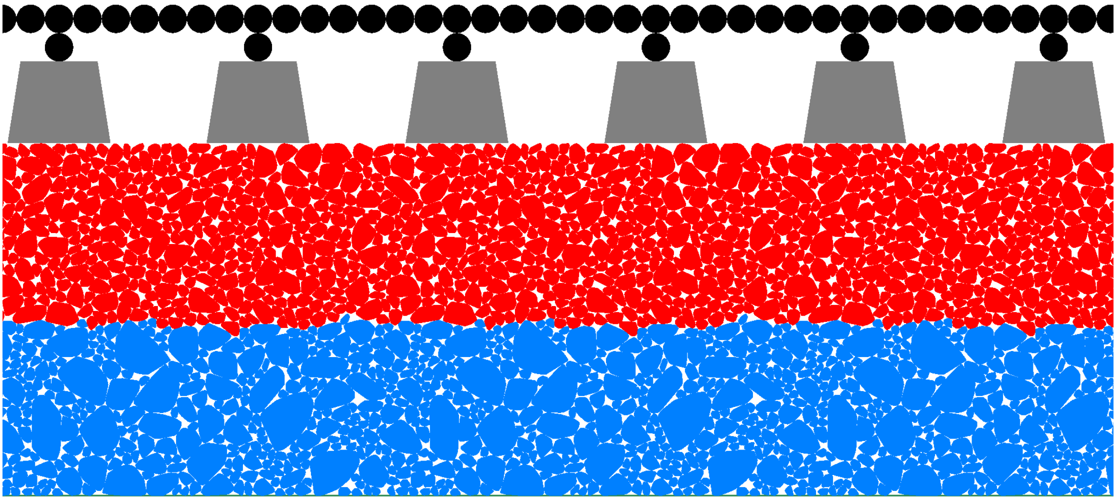
KTH ROYAL INSTITUTE
OF TECHNOLOGY

Licentiate Thesis in Civil and Architectural Engineering

Discrete element technique for modeling high-speed railway tracks

ALIREZA AHMADI



Stockholm, Sweden 2023

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Academic Dissertation which, with due permission of the KTH Royal Institute of Technology, is submitted for public defence for the Degree of Licentiate of Engineering on Tuesday the 30th May 2023 at 10:00 AM in Room B3, Brinellvägen 23, Stockholm.

Licentiate Thesis in Civil and Architectural Engineering
KTH Royal Institute of Technology
Stockholm, Sweden 2023

TRITA-ABE-DLT-2320
ISBN 978-91-8040-565-2

Printed by: Universitetsservice US-AB, Sweden 2023

Abstract

The Discrete element method (DEM) is a methodology to investigate the interactions among granular materials. It analyzes the behavior of particulate environments by solving force-displacement equations that adhere to Newton's second law of motion. Despite its usefulness, the DEM is not without limitations, and researchers are still facing certain challenges that restrict them from performing detailed analyses of granular materials. This study addresses two issues in DEM modeling of granular materials in railway embankments. Firstly, the long computational time required by the DEM for modeling fine angular particles in granular materials is addressed by exploring the effects of particle scaling on the shear behavior of granular material. This study investigates the impact of particle size distribution, particle angularity, and the amount of scaling on the accuracy and computational efficiency of DEM. Secondly, the limitations of DEM in including the continuous rail beam structure in the track are addressed by verifying a DEM model against physical measurements of a full-scale ballasted track and investigating the influence of including the rail beam structure on high-speed railway ballasted tracks. The results show that the use of particle scaling in the first study significantly improves the computational efficiency of the DEM while maintaining accuracy, and this method is used in the second study to investigate the influence of the rail beam structure on the behavior of railway tracks.

Keywords: Polygonal particles, Direct shear test, Particle scaling, Ballasted track, DEM

Sammanfattning

Diskreta elementmetoden (DEM) är en effektiv metod för att undersöka interaktioner i granulära material. Metoden analyserar samverkan mellan partiklar genom att lösa kraft-deformationsekvationer som följer Newtons andra lag. Trots dess användbarhet har DEM vissa begränsningar och forskare stöter fortfarande på vissa utmaningar som hindrar dem från att genomföra detaljerade analyser av granulära material. Denna studie tar upp två frågeställningar vid DEM-modellering av granulära material i järnvägsbankar. För det första behandlas den långa beräkningstiden som krävs för att modellera granulära material genom att utforska effekterna av partikelskalning på skjuvbeteendet. Studien undersöker effekten av partikelstorleksfördelning och spetsighet på noggrannheten och beräkningseffektiviteten. För det andra behandlas begränsningarna hos DEM när det gäller att inkludera den kontinuerliga rälsstrukturen i spåret genom att verifiera en DEM-modell mot fysiska mätningar av ett ballasterat spår i full skala och undersöka inverkan av att inkludera rälsstrukturen. Resultaten i den första studien visar att tillämpningen av partikelskalning avsevärt förbättrar beräkningseffektiviteten samtidigt som noggrannheten bibehålls. Partikelskalning används i den andra studien för att undersöka inverkan av rälsstrukturen på beteendet hos järnvägsspår.

