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**Particle-scale compaction mechanisms and free-boundary effects of
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Abstract

The earth-rock dam, as one of the most prominent types of dams at present, the quality of its compaction construction directly affects the structural stability and long-term service performance of the dam. This study investigates the particle-scale compaction mechanisms and free-boundary effects of rockfill under roller compaction without lateral confinement. Two PFC2D models were developed for sections parallel and perpendicular to the roller travel direction. The evolution of porosity, surface settlement ratio, particle displacement and rotation, transient velocity fields, and contact-force chains was examined. In both sections, the mean porosity decreased with the number of roller passes, showing rapid densification during the initial passes followed by gradual stabilization. Weak lateral confinement near the free boundaries promoted particle migration toward the free surfaces, causing a pronounced decrease in surface elevation without a commensurate reduction in porosity and thereby producing a distinct settlement–porosity mismatch. In the travel-direction section, the horizontal thrust induced by roller motion intensified particle translation and rotation, yielding a mean surface settlement ratio of 17.06% after compaction, compared with 11.46% in the transverse section. By contrast, the central zone developed a more stable load-bearing force-chain network and exhibited lower particle mobility. These findings demonstrate that settlement near an unconfined edge arises not only from pore compression but also from lateral particle migration and surface-profile reconstruction. Consequently, settlement-based indicators alone may overestimate the degree of compaction near free boundaries.

Keywords: rockfill; PFC2D; discrete element method; roller compaction; free boundary; particle-scale mechanism

1. Introduction

Earth–rockfill dams are widely used in hydraulic and hydropower engineering because they permit extensive use of locally available materials, are comparatively economical, adapt well to complex

topographic and geological conditions, and perform favorably under seismic loading (Liu, 2022); Wu and Zhang, 2018; Zhou et al., 2006). Rockfill, a discontinuous frictional granular material composed of gravel, crushed rock, and blocks over a wide size range, is commonly used in dam construction because of its availability, compactability, and high shear strength (Zhou et al., 2018). Repeated mechanical loading during roller compaction causes particles to overcome interparticle resistance and undergo translation, rotation, and rearrangement. These processes reduce void space, enhance interlocking, and increase the density, stiffness, and overall stability of the fill (Zhang, 2020). A sound understanding of the macro- and particle-scale responses of rockfill during compaction is therefore essential for improving fill-quality control.

Field compaction trials have long been the principal means of investigating rockfill response and selecting construction parameters. Zhu et al. examined placement standards for high rockfill dams through field trials (Zhu et al., 2019; Zhu, 2020), whereas An et al. optimized construction parameters using tests conducted at different roller speeds and vibration settings (An et al., 2020). Full-scale vibratory compaction tests have also been performed on asphalt mixtures, crushed stone, roller-compacted concrete, and other granular or composite materials (Dan et al., 2020); Tong, 2008; Liu et al., 2015; Zhu et al., 1999; Huang et al., 2010). Although field testing directly captures macroscopic compaction behavior under construction conditions, it is costly and time-consuming and cannot continuously resolve particle-scale translation, rotation, contact-network evolution, or local porosity changes.

Finite-element modeling has been used to reduce experimental costs and evaluate the influence of operating parameters. Kenneally et al., for example, analyzed the dynamic response of a vibratory roller-layered soil system (Kenneally et al., 2015), and Li et al. investigated the effects of drum mass,

excitation force, vibration frequency, and travel speed on the compaction of rockfill subgrades (Li et al., 2021). The finite element method (FEM) is well suited to continuum-scale stress and deformation analyses, but it does not directly represent particle rearrangement, rotation, local sliding, or force-chain reconstruction in strongly discontinuous materials such as rockfill.

The discrete element method (DEM) explicitly resolves particle contacts and motion and can therefore track structural rearrangement and load transfer during compaction at the particle scale. PFC- and EDEM-based studies have simulated the compaction of asphalt mixtures, subgrade fills, rockfill, and slag and have examined density or porosity, particle migration, parameter sensitivity, and contact-force evolution (Micaelo et al., 2011; Chen et al., 2024); Ma et al., 2023; Zhang, 2022; Xu et al., 2023; Li et al., 2018; Peng et al., 2024; Xu et al., 2025; Pei and Yang, 2018; Tang, 2008; Ma et al., 2013; Jiang, 2010; Wang et al., 2020; Peters et al., 2005). Collectively, these studies demonstrate that DEM can link macroscopic compaction response to particle motion, contact population, and load-bearing networks.

Most existing DEM studies of roller compaction focus on the number of passes, travel speed, vibration parameters, or overall compaction performance (Chen et al., 2021; Liu, 2016; Zhang, 2015); Cheng, 2012; Li et al., 2013). To limit computational cost, they also commonly employ small domains with rigid or periodic lateral boundaries. Previous studies have shown that rockfill and broadly graded particle assemblies are sensitive to specimen size and boundary conditions (Wu et al., 2024; Huang et al., 2014), and that particle rotation, sliding, and contact dissipation vary with lateral confinement (Liu et al., 2017). However, the manner in which outward particle migration near placement edges or exposed faces alters the relationship between surface settlement and pore compression remains insufficiently understood. To address this gap, two PFC2D models without vertical sidewalls were established for orthogonal sections. Particle displacement, rotation, velocity, and

contact forces were then used to elucidate the settlement–porosity mismatch near free boundaries.

2. PFC2D modeling of rockfill compaction

2.1 Numerical model and boundary conditions

Two-dimensional discrete element simulations were performed using Particle Flow Code 6.0 (PFC6.0; Itasca Consulting Group). The model consisted of a rockfill assembly and a roller-loading system and was designed to investigate particle displacement and micromechanical response during compaction with unconfined lateral edges. Circular particles represented the rockfill, a rigid wall formed the base, and rigid loading walls represented the roller. No vertical sidewalls were imposed. Instead, the assembly terminated in 45° loose-fill slopes so that edge particles could migrate outward under loading.

The model was 12 m wide at the base and 10.3 m wide at the crest, with an average loose-lift thickness of 0.85 m and side slopes of 45°. These dimensions accommodated both the roller-affected zone and the outward-migration zones at the edges. Free boundary denotes an inclined granular surface on which particles may move in both the normal and tangential directions, rather than a rigid boundary with prescribed zero displacement.

Based on previous studies and the objectives of this work, the roller was represented by a combination of rigid circular and planar walls. A rigid circle was used in the section parallel to roller travel, whereas an equivalent rectangular rigid platen was used to reproduce the transverse loading footprint in the perpendicular section.

During vibratory compaction, the principal external loads acting on the rockfill are the roller weight and the excitation force. Because the excitation force varies periodically and the roller can transmit compression but not tension, the applied roller force was expressed as:

$$F(t) = \begin{cases} G + F_{max} \sin(\omega t) & F(t) > 0 \\ 0 & F(t) \leq 0 \end{cases} \quad (1)$$

where G is the roller weight (N), F_{max} is the peak excitation force (N), and ω is the angular frequency of the roller eccentric mass (rad/s).

Table 1

Principal parameters of the vibratory roller

Parameter	Operating mass (kg)	Travel speed (m/s)	Frequency (Hz)	Drum diameter (mm)	Compaction width (mm)	Excitation force (kN)
Value	17000(front drum) 9000(rear drum)	1.1	27	1600	2170	435

2.2 Particle-size distribution and specimen generation

Particle-size distribution strongly affects compaction. To represent the field material as realistically as practicable, the particle assembly was generated from the measured grading of the test-section rockfill and was subsequently compacted from its loose placement state.

Following the particle-number estimation method based on sieve statistics proposed in Ref. [37], the number of particles in each size interval was calculated from the bulk density of the rockfill. This procedure allowed the target gradation and loose-placement state to be represented simultaneously in the DEM model. Because PFC particles are rigid and initial interpenetration was excluded, overlap was not permitted during particle generation.

The initial porosity is given by:

$$n = 1 - \frac{V_d}{V} \quad (2)$$

Assuming an approximately uniform solid density across all size classes, the mass fraction of each class can be approximated by its solid-volume fraction. The number of particles in size class i is then estimated as:

$$n_i = \frac{m_i V_d}{\pi r_i^2} \quad (3)$$

where V_d is the total solid volume of the particles, V is the bulk volume of the assembly, i denotes

the size-class index, n_i is the number of particles in class i , r_i is the representative particle radius (the mean of the minimum and maximum radii in that interval), and m_i is the fraction assigned to class i .

Particles in each size interval were generated randomly within the prescribed bounds in PFC2D. The arithmetic mean of the minimum and maximum radii was adopted as the representative radius r_i for particle-number estimation. Particles were first generated in a larger rectangular domain and allowed to settle under gravity to a loose equilibrium state. The settled assembly was then imported into the target geometry, and particles outside the prescribed boundary were removed. The resulting numbers of particles in each size interval are listed in Table 2.

