KL decomposition.

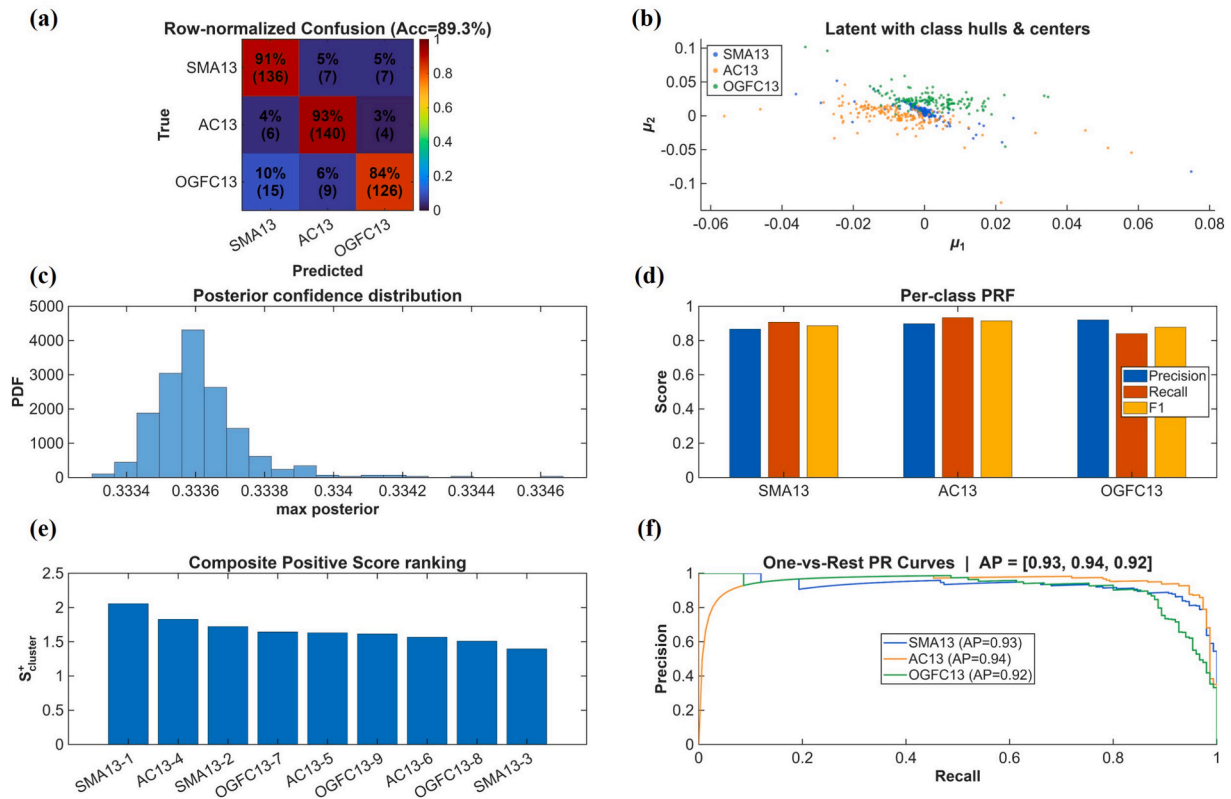


Fig. 30. Label acquisition in latent space via Gaussian mixture model (GMM): (a) row-normalized confusion matrix, (b) latent scatter with class hulls and centers, (c) posterior confidence distribution, (d) precision/recall/F1 scores per class, (e) composite positive score ranking, and (f) one-vs-rest precision–recall (PR) curves.