Nyckelord: Polygonala partiklar, direkt skjuvförsök, partikelskalning, ballastspår, DEM

Acknowledgements

First and foremost, I would like to express my sincere gratitude to my supervisors, Professor Stefan Larsson and Dr. Carl Wersäll, for their guidance, support, and encouragement throughout my research journey. Their insights, knowledge, and expertise have been invaluable in shaping my work and in helping me navigate the challenges that come with conducting a research project of this magnitude.

I also gratefully acknowledge the Swedish Transport Administration (Trafikverket) for their financial support of this research. Moreover, I appreciate all the members in the reference group meetings, especially Bo Johansson, Nils Ryden, Peter Zackrisson, and Johan Jonsson, and Andréas Andersson.

I would also like to acknowledge fruitful discussions and helps of Sacha Emam (Itasca), Emil Aggestam (Trafikverket), Mohammad Javad Mohajeri (Delft University), Dingena Schott (Delft University), Yuntian Feng (Swansea University), Martin Li (Trafikverket), Kenneth Viking (Trafikverket), Martin Schilke (Trafikverket), Magnus Ekh (Chalmers University), Jelke Dijkstra (Chalmers University), Jens Nielsen (Chalmers University), Karl Norberg (Sweco) and Kourosh Nasrollahi (Chalmers University).

I am also indebted to all my colleagues and friends, especially Mohammad Mohammadi and Amir Shabani, who have been with me every step of the way. Their unwavering support, encouragement, and camaraderie have been a constant source of inspiration and motivation, and have helped me maintain my focus and momentum throughout this journey.

Finally, I would like to express my heartfelt gratitude to my father, mother and brother. Their love, support, and encouragement have sustained me throughout my life, and have been a constant reminder of the importance of love, perseverance, and dedication.

Thank you all for your invaluable contributions to this project. I could not have done it without you.

Alireza Ahmadi,
Stockholm, May 2023

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List of Acronyms

T	Time-step of DEM, [s]
D_{max}	Largest particle size, [mm]
m	Mass of particle, [kg]
PSR	Particle size ratio, -
D_{min}	Smallest particle size, [mm]
K	Stiffness in the mass-spring system, [N/m]
R	Particle radius, [m]
k_{pn}	Parallel bond normal contact stiffness, [N/m]
k_{ps}	Parallel bond shear contact stiffness, [N/m]
E	Elastic modulus of rail, [Pa]
G	Shear modulus of rail, [Pa]
λ	Parallel bond radius multiplier, -
K	Normal to shear contact stiffness ratio , -

List of Definitions

DEM	Discrete Element Modeling
FEM	Finite Element Method
Particle Scalping	Scaling only fine range of particles

Chapter 1

Introduction

1.1 Background

In railway engineering, a transition zone is an area where the track structure changes from one type to another. It is a critical part of the railway track system, where the railway embankment transitions into a bridge, tunnel, or other type of structure. Transition zones can also occur where there is a change in the track alignment or slope.

The purpose of the transition zone is to ensure smooth and safe operation of the railway system by providing a gradual transition from one track structure to another. This is important to prevent derailments, excessive wear and tear on the track and rolling stock, and to ensure passenger comfort.

1.2 Research Aims

Sustainable development is a concept that has become increasingly important in the construction industry, as societies recognize the need for environmentally friendly and cost-effective structures and transport systems. The problem of settlements and stiffness variations in transition zones between embankments and stiff structures is a significant challenge in achieving sustainable construction. Sustainable structures require a long-term perspective and must be designed to minimize maintenance operations, reduce the cost of repairs, and minimize the impact on the environment.

The construction of high-speed railways presents a particular challenge. Therefore, great demands must be placed on the design of transition zones to ensure long-term sustainability. As such, it is necessary to study the mechanisms that govern accelerated settlements in transition zones and develop methods to prevent them. This will not only contribute to sustainable construction practices but also help to reduce the cost of repairs and maintenance.