Table 2

Number of particles in each size interval of the numerical model

Particle diameter (mm)	Cumulative percent finer by volume (%)	Number of particles	Particle diameter (mm)	Cumulative percent finer by volume (%)	Number of particles
300	100	9	40	41	1348
200	95	67	20	28	2896
100	80	115	10	21	5071
80	71	251	5	18	70819
60	59	687			

The particles were initially distributed randomly in a larger rectangular domain and deposited under gravity until the porosity reached approximately 0.16. The assembly was then imported into the target boundaries, and particles outside the geometry were deleted. Compaction commenced after static equilibrium was reached, defined by an average unbalanced-force ratio, $aratio$, below 10^{-5} .

2.3 Contact model and micromechanical parameter calibration

Micromechanical parameters such as normal stiffness, shear stiffness, friction coefficient, and rolling-resistance coefficient do not have unique relationships with macroscopic elastic modulus, strength, or compressibility. They must therefore be selected or calibrated with reference to the study objective, material behavior, and available experiments. Parameter ranges adopted in previous PFC

studies were first compared, as summarized in Table 3.

Table 3

Micromechanical parameters adopted in previous PFC studies

No.	Source	Material	Contact model	Model parameters
1	Tang [25]	Asphalt mixture	Linear contact model	$Kn=Ks=1 \times 10^8 \text{N/m}$
2	Zhang [32]	Roller-compacted concrete	Bonded contact model	$Kn=Ks=1 \times 10^8 \text{N/m}$ $n_bond=s_bond=2 \times 10^5 \text{N}$
3	Ma [26]	Gravelly soil foundation	Linear contact model	$Kn=Ks=1.5 \times 10^6 \text{N/m}$
4	Jiang [27]	Soil-rock mixture	Bonded contact model	$Kn=Ks=1 \times 10^9 \text{N/m}$ $n_bond=s_bond=2 \times 10^5 \text{N}$
5	Zhang [19]	Rockfill	Rolling-resistance linear model	$Kn=Ks=1 \times 10^8 \text{N/m}$ $\mu=0.47 \mu_r=0.5$

Most previous numerical studies of rockfill compaction have used laterally confined domains. Under such conditions, particle rotation and lateral displacement are suppressed, and rolling contributes relatively little to the overall compaction response. The present study instead focuses on displacement, rearrangement, and edge response under free-boundary conditions. In this setting, lateral flow and rotation become more prominent; a conventional linear contact model without rolling resistance may permit unrealistically free rotation and thus distort the predicted displacement pattern and local compaction response.

A rolling-resistance linear contact model was therefore adopted. By supplementing the linear contact law with rolling resistance, the model limits unrealistic particle rolling and better represents rotational resistance and energy dissipation at contacts between coarse particles. The model has been widely applied in DEM analyses of granular materials (Ai et al., 2011). The resisting moment comprises elastic and viscous contributions. The elastic rolling-resistance moment increases approximately linearly with rotation until a limiting value is reached and remains at that limit while the rolling direction is unchanged.

The sensitivity analysis indicated that normal and shear contact stiffnesses primarily govern

contact deformation and assembly stiffness and therefore control the macroscopic compressive response. The friction and rolling-resistance coefficients mainly affect sliding, rotation, and rearrangement. Calibration against the field-test response yielded $K_n = 1.0 \times 10^7 \text{ N/m}$, $K_s = 1.0 \times 10^7 \text{ N/m}$, $\mu = 0.5$, and $\mu_r = 0.5$. The calibrated model reproduced the observed bulk compression and particle rearrangement with reasonable fidelity and was therefore used in the subsequent free-boundary simulations. The adopted parameters are listed in Table 4.

Table 4
Micromechanical parameters of the rockfill DEM model

Parameter	Value
Initial porosity	0.16
Normal contact stiffness, K_n	$1 \times 10^7 \text{ N/m}$
Shear contact stiffness, K_s	$1 \times 10^7 \text{ N/m}$
Friction coefficient, μ	0.5
Rolling-resistance coefficient, μ_r	0.5
Particle density	2760 kg/m^3

2.4 Monitoring scheme and evaluation metrics

The analysis focused on the evolution of porosity, surface settlement, and particle displacement at different locations and after successive roller passes. Two monitoring systems were implemented: surface-elevation sampling and internal porosity measurement.

2.4.1 Surface settlement measurement

Fixed x-coordinates were assigned along the model surface at an interval of 0.01 m, and a total of 990 balls with a radius of 0.005 m were used as sampling points. After each pass, the surface elevation at every x-coordinate was reidentified and compared with its initial value to obtain the surface profile and the spatial distribution of settlement ratio. These points were used only for post-processing and did not participate in particle contacts.

This measure describes the geometric change in surface elevation at a fixed spatial coordinate rather than the vertical displacement of a particular particle. Consequently, when particles migrate

laterally, the elevation loss at a fixed x-coordinate reflects vertical densification, particles leaving the sampling line, and surface-profile reconstruction.

The surface settlement ratio was calculated as:

$$s_i = \frac{h_{i0} - h_{i1}}{h_{i0}} \quad (4)$$

where s_i is the surface settlement ratio at location i , h_{i0} is the surface elevation before compaction, and h_{i1} is the elevation after compaction.

2.4.2 Local porosity measurement

Twenty-nine measurement circles were arranged horizontally within the model (Fig. 1.). Each circle had a diameter of 0.66 m and a center elevation of 0.33 m. PFC2D calculated the two-dimensional local porosity from the particle area within each circle. The values were used to compare relative densification at different locations and after different numbers of passes within the same two-dimensional model. Adjacent circles overlapped to provide a quasi-continuous profile with distance from the boundary.

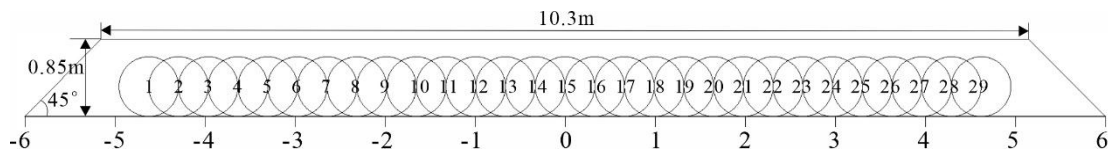


Fig. 1. Arrangement of measurement circles for local porosity

2.5 Simulation of the roller-compaction process

2.5.1 Definition of simulation cases

Roller compaction is inherently three-dimensional. In a longitudinal section parallel to roller travel, particles are subjected to both vertical contact loading and the horizontal action generated by forward rolling. In a transverse section perpendicular to travel, the response primarily reflects load distribution across the drum width, overlap between adjacent lanes, and lateral extrusion. To separate these dominant directional mechanisms, two orthogonal PFC2D models were established, as illustrated in Fig. 2.

The travel-direction model used a rolling rigid circle to reproduce particle translation and rotation as the drum approached, contacted, and moved away from a location. The transverse model used a rectangular rigid platen with lane-by-lane loading to represent extrusion and overlap across the drum width. Both sections retained free edges so that the response of the weakly confined boundary zones could be compared with that of the central zone.

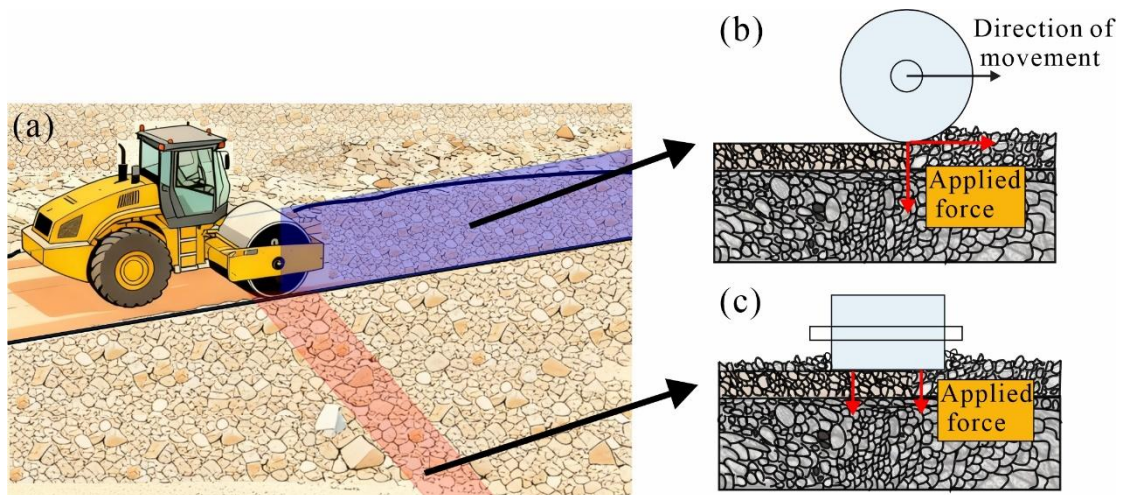


Fig. 2. Conceptual representation of the two orthogonal PFC2D sections

Modeling the two directions separately reduces computational cost while isolating their principal mechanical contributions, thereby facilitating identification of the mechanisms responsible for anomalous edge response.