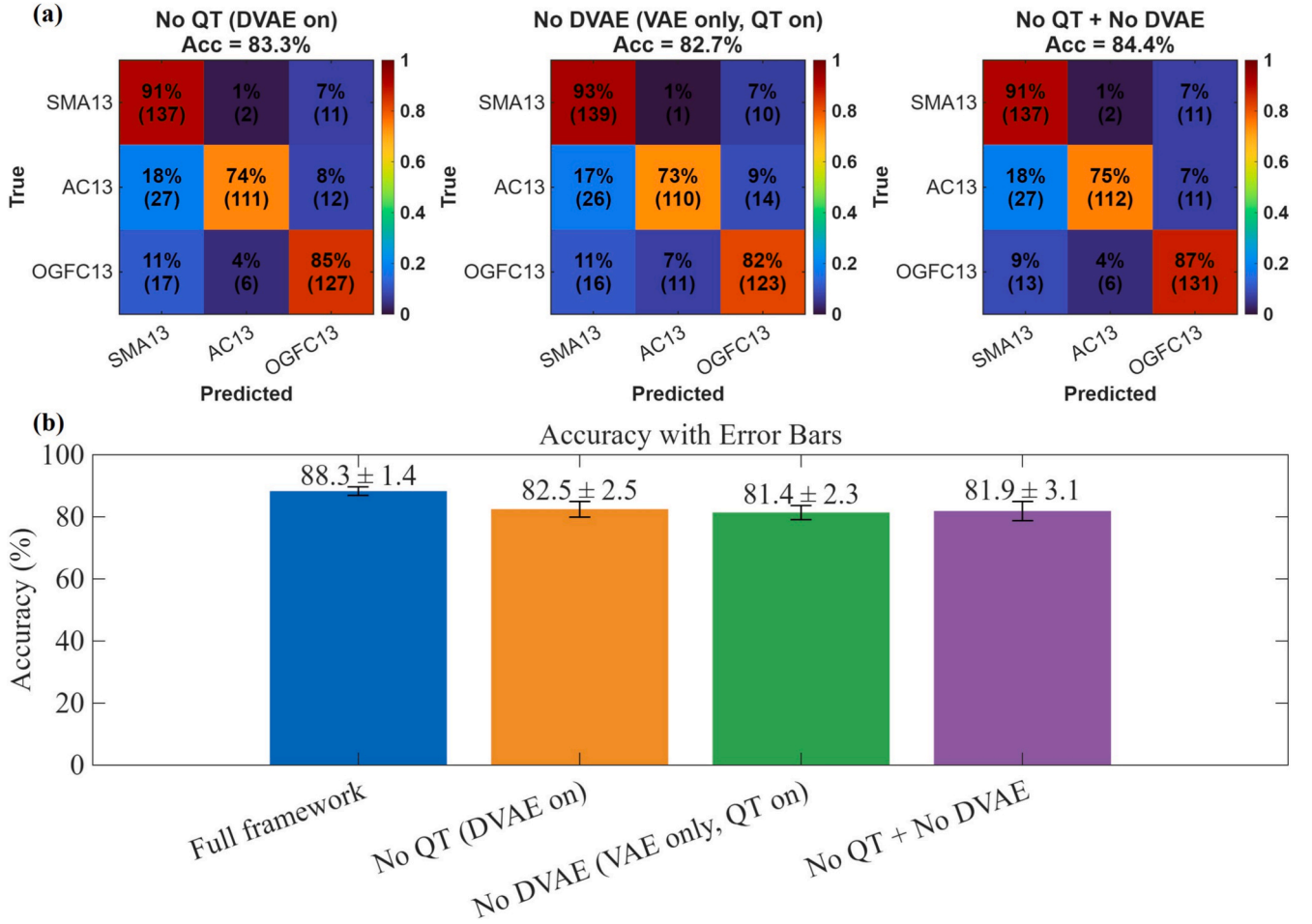


Fig. 31. Research on the stability of the automatic feature evaluation framework: (a) ablation study of QT and DVAE: impact on pre-compaction class prediction (confusion matrices), (b) accuracy of ablation experiments with repeated random initializations (20 repetitions per group).

residuals exhibited a wider dispersion and a weak trend with the fitted values, revealing modest heteroscedasticity and a small structure remaining unexplained at the extremes of the prediction range.

The predicted–actual comparisons (see Fig. 32 (b)) showed an almost perfect alignment with the 1:1 line on the training data ($R^2 = 0.9977$ with small RMSE and MAE), whereas the test scatter was more diffuse ($R^2 = 0.8444$). The fitted line on the test panel lay below the 1:1 reference for larger targets and above it for smaller targets, implying a slight tendency to under-predict high responses and over-predict low responses. Despite this shrinkage toward the mean, the error magnitudes remained within a moderate range (test RMSE and MAE near 1.27 and 0.93, respectively) and the ranking of samples was largely preserved.

Together, these diagnostics indicated that the model learned a stable mapping with excellent in-sample fit and reasonable out-of-sample accuracy, while leaving room to reduce the generalization gap and the mild bias at the extremes (e.g., through additional variability in the training data or calibrated regularization).