One method of studying these mechanisms is through the use of simulation by discrete element modeling (DEM). DEM allows for the behavior of embankment material and sub-ballast to be studied at particle level, taking degradation and rearrangement into account. By understanding the mechanisms that cause settlements in transition zones, it will be possible to optimize construction methods in terms of cost and climate impact.

The transition zone between embankment and bridge is a critical area for study, as settlements are greater in this zone than in the rest of the embankment. This is due to a combination of mechanisms, including reduced friction at the boundary layer between embankment and bridge, dynamic stress concentrations due to a rapid change in stiffness, and the influence of horizontal bridge movements. An understanding of these mechanisms will enable cost-effective design and maintenance measures, leading to sustainable constructions that contribute to a sustainable society.

1.3 Research Objectives

This thesis presents the first phase of a research project on discrete element modeling (DEM) of transition zones between railway embankments and bridges. The initial phase involves calibrating the numerical modeling procedure of the discrete element method, which includes determining the shape, material properties, and contact models of the particles. The particle size distribution is modified using a particle scaling approach, and a ballasted railway track is constructed to study the structural elements using the discrete element method. In the second phase of the research, the model will be expanded to include a slab-track railway, with a breakage mechanism added for granular material. The transition zone will also be included in the model to study the long-term differential settlement of high-speed railway transition zones. Figure 1.1 displays steps for this research.

1.4 Research limitations

There are limitations concerning computational time, particle size and structural elements in DEM. Details regarding significant limitations and simplifications, which are necessary for the modeling and the scope of the study, are stated and discussed continuously in this thesis and the papers.

1.5 Research Contributions

This study makes two important contributions. Firstly, it improves the discrete element methodology for numerical modeling in two ways. The first improvement involves investigating particle scaling and using polygonal shapes for granular material. This advancement can facilitate faster and more accurate modeling in DEM, making the models more realistic. The second improvement is exploring the impact of incorporating structural elements into railway models, which enhances the approach to railway modeling using DEM. Secondly, the study demonstrates that by using more detailed and realistic models in DEM, practical results can be obtained from numerical research. This can be helpful in solving real-world industry problems.

1.6 Outline of the Thesis

This thesis is organized in seven chapters as follows:

- Chapter 1 discusses the introduction and the motivation of the research project.
- Chapter 2 discusses the literature review of discrete element method and modeling the railway tracks.
- Chapter 3 introduces the methodology that is chosen for this research.

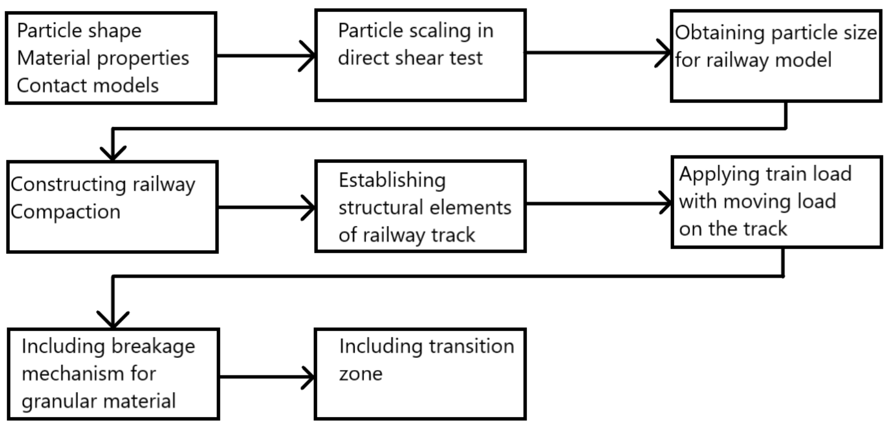


Figure 1.1: Schematic diagram of research project

- Chapter 4 discusses the limitations of this research.
- Chapter 5 presents the method of particle scaling to improve the computational speed of discrete element method.
- Chapter 6 discusses the challenges and methods of modeling railway tracks in discrete element method.
- Chapter 7 summaries of the two papers of this research.
- Chapter 8 presents the conclusion and the future work of the second phase of this research.

Chapter 2

Literature review

This chapter includes a literature review that is divided into two main sections. The first section provides a general overview of the discrete element method (DEM), highlighting its strengths and limitations. The literature review covers the principles and assumptions of DEM, as well as its applications in different fields. Additionally, the section discusses the challenges associated with using DEM, including computational time, particle size distribution, and the choice of contact model. Furthermore, the section explores the advancements that have been made to address these challenges, such as particle scaling and parallel computing.