2.5.2 Section parallel to roller travel

The travel-direction model is shown in Fig. 3. It was used to analyze particle motion under the combined vertical load and longitudinal horizontal action generated by a moving roller. A rigid circular wall with a radius of 0.8 m represented the roller.

The roller weight and excitation force supplied the vertical load, whereas forward rolling transferred a horizontal action to particles in contact with the drum, producing longitudinal translation, local spreading, and rotation. This model was used to identify the influence of rolling on particle migration, surface settlement, and contact-network evolution and is hereafter referred to as

Case 1.

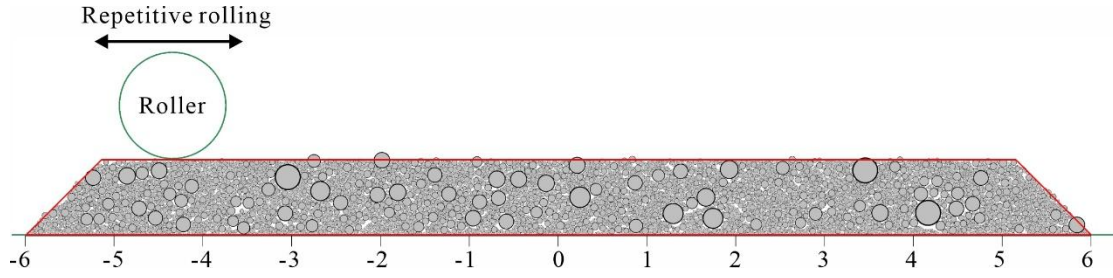


Fig. 3. Rolling-compaction model for the section parallel to roller travel

2.5.3 Section perpendicular to roller travel

The transverse loading model is shown in Fig. 4. It represents the stress and deformation response across the roller width and was used to compare compaction in the central and free-boundary zones under lateral extrusion.

A rectangular rigid platen 2.17 m wide and 1.6 m high represented the transverse contact footprint of the roller. The platen was advanced from left to right in discrete lanes along the model surface. Adjacent lanes overlapped by 20%, consistent with the field construction parameters, to reproduce overlapping roller passes.

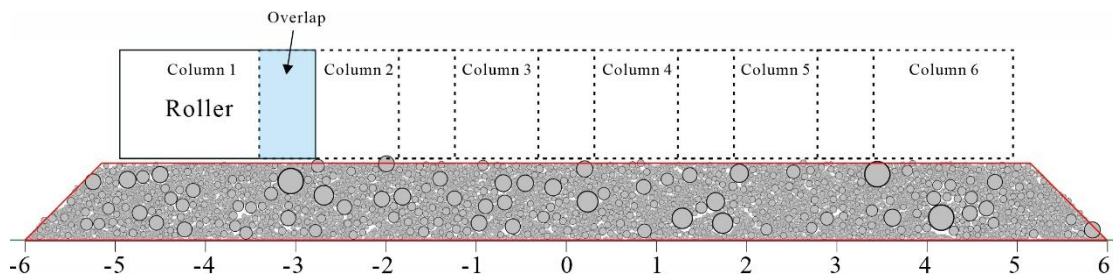


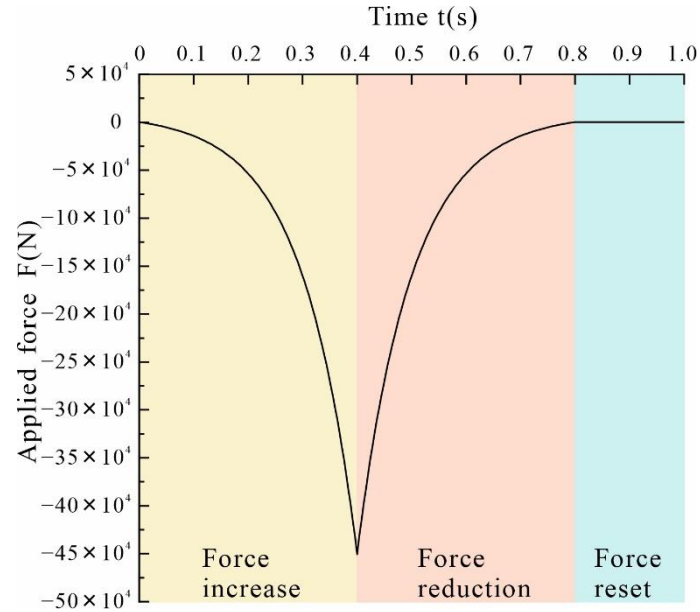
Fig. 4. Lane-based overlapping loading model for the section perpendicular to roller travel

In the transverse section, the contact area between the roller and rockfill was approximated as rectangular; the equivalent vibratory contact stress was therefore expressed as:

$$P(t) = F(t)/LB \quad (5)$$

where L is the roller width and B is the roller-ground contact length. From roller geometry, $B = (D/2)\sin\beta$, where D is the roller diameter and β is the rolling-resistance angle; $\beta \approx 51^\circ$ was adopted for

237 the field roller.



238
239 Fig. 5. Loading-unloading cycle at a single platen position

240 To represent the time-varying load at a fixed location as the roller passed, a complete loading-unloading cycle was applied at each platen position (Fig. 5). As the roller approached, covered, and left a location, the local force increased, reached its peak, and then decreased. Each cycle comprised three stages to allow sufficient time for force transmission and particle rearrangement:

244 (1) Loading: the roller enters the local zone and the force increases gradually from zero to its peak value;

246 (2) Unloading: the vertical force decreases progressively to zero;

247 (3) Rebound and relaxation: the rockfill material rebounds and rearranges until a quasi-static equilibrium is recovered.

249 After completing a loading cycle, the platen moved to the next lane until the entire model surface had been covered. This model is hereafter referred to as Case 2.

3. Compaction response and free-boundary effects

3.1 Overall compaction behavior

3.1.1 Macroscopic deformation and porosity evolution

Fig. 6 shows the overall deformation of the rockfill during ten passes in Case 1. The initial surface was approximately level. Repeated roller loading caused progressive rearrangement of the surface and shallow particles and migration toward the free edges of the section. In the absence of rigid side confinement, edge particles gradually moved beyond the initial outline and formed outward-spreading zones. The surface geometry and internal structure of the central zone approached a stable state after approximately four passes, whereas outward migration and loose accumulation remained evident near the free boundaries, indicating a response distinct from that of the model center.

Fig. 7 presents the corresponding porosity evolution. The mean porosity decreased with the number of passes, with the largest reduction occurring during the first two passes, followed by progressively smaller changes (Fig. 7a). This trend marks a transition from rapid initial rearrangement to a comparatively stable interlocked structure. The local porosity within measurement circle M15 also decreased overall but fluctuated briefly within individual passes because particles entered or left the measurement area and the local fabric adjusted (Fig. 7b). Within a single cycle, local porosity alternated between loading-induced densification and unloading-related adjustment (Fig. 7c).