3.3.5. Explainable evaluation

Fig. 33 shows feature-wise SHAP dependence plots for the XGBoost model, with each subplot depicting sample-level SHAP values against a single feature; point color encodes the raw feature value and a LOESS curve summarizes the central trend. Several consistent patterns emerged. First, a subset of predictors displayed approximately monotonic decreasing effects on the model output. Typical examples included the void decrease ratio (VDR), the mechanical coordination number Z_M , and the proportion of high stress particles (P_{HSP}), where larger values

were associated with more negative SHAP contributions. The LOESS curves in these subplots trended downward and often flattened at high feature levels, indicating saturation after an initial steep decline. Color gradients concentrated near the tails further suggested that extreme values dominated the strongest negative contributions. Second, other predictors exhibited approximately monotonic increasing effects. The proportions related to weak or total force chain participation (e.g., P_{WFC} , P_{PFC}) generally contributed positively as their values increased. These subplots showed upward LOESS trends with mild curvature, and color bars indicated that higher feature magnitudes clustered with larger positive SHAP values. In several cases the increase was sublinear, again suggesting saturation. Third, several features showed non-monotone or threshold-like responses. Average force metrics (e.g., $\bar{F}_{sp}^C$, $\bar{F}_T^C$) and angular/ratio descriptors (e.g., a_n from $F_p^C(\beta)$ and from $P_{FCD}(\beta)$) presented turning points: SHAP values were near zero at low levels, grew in magnitude over an interior range, and then tapered or reversed at the upper tail. The corresponding LOESS curves showed clear inflection or S-shaped behavior, consistent with nonlinear sensitivity of the prediction to those variables. Across panels, the vertical color variation at a fixed x-value frequently changed from cool to warm, revealing interaction signals: the contribution of a given feature depended on the configuration of others. This was most visible for force chain proportion and length variables (e.g., $\bar{L}_{FC}^S$, $\bar{L}_{FC}^W$), where points with similar abscissa but different colors had noticeably different SHAP values, implying conditional effects modulated by the broader contact network state. Finally, dispersion patterns conveyed uncertainty and heteroscedasticity. Features with tight SHAP clouds around the LOESS curve (e.g., some