The second section of the literature review focuses on the application of DEM in modeling high-speed railway tracks. This section covers the unique features of railway tracks that make them challenging to model with DEM. It also discusses the available techniques for incorporating the rail structure and the granular layers in DEM models. Additionally, the section presents the advantages and limitations of DEM in railway track modeling and explores the recent research on this topic.

2.1 Discrete element method

DEM is a numerical simulation technique used to model the interaction between discrete particles. The interaction between particles is resolved using Newton's second law of motion in terms of force-displacement, which was first introduced by Cundall and Strack (1979).

DEM is versatile and can be applied to analyze both rounded and angular particles under various loading conditions. It has become an efficient alternative to experimental and field studies for analyzing the behavior of granular materials.

This is because it can capture both microscopic and macroscopic responses of granular media, making it a more cost-effective and controllable option compared to field tests, which require expensive large-scale instruments (Coetzee, 2017; O'Sullivan, 2011).

Moreover, DEM is capable of providing precise information about particle interactions that is not possible with laboratory tests. This is because laboratory tests only provide limited information on the macroscopic behavior of granular materials due to the complexity of the system. In contrast, DEM simulations can provide detailed information about the motion and interaction of individual particles, allowing researchers to study the behavior of granular materials at a microscopic level (O'Sullivan, 2011).

Compared to other numerical methods like the finite element method (FEM), DEM has several advantages. It can simulate the contact force distribution, particle rearrangement, particle shape and size effect, and particle breakage, allowing it to capture and visualize the microscopic behavior of granular material. On the other hand, FEM models the entire system as a continuum layer and cannot consider the non-uniformity of contact force distribution and particle deformations throughout the granular assembly, as discussed by O'Sullivan (2011).

2.1.1 Application of DEM in industrial problems

In recent years, DEM has been increasingly used to model industrial problems, particularly those related to granular media. One such application is the modeling of railway ballast, sub-ballast, and embankment materials, which typically contain a wide range of particle sizes and shapes. However, the main challenge in using DEM to model such materials is the long computational time required, which has been discussed in previous studies (Alabbasi and Hussein, 2021; Roessler and Katterfeld, 2016). This is because DEM solves the equations of motion for all particles in small time-steps, and more particles result in longer computational times. As a result, most DEM simulations typically involve only a few thousand particles and cycles, as seen in studies by de Frias Lopez et al. (2021); Indraratna et al. (2020); Jing et al. (2020); Guo et al. (2020b); Zhao and Chen (2020); Feng et al. (2019); Bian et al. (2019); de Frias Lopez et al. (2019), and Liu et al. (2019). Despite this limitation, DEM offers insightful results on the behavior of granular media, particularly in comparison to expensive and less controllable field tests or less realistic continuum-based numerical methods like the finite element method (FEM), which cannot capture the microscopic behavior of granular materials as effectively as DEM.

2.1.2 Importance of particle shape

By simplifying the particle shape, the computational cost is reduced, allowing for larger-scale simulations with more particles (e.g., (de Frias Lopez et al., 2021; Zeng et al., 2020; Jing et al., 2019; Li and McDowell, 2018; Suhr et al., 2018; Jiang et al., 2018; Zhang et al., 2017; Khatibi et al., 2017; Zhang et al., 2016; Ngo et al., 2016; Vizcarra et al., 2016; McDowell and Li, 2016; Wang et al., 2015; Chen et al., 2015, 2014). However, it is important to note that the choice of particle shape can have a significant impact on the accuracy of the simulation results. Some studies have shown that using spherical particles can lead to wrong estimations of the material strength and stiffness compared to using more realistic, angular particle shapes (Seyyedan et al., 2021; Bian et al., 2019; Ouhbi et al., 2016). Therefore, it is necessary to carefully consider the trade-off between computational efficiency and accuracy when choosing particle shapes for DEM simulations. Rounded particles have a major drawback of not producing sufficient interlocking among particles due to their ability to rotate freely (Alabbasi and Hussein, 2021; Guo et al., 2020a; Nie et al., 2020; Coetzee, 2020; Zhou et al., 2020; Zhang et al., 2017). As a result, researchers have tried to simulate the angularity of particles by adding rolling friction to the contact properties of spherical particles. However, this approach has not always been effective because rolling friction resists particle rotation, while particle angularity can either encourage or resist particle rotation (Coetzee, 2017; Sinnott and Cleary, 2016; Wensrich et al., 2014; Wensrich and Katterfeld, 2012; Ai et al., 2011). Some researchers have used sphero-polyhedrons and sphero-polygons to simulate real particle shapes, but these shapes may be computationally expensive for large-scale industrial projects dealing with millions of particles (Jiang et al., 2020, 2019; Ji et al., 2015; Alonso-Marroquin, 2008). It is important to note that the effect of real particle shapes on industrial DEM problems needs more attention because it strongly affects the results (Govender, 2021; Windows-Yule et al., 2016; Lu et al., 2015; Eliáš, 2014).