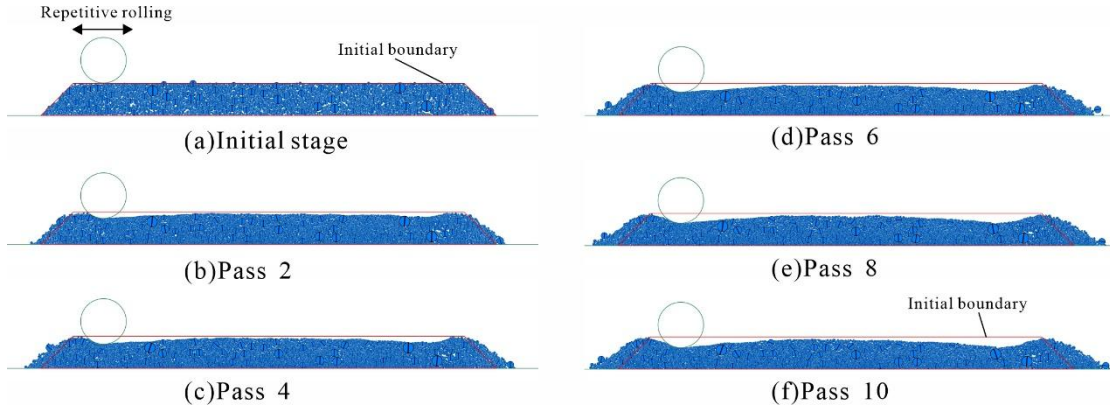


Fig. 6. Evolution of overall deformation during compaction in Case 1

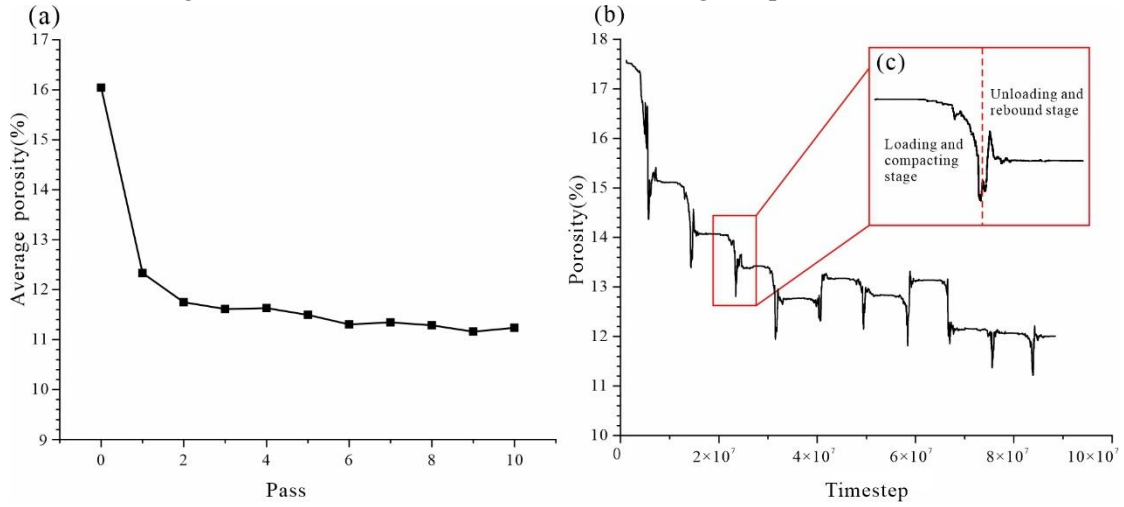


Fig. 7. Porosity evolution in Case 1: (a) mean porosity versus number of passes; (b) porosity history in measurement circle M15; and (c) local porosity changes during one compaction cycle

Fig. 8 shows deformation in Case 2. Unlike Case 1, this section excludes the longitudinal particle push directly generated by forward rolling and therefore exhibits a more coordinated overall deformation pattern. As the number of passes increased, the central zone densified progressively. Lateral migration and outward spreading still occurred near the free surfaces, but their extent and magnitude were smaller than in Case 1, confirming that the horizontal action of rolling intensifies particle migration near a free boundary.

Fig. 9 shows the porosity evolution in Case 2. Mean porosity again decreased rapidly during the initial passes and then approached a stable value. Local porosity in M15 decreased overall. Because adjacent loading lanes overlapped, two distinct reductions could occur within one complete cycle (Fig. 9c) as the M15 region was successively loaded by neighboring lanes. Overlapping compaction therefore

reduced locally undercompacted zones and improved uniformity.

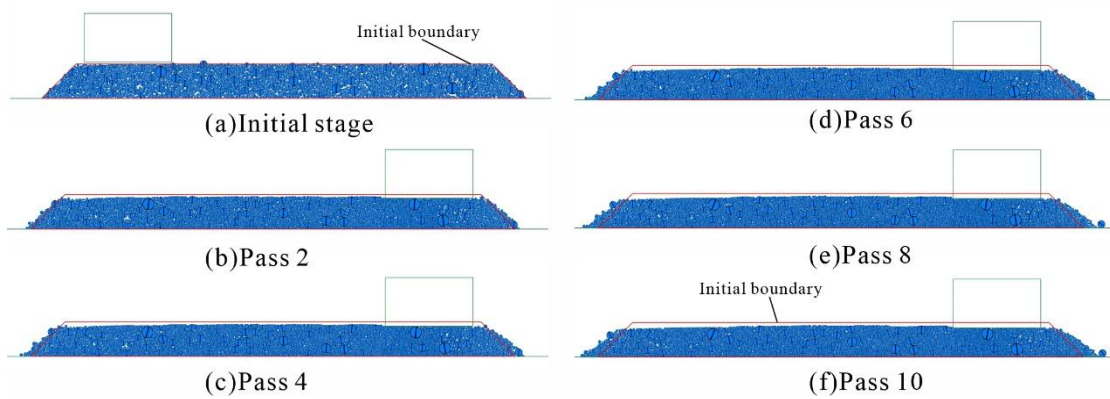


Fig. 8. Evolution of overall deformation during compaction in Case 2

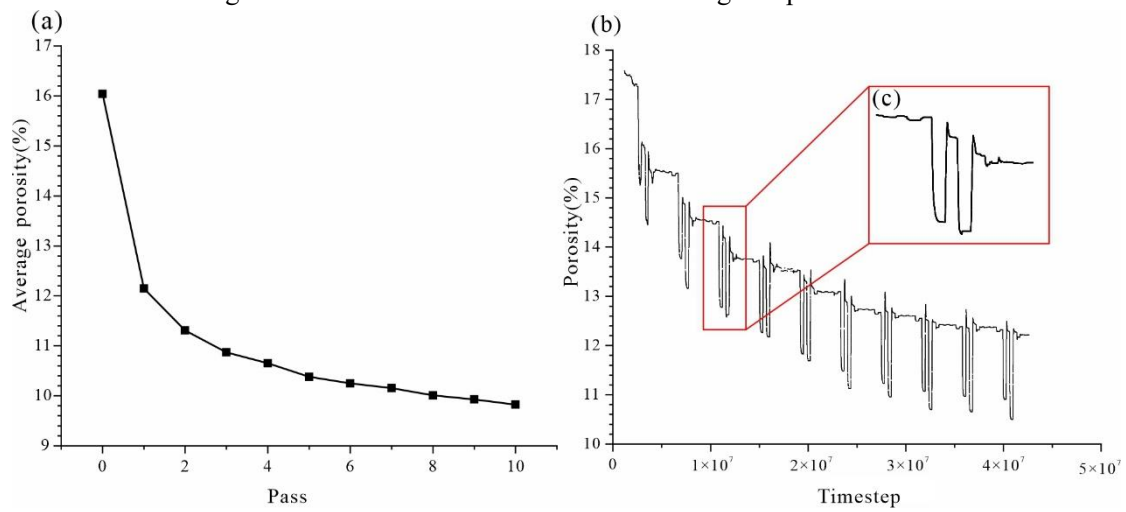


Fig. 9. Porosity evolution in Case 2: (a) mean porosity versus number of passes; (b) porosity history in measurement circle M15; and (c) local porosity changes during one compaction cycle

3.1.2 Particle kinematics

The free boundaries on both sides permitted pronounced horizontal migration and spatial redistribution during compaction. Fig. 10 shows the total particle displacement in Case 1. After compaction, the outermost particles on the left and right had moved to $x = -6.719$ and 6.955 m, respectively, beyond the initial boundaries at $x = \pm 6$ m. The larger displacements were concentrated near the free edges and surface, indicating that rolling drove particles toward the free surfaces in addition to producing vertical densification.

Fig. 11 further shows the horizontal particle-displacement field in Case 1. The larger horizontal displacements were concentrated at the lateral edges and in the surface layer, whereas particles in the

central and deeper zones moved relatively little and primarily underwent local rearrangement. This spatial contrast demonstrates that a free boundary provides an additional deformation-release pathway.

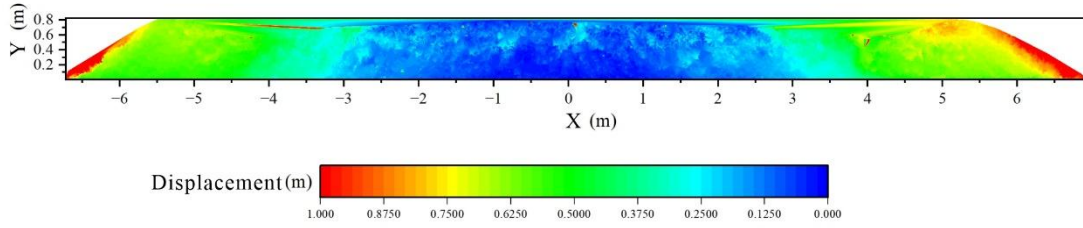


Fig. 10. Total particle-displacement field in Case 1

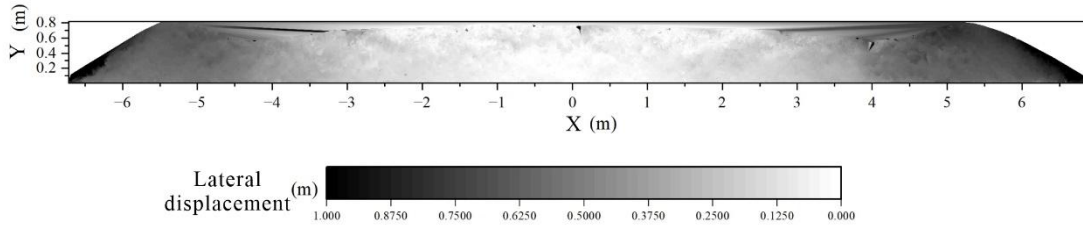


Fig. 11. Horizontal particle-displacement field in Case 1

Case 2 exhibited smaller overall displacements and less outward spreading. The outermost particles reached $x = -6.408$ and 6.482 m (Fig. 12), smaller extensions than those in Case 1. Fig. 13 shows that horizontal displacement was concentrated near the free boundaries and in local pore-adjustment zones; the broad surface migration observed in Case 1 did not develop. Thus, in addition to transverse rearrangement caused by interparticle extrusion, the longitudinal action generated by roller motion is an important driver of particle migration.