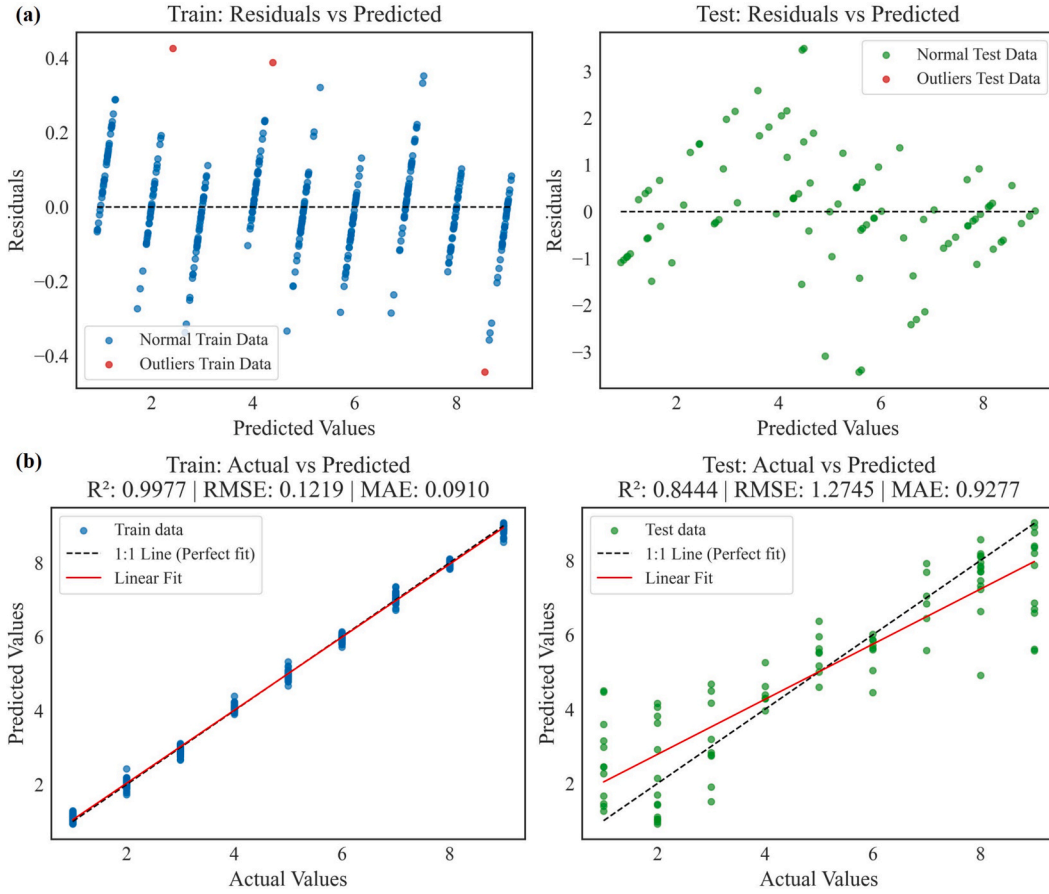


Fig. 32. Supervised regression diagnostics for XGBoost model: (a) residuals vs. predicted for training and test sets, (b) predicted vs. actual with 1:1 and linear fits (R^2 , RMSE, MAE).

coordination/ratio measures) exerted stable effects across samples, whereas broader, fan-shaped clouds (e.g., average contact forces) indicated larger case-to-case variability. Together, these dependence plots corroborated the global importance rankings while clarifying where effects were linear vs. nonlinear, increasing vs. decreasing, and additive vs. interaction-dominated, thereby guiding interpretation of the pre-compaction quality determinants.

Fig. 34 shows cumulative SHAP trajectories for all samples, ordered by global importance (top to bottom). Curves start at the model's base value (vertical reference near 5.0 on the x-axis) and accumulate feature contributions as they proceed downward; rightward deflections increase the prediction, whereas leftward deflections decrease it. The color bar at the top maps lower to higher final outputs. Dominant positive drivers appeared at the top of the stack. The largest and most consistent rightward shifts occurred at P_{PWFC} , followed by $\bar{F}_T^C$ and $\bar{F}_p^C$, indicating that a higher proportion/average strength of force chain contacts strongly pushed predictions upward across nearly all cases. Z_M and P_{HSP} produced additional rightward movement for most trajectories, suggesting that higher mechanical coordination number and a larger share of high stress particles supported higher predicted scores. $SCFR$ and P_{LSP} contributed at a secondary level, with modest but systematic rightward steps. Mid-ranked variables ($\bar{L}_{FC}^W$, CI_{SP} , and a_n from $\bar{F}_p^C(\beta)$) showed mixed effects: many trajectories shifted right, but several bent left, pointing to sample-dependent influences and potential interactions. Lower-ranked variables toward the bottom (P_{WFC} , P_{PSFC} , $\bar{L}_{FC}^S$, P_{PFC} , VDR , P_{PNFC} , CI_T , $\bar{n}_C$, a_n from $P_{FCD}(\beta)$, Φ_D) produced only small incremental changes, with contributions that were comparatively weak and often canceling. The overall shape of the fan—narrow spread near the start and diverging as major features accrue—indicates that most between-sample variation in the

final output is explained by the top few force chain-related descriptors. The concentration of large rightward steps in those descriptors confirms that the model's decisions are primarily governed by micro-mechanical connectivity and stress concentration features, whereas void metrics and baseline contact counts play a limited role.

The global bar plot ranked predictors by mean absolute SHAP value, with an inset radial chart summarizing relative shares (see Fig. 35). The proportion of particles on weak force chains (P_{PWFC}) dominated the explanation, accounting for 25.1% of total importance. The void decrease ratio (VDR) followed at 12.9%, and a small group of micro-mechanical descriptors—mechanical coordination number (Z_M), average tamper-particle contact force ($\bar{F}_T^C$), and the proportion of high stress particles (P_{HSP})—each contributed approximately 7–8%. Subsequent contributors, including the average length of strong force chains ($\bar{L}_{FC}^S$), particles located on force chains ($\bar{F}_p^C$), particles on force chains (P_{PFC}), and particles on strong force chains ($\bar{F}_{SP}^C$), formed a mid-tier with noticeable but smaller effects. The remaining variables (e.g., tamper and screed plate contact impulses CI_T/CI_{SP} , non-force-chain particles P_{PNFC} , weak/strong force chain ratios and length measures, and angular descriptors) each contributed $\leq 6\%$, producing a long-tailed importance profile. Two patterns emerged (see Fig. 35). First, contact network topology and force chain morphology (e.g., P_{PWFC} , Z_M , $\bar{L}_{FC}^S$, P_{PFC} , and P_{SPFC}) collectively explained a large fraction of model variability, indicating that how particles participate in, and organize along, force chains were critical for predicting pre-compaction quality. Second, pre-compaction effectiveness indicators (VDR , tamper/screed plate interaction features) also ranked highly, suggesting that macroscopic densification signals complemented microstructural descriptors rather than replacing them. Overall, the SHAP analysis showed that a small subset of features