2.1.3 Particle scaling

Several studies have investigated particle scaling as a solution to the aforementioned challenges. Particle scaling is an innovative technique that could enhance the speed of calculations while also integrating more lifelike particle shapes into simulations. When the size of the particles is increased, the total number of particles in the model decreases. Additionally, the critical time-step is directly related to the particle diameter, implying that larger particles result in larger time-steps (Cundall and Strack, 1979). Up until now, various methods of particle scaling have been studied by researchers, including exact scaling which has been investigated in studies such as those conducted by Wang et al. (2022); Feng and Owen (2014) and Feng et al. (2009), coarse-graining which has been studied by researchers such as Cerfontaine et al. (2021); Mohajeri et al. (2020); Coetzee (2019); Lommen et al. (2019); Weinhart et al. (2016); Lee et al. (2012) and Bagherzadeh-Khalkhali and Mirghasemi (2009), density scaling which has been examined by researchers such as Yousefi and Ng (2017), and particle scalping or cut off which has been explored in studies such as those conducted by Roessler and Katterfeld (2018) and Roessler and Katterfeld (2016).

Each scaling method has its advantages and limitations. The main advantage of scaling is that it can reduce computation time while maintaining accuracy in the behavior and mechanism, as noted in studies by Thakur et al. (2016) and Ciantia et al. (2015). However, exact scaling (which involves scaling both the particles and geometry by the same factor) does not seem to result in significant computation time reduction, according to studies by Wang et al. (2022); Coetzee (2019) and Feng and Owen (2014). On the other hand, it is still unclear if the coarse-graining method (which involves scaling only the particles without scaling the geometry) is applicable for polygonal particles, as indicated by studies by Torres-Serra et al. (2021) and Govender (2021). Additionally, there are discrepancies between some studies on the effectiveness of the coarse-graining method, as pointed out by Lommen et al. (2019); Roessler and Katterfeld (2018) and Feng and Owen (2014). Density scaling, which involves increasing the particle mass, can lead to unrealistic results as noted by Tu and Andrade (2008) and Yousefi and Ng (2017). The impact of particle scalping, which only scales smaller particles, on granular material shear strength is still not well understood, as reported by Coetzee (2019); Roessler and Katterfeld (2016); Weinhart et al. (2016); Schott et al. (2015) and Le Pen et al. (2013).

Particle scaling faces a significant challenge in determining the appropriate scaling factor and conditions (Feng et al., 2009). Moreover, the effectiveness of scaling may vary depending on the specific case being studied. For example, Yousefi and Ng (2017) found that the mechanical behavior of a scaled model was different from that of an unscaled model. Furthermore, there is no guarantee that a scaled model will accurately represent the original model (Wang et al., 2022), and the influence of particle size and shape on scaling is not yet fully understood (Le Pen et al., 2013). Therefore, it is necessary to explore the scaling method for each individual system (Jiang et al., 2018).

2.2 Railway in discrete element method

It is a difficult task to model the rail beam and other structural elements of railway tracks using the DEM due to the way in which DEM represents materials as discrete particles interacting through contact forces. This makes it challenging to capture the smooth deformation and continuous stresses that occur in a railway beam under applied loads. As a result, most research on railway modeling using DEM does not consider the rail beam structure (Chen et al., 2023; de Frias Lopez et al., 2021; Feng et al., 2019). Some researchers have attempted to address this issue by conducting cyclic loading tests on ballast without the rail structure to study the behavior of the build-up of granular materials (Indraratna et al., 2020; de Frias Lopez et al., 2019; McDowell and Li, 2016). However, it has been suggested that this approach may be insufficient in accurately representing the principal stress rotation phenomena caused by moving loads of the train (Bian et al., 2020). Therefore, it is necessary to incorporate the rail and other structural elements of the track in DEM in order to capture the true behavior of the railway during the train passage.