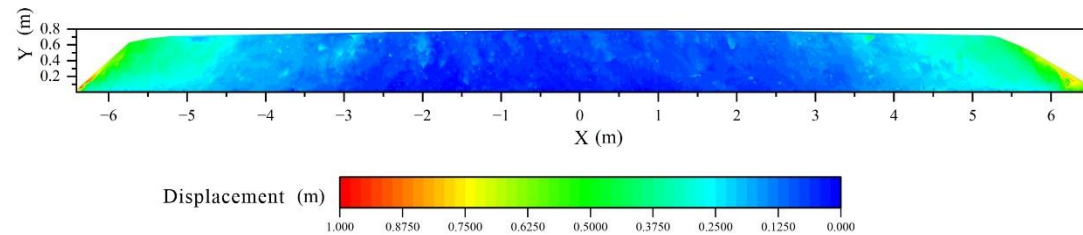


Fig. 12. Total particle-displacement field in Case 2

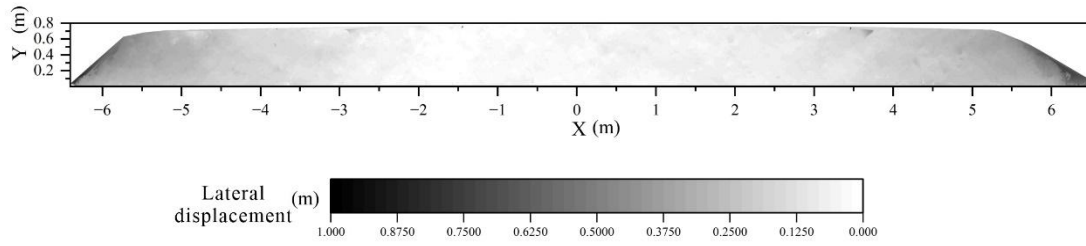


Fig. 13. Horizontal particle-displacement field in Case 2

Figs. 14 and 15 show the spatial distributions and pass-by-pass evolution of the surface settlement ratio in the two cases. The mean ratio increased with the number of passes in both models. At the end of compaction, the mean value was 17.06% in Case 1 and 11.46% in Case 2 (Figs. 14(a) and Fig. 15(a)). Together with the displacement fields, these results indicate that the larger settlement in Case 1 reflected not only vertical densification but also greater horizontal migration and boundary spreading.

Figs. 14(b) and Fig. 15(b) show the average surface settlement ratio at the corresponding positions for different monitoring circles. In both cases, settlement ratios were larger near the edges than in the central zone, demonstrating that migration amplified the apparent geometric settlement near free boundaries.

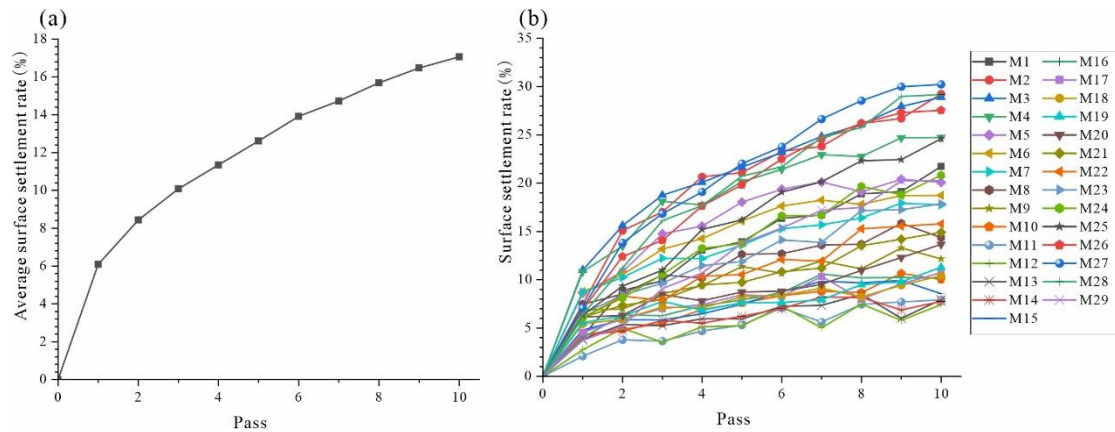


Fig. 14. Evolution of the surface settlement ratio in Case 1

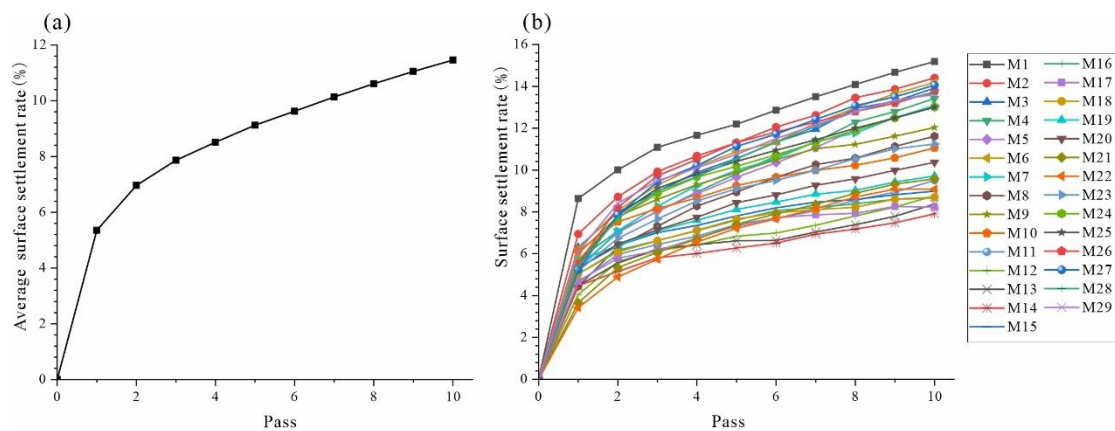


Fig. 15. Evolution of the surface settlement ratio in Case 2

Fig. 16 compares particle rotation after compaction. Rotation was more pronounced in Case 1 and was concentrated near the lateral edges and in the upper and middle portions of the fill, indicating that the tangential action of the moving roller promoted rolling and rearrangement. In Case 2, particles with large rotations were largely confined to the edges, while rotation in the central zone remained limited. Compaction in the transverse section was therefore dominated by vertical compression and local extrusion-induced rearrangement.

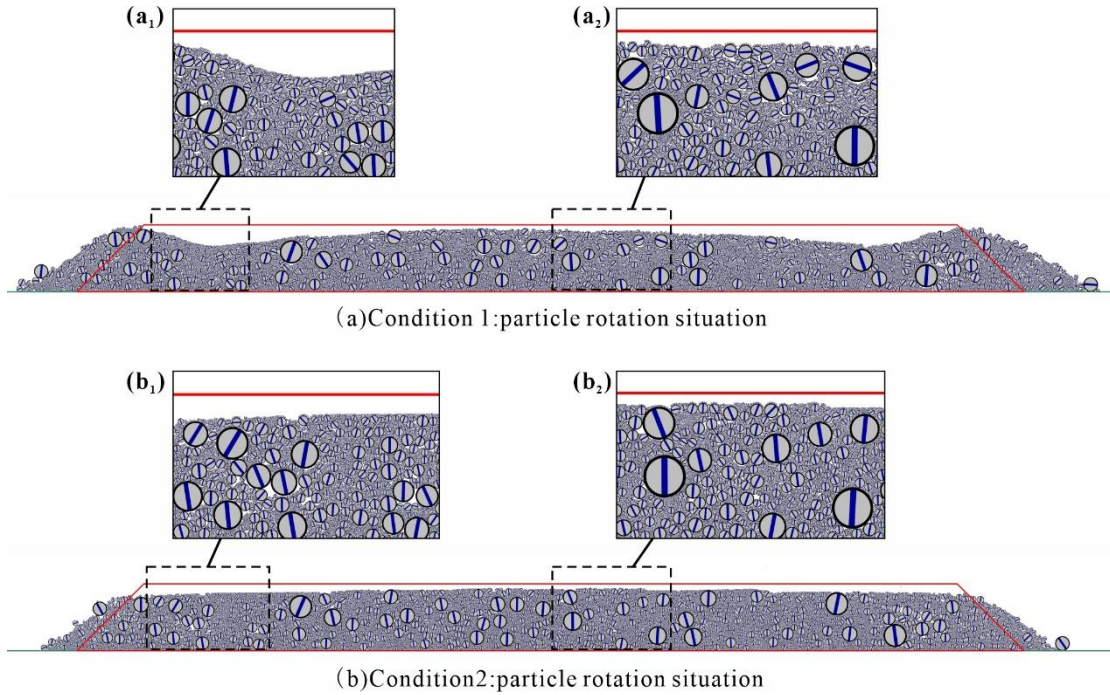


Fig. 16. Particle rotation after compaction: (a) Case 1 and (b) Case 2

3.1.3 Evolution of contact-force chains

Figs. 17 and 18 show the particle contact-force chains after 2, 4, 6, 8, and 10 passes in the two cases. Both models exhibited a marked separation between strong and weak chains. Force chains were comparatively continuous in the central zone but sparse near the two free boundaries. Without lateral confinement, edge particles more readily dissipated the applied load through translation and rotation, inhibiting the development of stable local load-bearing chains.