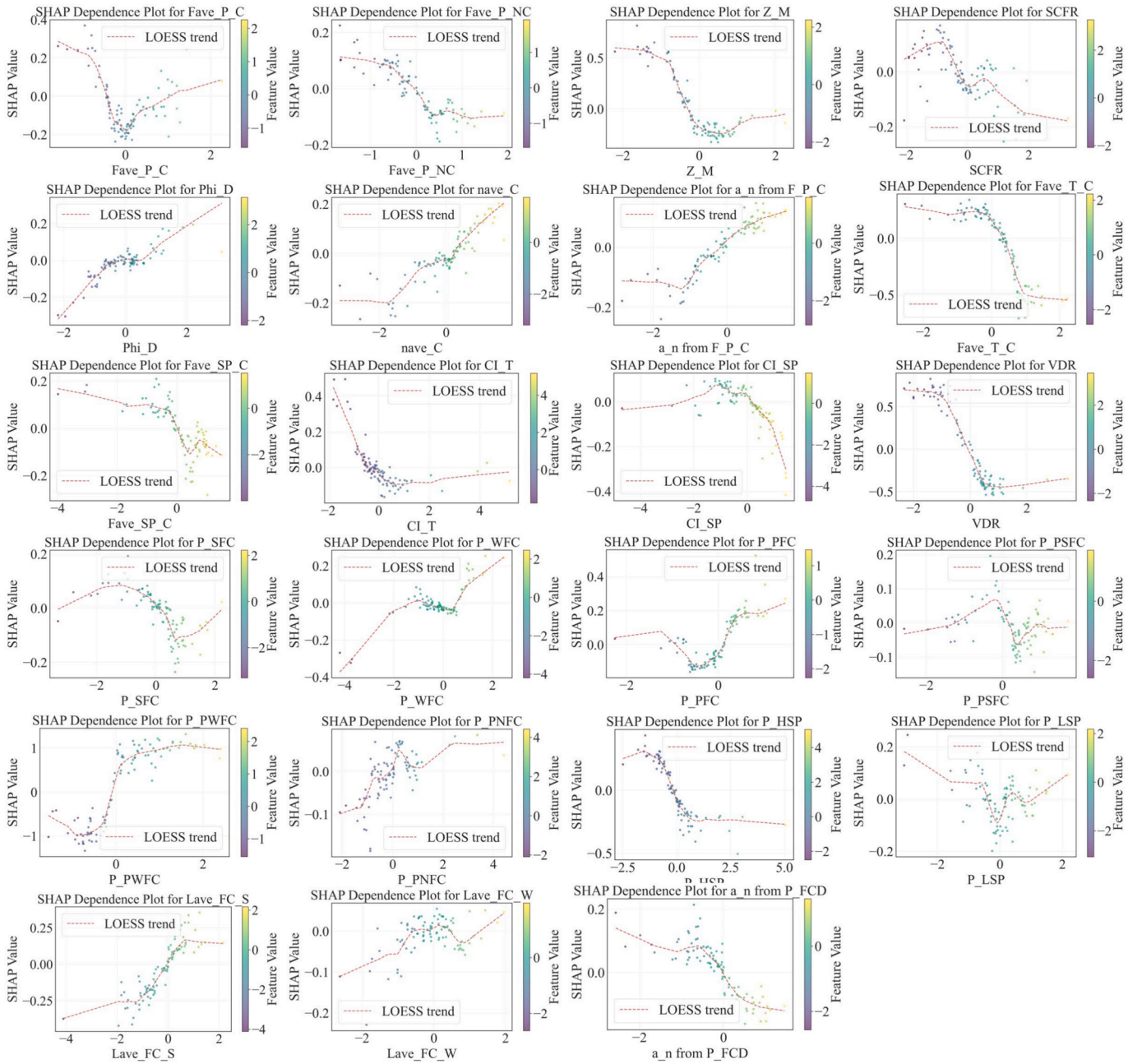


Fig. 33. Feature-wise SHAP dependence for XGBoost, with LOESS trends and color-mapped feature values.

concentrated most explanatory power, led by P_{WFC} and VDR , while a broader set of contact and loading descriptors provided incremental refinements. This hierarchy supports the interpretation that reductions in weak force chain prevalence together with improved densification were the primary drivers captured by the learned model.