Contact forces were quantified after each selected pass (Table 5). In both cases, the mean force was substantially greater than the median. For example, after six passes in Case 1, the mean force was 91.49 N whereas the median was only 4.04 N; after ten passes in Case 2, the corresponding values were 74.81 and 4.53 N. Thus, most contacts carried relatively small forces, while a small population of highly loaded contacts formed the strong force-chain skeleton.

The proportions of high-force contacts further distinguish the load-bearing structures. Contacts carrying at least 1000 N accounted for approximately 1.16%–1.44% in Case 1 but only 0.71%–0.97%

in Case 2. The corresponding proportions for forces of at least 3000 N were approximately 0.044%–0.075% and 0.014%–0.041%, respectively. Although uncommon, these highly loaded contacts carried a substantial share of the local load and formed the backbone of the strong force-chain network.

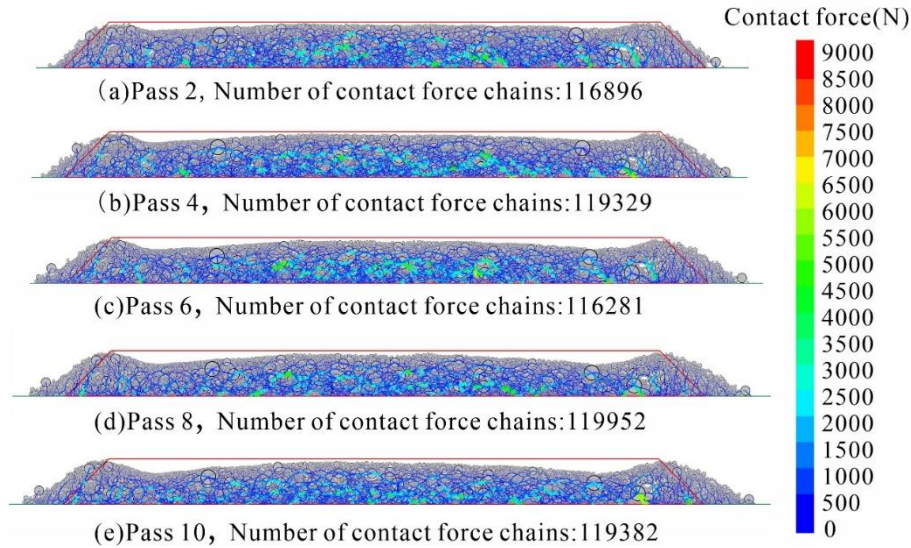


Fig. 17. Contact-force chains after different numbers of passes in Case 1

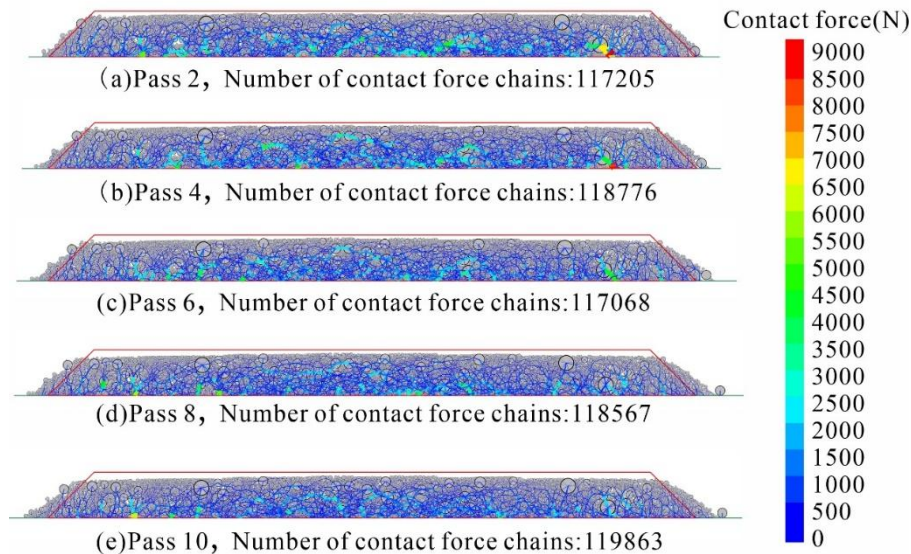


Fig. 18. Contact-force chains after different numbers of passes in Case 2

In Case 1, the mean contact force increased from 80.19 N after two passes to 91.49 N after six passes and then fluctuated between 81.53 and 89.74 N, indicating early strengthening followed by stabilization. The median increased from 3.60 N after two passes to 4.42 N after ten passes, showing a gradual rise in the overall contact level and progressive stabilization of the load-bearing skeleton.

In Case 2, the mean contact force remained within a narrow range of approximately 71.90–75.96 N and did not increase persistently. The proportions of contacts carrying more than 1000 and 3000 N generally decreased with additional passes. Continued pore filling and rearrangement therefore redistributed the load across a more stable and uniform contact network, reducing strongly localized force concentrations.

Table 5.
Contact-force statistics for the two simulation cases

Case	Passes	Number of contacts	Mean contact force (N)	Median (N)	P95 (N)	F $\geq$ 1000 N/%	F $\geq$ 3000 N/%
Case 1	2	116896	80.19	3.60	419.94	1.173	0.053
Case 1	4	119329	86.83	3.68	456.93	1.373	0.064
Case 1	6	116281	91.49	4.04	471.34	1.439	0.075
Case 1	8	119952	81.53	3.93	425.12	1.156	0.044
Case 1	10	119382	89.74	4.42	477.12	1.442	0.046
Case 2	2	117205	75.96	3.51	402.02	0.974	0.041
Case 2	4	118776	74.49	3.62	383.07	0.929	0.031
Case 2	6	117068	71.90	3.65	381.91	0.774	0.028
Case 2	8	118567	74.97	4.10	392.17	0.756	0.027
Case 2	10	119863	74.81	4.53	384.03	0.709	0.014

The displacement and velocity results provide a consistent interpretation. Strong confinement by surrounding particles limited movement in the central zone and converted a larger fraction of the applied load into interparticle contact forces, thereby sustaining continuous load-bearing chains. Near a free boundary, greater lateral freedom allowed part of the load to be released through outward migration, resulting in less continuous force chains and lower local load-bearing capacity. Thus, despite exhibiting large surface settlement, the edge zone did not develop a commensurately stronger internal skeleton. This observation corroborates the larger edge settlement but limited porosity reduction reported above and indicates that much of the geometric change near a free boundary results from lateral migration rather than proportional internal densification.

3.1.4 Transient velocity-field response

To characterize transient particle motion during compaction, velocity fields were examined in both cases. Figs. 19 and 20 show the instantaneous velocity distributions when loading was applied near the left edge, at the center, and near the right edge.

Both cases exhibited a clear edge effect. When the load approached a free boundary, edge-particle velocities increased and the velocity vectors generally pointed toward the free surface. When loading was applied at the model center, both the extent and magnitude of particle motion decreased. A free boundary therefore acts as a low-confinement deformation pathway through which edge particles can release applied loading by horizontal migration.

In Case 1, particle velocities contained a pronounced longitudinal component in addition to the vertical component, reflecting the pushing action of the moving roller on surface particles. The horizontal component was weaker in Case 2, where motion was dominated by vertical compression and lateral extrusion near the free boundaries. These differences are consistent with the displacement and rotation fields.

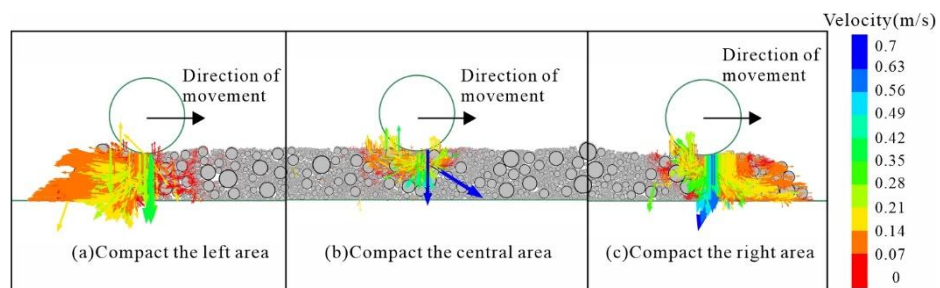


Fig. 19. Instantaneous particle-velocity fields at different loading positions in Case 1: (a) Compact the left area; (b) Compact the central area; (c) Compact the right area

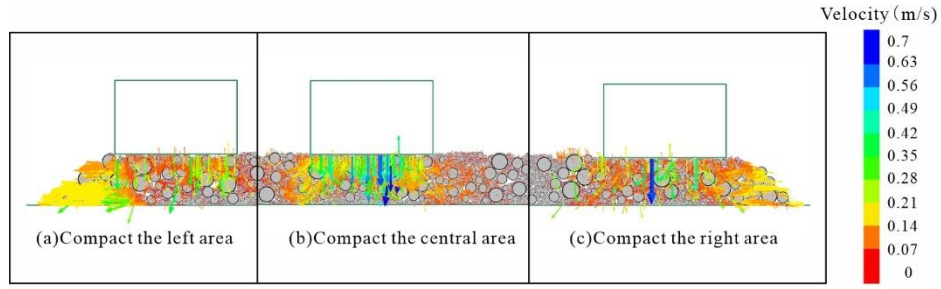


Fig. 20. Instantaneous particle-velocity fields at different loading positions in Case 2: (a) Compact the left area; (b) Compact the central area; (c) Compact the right area

3.2 Local compaction response and settlement–porosity mismatch near free boundaries

3.2.1 Distance from the free boundary and evaluation metrics

To quantify the influence of a free boundary on local compaction, the horizontal distance from the center of each porosity measurement circle to the nearest free boundary was adopted as the spatial variable d . The 29 circles were arranged approximately symmetrically about the model center, with distances ranging from 0.53 to 5.15 m. Because random particle packing and isolated coarse particles can cause local fluctuations, values from the two circles located at the same distance on opposite sides were averaged to represent the local compaction state at that distance.

For measurement region i , the two-dimensional porosities before and after compaction are denoted by $n_{0,i}$ and n_i , respectively. The local porosity reduction is defined as:

$$\Delta n_i = n_{0,i} - n_i \quad (6)$$

A larger Δn_i indicates a greater reduction in internal void space and therefore stronger local densification.

Because surface settlement can arise from pore compression, lateral migration, and changes in surface geometry, an equivalent local compression ratio was derived from the porosity change. Assuming that the solid particle area within a measurement region remains approximately constant, that cross-boundary migration is negligible, and that deformation is predominantly vertical, the pre- and post-compaction porosities yield:

$$s'_i = \frac{n_{0,i} - n_i}{1 - n_i} \quad (7)$$

where s'_i is the equivalent settlement ratio derived from porosity change and s_i is the surface settlement ratio measured at a fixed spatial coordinate. The two should agree when deformation is dominated by internal densification. Pronounced lateral migration or surface-profile reconstruction may instead produce $s_i > s'_i$.

To quantify the correspondence between surface settlement and pore compression, the compaction correspondence coefficient R_c is defined as:

$$R_c = \frac{s'}{s} \quad (8)$$

When R_c approaches 1, surface settlement corresponds closely to pore compression. A value of R_c well below unity indicates that the observed settlement exceeds the equivalent compression attributable to porosity reduction and therefore contains a substantial non-densification component.

3.2.2 Settlement–porosity mismatch in the travel-direction section

Case 1 exhibited a particularly pronounced settlement–porosity mismatch. In addition to vertical loading, the moving circular roller exerted a forward horizontal thrust, causing substantial horizontal migration during densification and amplifying surface-geometry changes near the free boundaries.

At distances of 0.86 and 1.19 m from the free boundary, the mean surface settlement ratios reached 29.21% and 29.56%, respectively, far above the approximately 14% values at the corresponding locations in Case 2. The associated porosity reductions were only 0.0368 and 0.0570 and did not increase in proportion to settlement. The correspondence coefficients were 0.142 and 0.214, indicating that pore compression explained only a small fraction of the observed settlement.

With increasing distance from the free boundary, the surface settlement ratio in Case 1 generally decreased and stabilized at approximately 9%–12% in the interior. Meanwhile, R_c generally increased,

indicating a progressive reduction in boundary-induced settlement amplification. Unlike Case 2, however, R_c remained well below unity even near the model center. The mismatch in the travel-direction section therefore cannot be attributed solely to the free boundary; the forward pushing action of the roller also altered particle positions and surface geometry.

Zone-averaged statistics provide further evidence. In Case 1, the mean surface settlement ratio in the near-edge zone was approximately 25.65%, 2.7 times the 9.54% value in the interior. By contrast, the mean porosity reductions were 0.0475 and 0.0441, respectively, and differed only slightly. The greatly amplified edge settlement in the travel-direction section thus arose primarily from horizontal particle migration and geometric spreading rather than stronger internal densification.

Taken together, the two cases show that a free boundary weakens lateral confinement and produces varying degrees of settlement–porosity mismatch. The mismatch was substantially greater in Case 1 because of the additional horizontal thrust. This interpretation is consistent with the displacement, velocity, and contact-force fields: the boundary zones showed larger particle displacements and transient velocities but comparatively limited pore compression and less stable contact networks. Large settlement near an edge therefore cannot be equated directly with a high degree of compaction, and both boundary conditions and lateral particle migration must be considered when surface deformation is used to assess rockfill compaction quality.

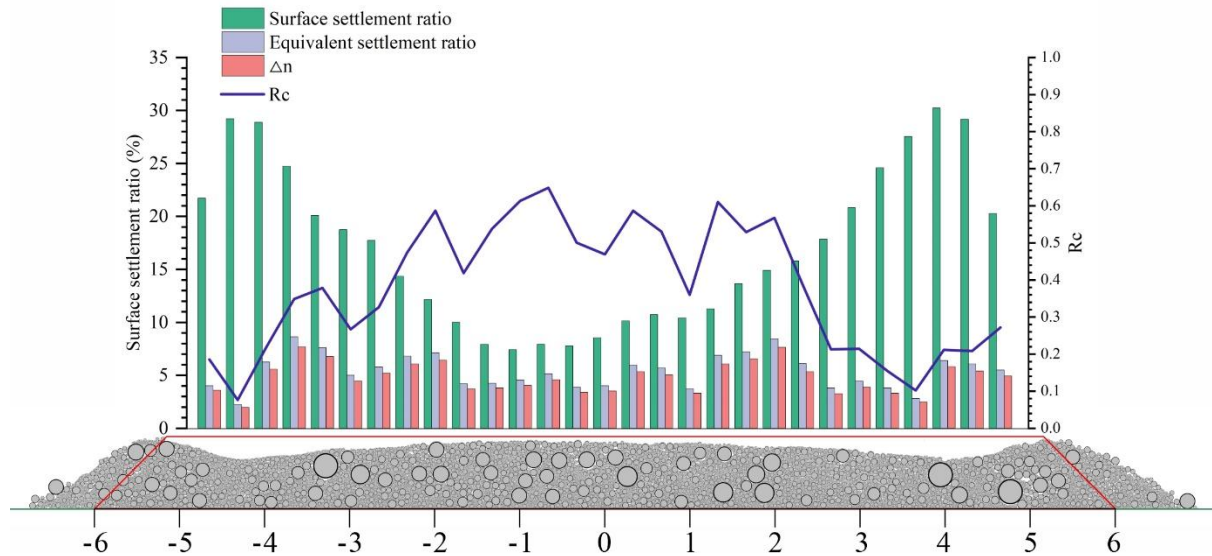


Fig. 21. Spatial distributions of the measured surface settlement ratio and porosity-derived equivalent compression ratio in Case 1

3.2.3 Boundary response in the transverse section

Fig. 22 shows the surface settlement ratio, porosity reduction, and settlement–compaction correspondence coefficient at different distances from the free boundary in Case 2. The measured settlement ratio decreased markedly with distance, confirming a strong influence of the free boundary on surface deformation. At distances of 0.53, 0.86, and 1.19 m, the mean ratios were 14.39%, 14.05%, and 13.98%, respectively; at 4.49–4.82 m, they decreased to approximately 8.3%.