3.4. Discussion

This study developed and validated an automated evaluation process for quantitatively assessing pre-compaction quality through micro-mechanical characteristics related to particle contacts and force chains, derived from DEM simulations. However, this approach still exhibits several limitations.

First, particles were idealized as 2D disks, which underrepresents real aggregate angularity, surface roughness, and interlocking; this may bias contact orientation, coordination, and force chain continuity

relative to 3D angular particles. Extending the framework to poly-disperse, non-spherical 3D particles (e.g., clumps or superquadrics) would better capture geometry-driven anisotropy and dilatancy. A practical next step is to replicate a subset of representative cases in 3D with angular particle proxies and compare the resulting key indicators to quantify the 2D-to-3D transferability.

Second, only coarse fractions and a reduced pre-compaction domain were modeled; fines, mastic migration, and scale effects were therefore implicit rather than resolved. A multi-scale coupling that includes fines (and their bridging roles) would improve transferability. Future work can explicitly introduce a fines-mastic phase (or coupled mortar model) and evaluate how fines content alters void evolution and force chain persistence.

Third, the asphalt-binder contact law was treated with fixed parameters, whereas binder rheology is temperature-, rate-, and aging-dependent; incorporating thermo-viscoelastic/viscoplastic evolution

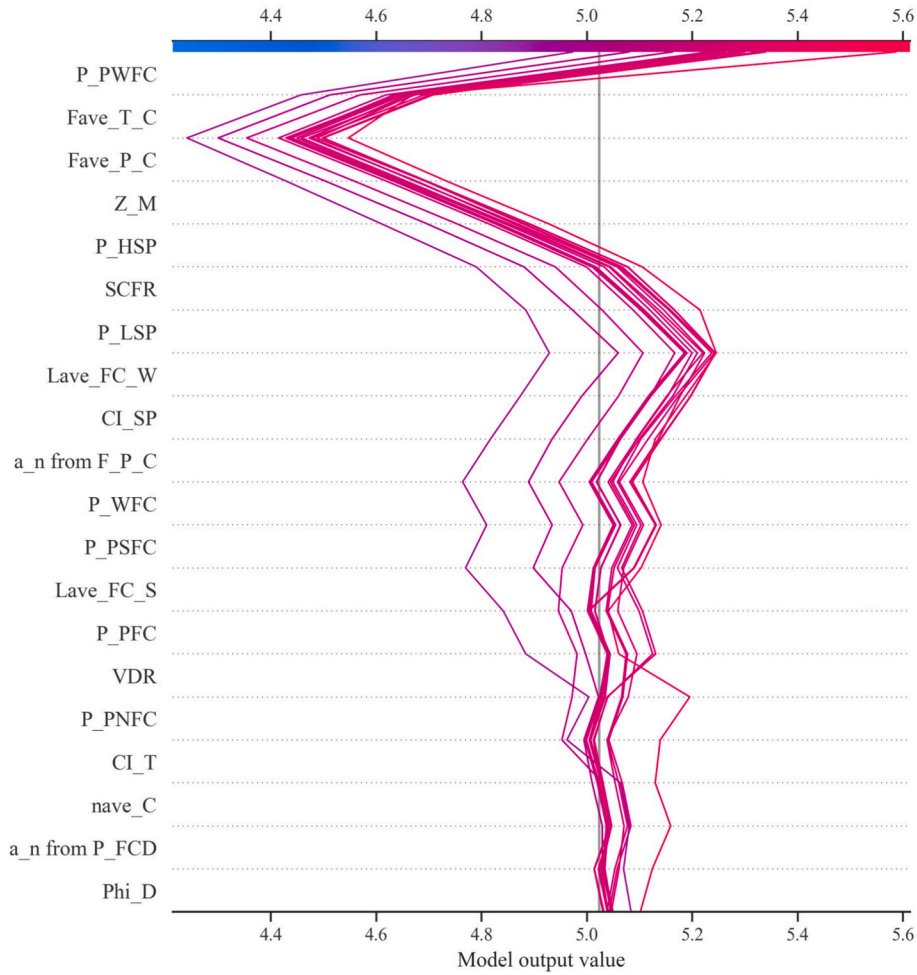


Fig. 34. SHAP decision plot for XGBoost: cumulative feature contributions to the model output across samples (top-20 features).