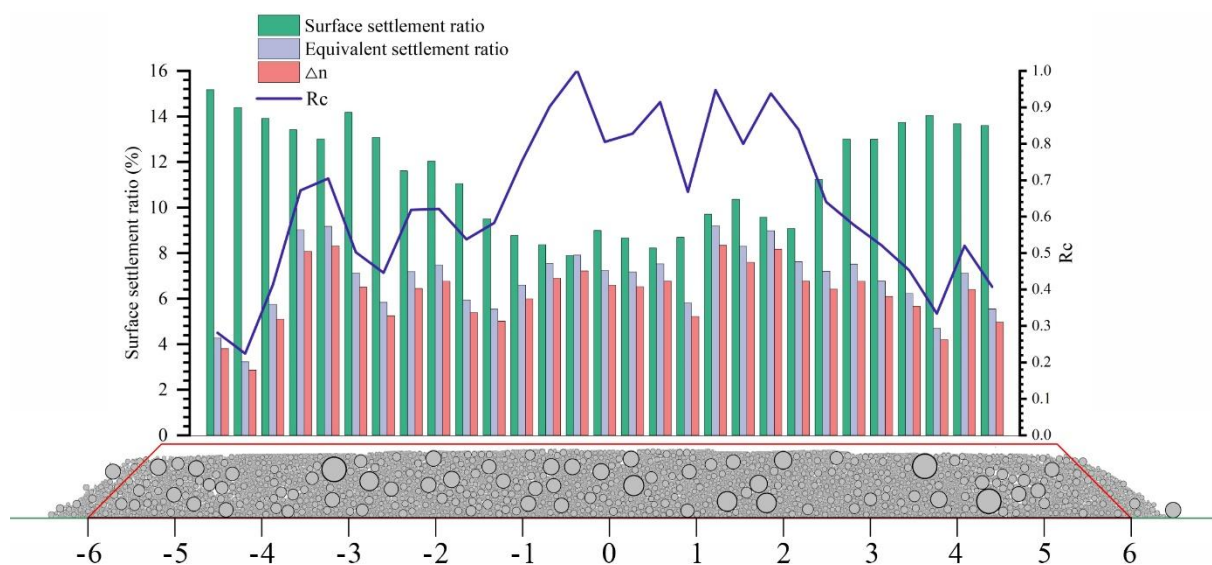


Fig. 22. Spatial distributions of the measured surface settlement ratio and porosity-derived

equivalent compression ratio in Case 2

Porosity reduction did not exhibit the same spatial pattern. At 0.53 m from the boundary, the mean porosity reduction was only 0.0439, corresponding to an equivalent compression ratio of 4.91%, substantially below the measured settlement ratio of 14.39%. The associated R_c was only 0.341. Thus, the pronounced surface-elevation loss near the free boundary was not accompanied by a commensurate reduction in internal void space.

The correspondence between settlement and densification generally improved with increasing distance from the boundary. At $d = 4.49$ m and 4.82 m, R_c increased to 0.908 and 0.911, respectively. Away from the free boundary, lateral particle motion was constrained by the surrounding material, and surface settlement became increasingly dominated by internal rearrangement and pore compression.

For regional comparison, the measurement locations were divided into near-edge, transition, and interior zones according to their distance from the free boundary. The mean settlement ratio in the near-edge zone was 13.80%, compared with 9.11% in the interior; however, the corresponding porosity reduction was 0.0555, lower than the interior value of 0.0652. The coefficient R_c increased from 0.45 near the edge to 0.80 in the interior. The free boundary therefore amplified surface settlement in the transverse section, and settlement alone did not fully represent the actual degree of densification.

3.3 Particle-scale mechanism and applicability of the free-boundary effect

The mechanism underlying the free-boundary effect can be synthesized from the macroscopic deformation, porosity, particle displacement and rotation, velocity, and contact-force results (Zhai et al., 2019).

First, the free boundary is the prerequisite for the edge effect. In the central zone, confinement by surrounding particles creates a relatively enclosed and stable load-transfer environment. Motion is dominated by vertical densification and local rearrangement, and surface settlement, porosity reduction,

and contact-force strengthening correspond reasonably well. At an edge, the free surface allows particles to move outward as well as downward under roller loading. This contrast in confinement produces fundamentally different compaction responses in the edge and central zones.

Second, lateral particle migration is the most direct kinematic manifestation of the edge effect. In both orthogonal sections, edge particles exhibited larger displacement and velocity than central particles, and their velocity vectors generally pointed toward the free surface. Edge particles therefore moved laterally more readily under external loading. This effect was particularly strong in Case 1, where the moving roller imposed an additional horizontal shear thrust and pushed edge particles beyond the initial boundary while compressing them vertically. The resulting settlement amplification was therefore attributable not only to pore compression but also, to a substantial extent, to lateral migration and geometric spreading.

Third, strengthening of the internal load-bearing structure was substantially weaker at the edges. Although both assemblies developed stronger force networks with additional passes, force-chain density and intensity remained greater in the central zone. Constrained central particles developed stronger interlocking and more concentrated stress-transfer paths. Near a free boundary, stress was released and redistributed through outward motion, preventing development of a load-bearing structure commensurate with the observed settlement. In other words, large geometric deformation at the edge was not accompanied by proportional strengthening of the particle skeleton or pore compression.

The porosity results support the same interpretation. Despite much larger surface settlement near the edges, local porosity reduction did not increase proportionally. The additional settlement therefore represented particle redistribution and surface-profile adjustment rather than an equal amount of internal densification. This boundary-induced amplification reduces the ability of surface settlement to serve as

a direct proxy for true compaction.

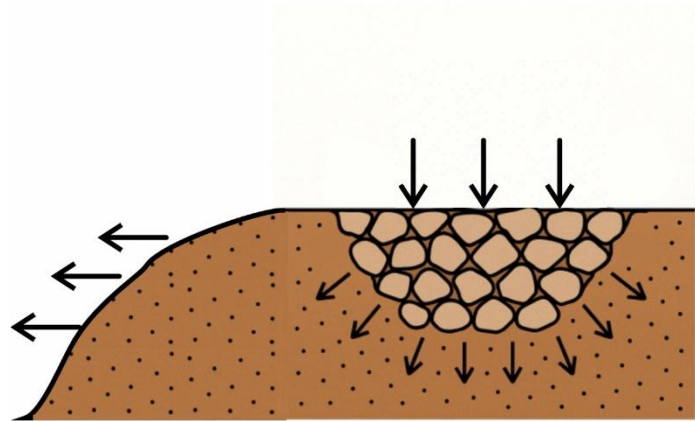


Fig. 23. Particle-scale mechanism of the free-boundary effect

The free-boundary effect can thus be summarized as follows: under roller loading, edge particles have additional pathways for horizontal migration and stress release (Fig. 23.). Outward particle movement and profile reconstruction amplify the settlement measured at fixed spatial coordinates, whereas pore compression and strengthening of the load-bearing skeleton do not increase proportionally. In zones with pronounced free boundaries, compaction assessments based solely on surface settlement or geometric volume change may therefore overestimate actual densification. Internal density-related metrics or an explicit boundary correction should be incorporated.

4. Conclusions

PFC2D simulations were used to decompose the three-dimensional roller-compaction process into two orthogonal sections parallel and perpendicular to roller travel. The analysis focused on particle migration near free boundaries and its influence on the relationship between surface settlement and porosity. The main conclusions are as follows:

(1) A PFC2D model without rigid lateral confinement was established using the field particle-size distribution and construction parameters. A rolling-resistance linear contact model represented particle interaction. Surface elevations at fixed coordinate balls and 29 measurement circles provided spatially

consistent measures of surface settlement ratio and two-dimensional local porosity, respectively.

(2) A rigid circular wall in the travel-direction section reproduced the coupled vertical loading and longitudinal action of the moving roller. Lane-based overlapping loading by a rectangular platen in the transverse section represented vertical compression and lateral extrusion across the drum width. The two models separated the dominant directional responses of roller compaction.

(3) Mean porosity decreased with the number of passes in both cases, with rapid initial densification followed by gradual stabilization. Because the horizontal action of rolling was superimposed in Case 1, particle displacement and rotation were more pronounced, and the final mean surface settlement ratio reached 17.06%, compared with 11.46% in Case 2.

(4) The displacement, rotation, velocity, and contact-force fields consistently showed that particles near a free boundary migrated more readily toward the free surface, attained higher transient velocities, and formed less stable load-bearing chains. Stronger confinement in the central zone limited particle motion to local rearrangement and vertical densification. Consequently, surface settlement increased markedly near the edges without a proportional porosity reduction, producing a settlement–porosity mismatch. Settlement near a free boundary therefore contains a substantial migration-induced component, and using settlement alone may overestimate local compaction.

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Competing Interests

The authors declare that they have no known competing financial interests or personal

relationships that could have appeared to influence the work reported in this paper.

Author Contributions

G.L. and J.Z. conceived and designed the study. G.L., J.C. and B.Y. prepared and analyzed the data. G.L., B.W. and B.Y. performed the numerical simulations and prepared the figures. J.C., B.W. and W.L. contributed to the analysis and discussions. J.Z. and W.L. supervised the research and revised the manuscript. G.L. and B.Y. wrote the original draft. All authors reviewed and approved the final manuscript.

Data availability

The datasets used and analyzed during the current study are available from the corresponding author upon reasonable request.

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