and temperature fields would allow more realistic stick-slip and energy dissipation pathways. In the present study, temperature was effectively idealized as spatially uniform, and the thermal-mechanical coupling as well as temperature gradients within the mat were not explicitly resolved. In practice, thermal segregation during paving can create local hot and cold spots, which may substantially change binder stiffness, adhesive contact response, and consequently the formation and persistence of force chains and contact networks compared with the idealized isothermal assumption. Therefore, a time-dependent JKR contact model can be considered for future implementation [4]. A concrete improvement is to implement a thermo-viscoelastic, rate-dependent contact law calibrated with temperature-controlled mastic/binder tests and then rerun pre-compaction scenarios across representative paving temperatures.

Fourth, screed device boundary conditions (tamper and screed plate kinematics, a fixed 15 s window) were prescribed and idealized. Hardware-in-the-loop calibration or instrumented field trials could reduce boundary condition bias. Future studies can incorporate measured screed kinematics and contact forces from instrumented equipment to calibrate the boundary inputs and validate the simulated response.

Fifth, although the proposed force-chain indicators are micro-scale quantities that are not directly observable during real paving operations, they can be conceptually linked to measurable field variables through their macro-scale manifestations. In particular, variations in contact network connectivity and force-chain persistence are expected to influence bulk responses that are routinely monitored or can be measured in practice, such as pre-compaction density, stiffness or

modulus-related measures, segregation patterns, and the sensitivity of the mat response to vibration and loading. A practical next step is to establish quantitative mappings between these micro-indicators and field-observable signals by jointly analyzing DEM outputs and sensor data (e.g., screed vibration, tow-point or screed contact forces, hydraulic pressures, paving speed, layer thickness, and mat temperature fields from infrared imaging). Such mappings would enable the micro-scale indicators to be inferred rather than directly measured, using calibrated DEM simulations and machine-learning surrogates.

Moreover, key operating parameters such as screed vibration frequency, vibration amplitude, and paving speed were not systematically varied in the present numerical campaign [1]. Future parametric studies that treat these operating variables as controllable inputs would help quantify their influence on the proposed indicators and improve the framework's direct applicability to field decision-making. Finally, labels for supervised learning arose from latent space clustering and may inherit clustering biases; cross-dataset testing and alternative label sources (expert or field data) would help assess robustness. In future work, labels can be anchored to independent quality measures (e.g., density/void targets or field pre-compaction metrics) to benchmark the learned categories and reduce dependence on clustering.

4. Conclusion

This study proposed a DEM-based particle-force chain informatics framework for the simulation and data-driven evaluation of pavement pre-compaction beneath a vibrating screed. The framework couples a physics-based discrete element model with an automated analytics

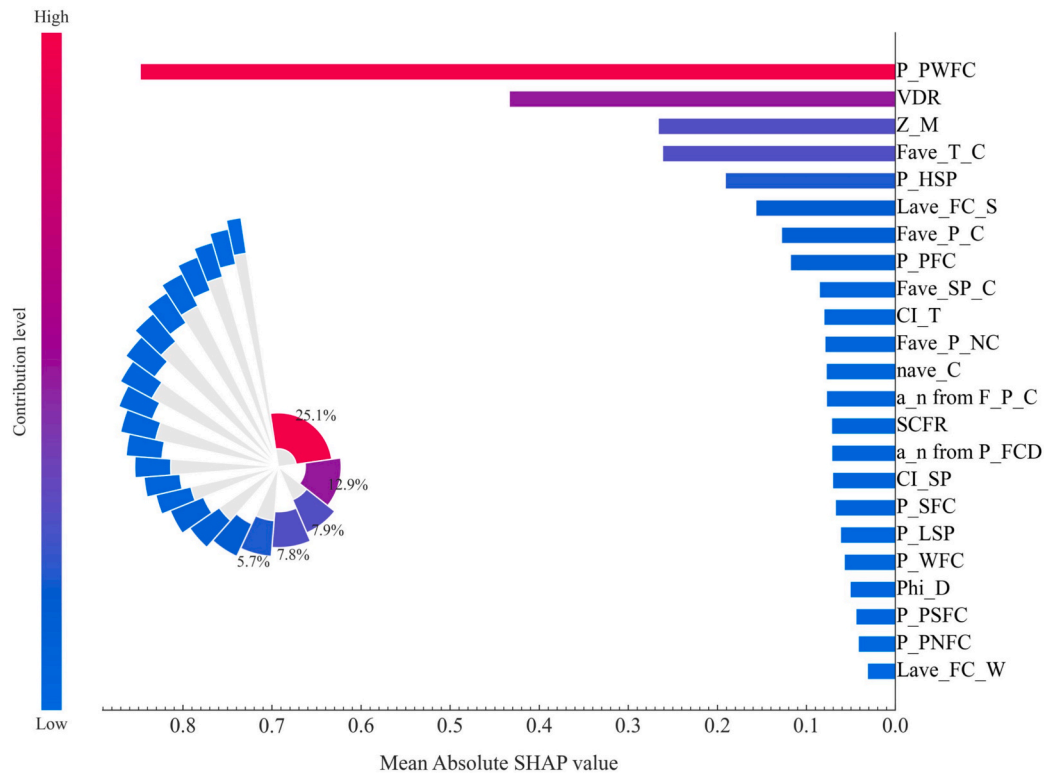


Fig. 35. Global feature importance from SHAP: mean absolute contributions and radial share (top features).

pipeline for feature extraction, latent space clustering, supervised prediction, and explainable post-processing. Its objective is to transform detailed particle contact and force chain information into quantitative indicators of pre-compaction quality that are suitable for informatics-driven analysis. The main conclusions of this study are as follows:

- The DEM model simulated screed device–aggregate interaction for three representative gradation families (SMA-13, AC-13, OGFC-13, each with three cases) and produced coordinated streams of particle-to-particle and force chain data. From these simulations, 23 micro-mechanical descriptors were extracted, jointly characterizing fabric anisotropy, coordination, force chain morphology, and stress heterogeneity, and providing a quantitative basis for pre-compaction assessment.
- Across all gradations and cases, pre-compaction was found to reorganize the granular skeleton in a consistent pattern: weak short force chain segments were removed, short-to-medium segments were strengthened, average force chain length increased slightly, and force chain orientations aligned with the loading direction. High stress particles became increasingly concentrated along these reinforced chains. These mechanisms clarify how gradation influences the development of stable load-bearing networks in the pre-compaction stage.
- The automatic feature evaluation pipeline—QuantileTransformer (QT), denoising variational autoencoder (DVAE), Gaussian mixture model (GMM), and XGBoost—standardized heterogeneous features, learned a compact latent representation, generated data-driven labels, and produced predictive scores for pre-compaction quality in a fully automated manner. By reducing manual intervention in feature handling and labeling, this informatics workflow enables scalable and repeatable processing of large DEM datasets and systematic comparison of different aggregate gradations and operating conditions.
- SHAP-based explainable evaluation further related the predictive scores to a compact set of dominant indicators (e.g., proportion of

weak force chain particles, void decrease ratio, mechanical coordination number, and high stress particle ratio), yielding physically interpretable surrogate models. The resulting explanations help to identify the most influential micro-mechanical mechanisms and to quantify their relative importance across gradations within a unified data-driven framework.

- For engineering use, this study recommends a compact, robust indicator set in which the share of particles on weak force chains (P_{PWFC}) serves as the primary metric (lower values indicate better pre-compaction), complemented by the void decrease ratio (VDR) as a macroscopic densification measure. As secondary diagnostics, mechanical coordination (Z_M), tamper–particle contact force ($\bar{F}_T^C$), and the high stress particle ratio (P_{HSP}) are useful, because higher values respectively reflect stronger contact connectivity, stronger device–aggregate coupling, and more consolidated load paths. For added nuance, strong force chain length ($\bar{L}_{FC}^S$), particles on force chains (P_{PFC}), and particles on strong force chains (P_{PSFC}) may be reported, but they are not essential for first-pass ranking and decision-making.

Overall, the results demonstrate that combining DEM simulations with latent-variable learning, probabilistic clustering, and explainable supervised models can upgrade pre-compaction analysis from isolated, problem-specific indicators to a structured, predictive, and interpretable indicator system. The proposed particle–force chain informatics framework provides a general template for extracting reduced-order, yet physically meaningful, descriptors from particle-scale simulations, and it can be extended to other granular compaction problems and to more complex 3D screed–pavement interaction models.

CRediT authorship contribution statement

Dong Feng: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Resources, Methodology,

Investigation, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

The authors declare no competing financial interests or personal relationships that could have influenced the work reported in this paper.

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Data availability

Data will be made available on request.

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