To more precisely model railway tracks using DEM, one option is to integrate it with other methods such as FDM or FEM, resulting in a coupled DEM-FDM/FEM method. This technique can more precisely depict the deformation and stress distribution occurring in the railway track. By combining DEM with FDM or FEM, the granular material interactions are solved using DEM, while FDM or FEM is utilized to model the behavior of the rail and other structural components of the track. The force-displacement at the interface between these two methods is then shared, providing a more accurate and authentic simulation of the dynamic behavior of the railway track. This technique has been used in some studies (for instance, (Shi et al., 2021a, 2020b,a)).

Chapter 3

Methodology

In this chapter, more details about discrete element modeling is discussed. Also, the methodology that was chosen for this research is motivated.

3.1 FEM vs DEM

The finite element method (FEM) discretizes a continuous domain into smaller elements and solves the governing equations of the system being modeled. This method is well-suited for continuous media, like fluid dynamics and structural analysis, and it's generally computationally efficient compared to DEM.

Conversely, discrete element method (DEM) is ideal for systems made up of interacting particles, like granular materials and rock mechanics. DEM represents each particle as an individual element and models interactions between particles via contact forces. It's a valuable tool for studying complex systems that show discontinuous behavior and particle-particle interactions, but can be computationally demanding.

In this research, DEM has been employed due to its ability to simulate the interaction among granular particles under the rail structure. Also, the ability of DEM to represent the particle breakage and abrasion is another advantage of DEM over other numerical methods.

3.2 2D vs 3D

One of the crucial questions to be answered while choosing the methodology of the research is whether the simulations should be done in 2D or 3D. The decision of whether to use a 2D or 3D model in DEM depends on the nature of the problem being studied. In cases where the problem has symmetry or translational invariance, such as in geotechnical engineering involving soil slopes, retaining walls, or plain strain problems, 2D models are often used. Similarly, when the problem is driven primarily by gravity, such as granular flows down a slope, 2D models are appropriate. However, for problems that lack a single plane or axis of symmetry or involve complex particle shapes, 3D models are necessary in order to capture the full complexity of the problem. Additionally, 3D models are used when considering problems with fluid flow or where the third dimension is crucial, such as the transport of particles in a pipe or the motion of particles in a vertical chute.

Numerous research works have indicated that 2D models are capable of capturing the essential aspects of granular interactions with a satisfactory degree of precision (e.g., (Salazar et al., 2015; O'Sullivan, 2011; Thornton and Zhang, 2003; Masson and Martinez, 2001)). In addition, 2D models possess higher computational speed, enabling the simulation of intricate polygonal particles, which are known for their precision in terms of particle shape (Lee et al., 2012). Therefore, in this research, 2D simulation was chosen due to its faster simulation and sufficient accuracy.

3.3 Discrete element modeling

Discrete element modeling refers to a computer-based simulation technique that models granular materials such as soil by taking into account the behavior of individual particles and their interactions. This method deviates from the conventional approach of continuum mechanics, which presumes that soil behaves as a continuous material and neglects particle movements and rotations. DEM simplifies particle shapes and contact models, making it computationally efficient while still capturing important soil behavior features. The technique has become increasingly popular among geotechnical engineers due to advances in computing power. DEM is used in various fields, including food technology and mining engineering (O'Sullivan, 2011; Cundall and Hart, 1993; Cundall and Strack, 1979).

There are some main reasons why researchers and practitioners in geomechanics use DEM. One of the key advantages of using DEM is the ability to simulate physical laboratory tests virtually, enabling the application of loads and deformations to virtual samples. Additionally, it facilitates the monitoring and analysis of particle scale mechanisms that underlie the overall material response, which may be difficult or impossible to obtain through physical tests. Furthermore, DEM provides a valuable set of tools that complement existing techniques for studying soil behavior and enhance our capacity to predict response in the field.

In addition, it enables the analysis of mechanisms involved in large-displacement problems that cannot be easily modelled using continuum approaches such as the finite element method. The significance of DEM in geomechanics lies in its ability to inform our understanding of critical failure mechanisms, which often involve significant displacements or deformations. Therefore, DEM is now widely recognized as a crucial tool in basic geomechanics research (O'Sullivan, 2011).

3.3.1 Simulation procedure

In order to perform a DEM simulation, the geometry of the system to be analyzed is defined as the first step step, including the particle coordinates and boundary conditions. The material properties, such as stiffness and friction coefficient, are usually specified through contact model parameters. At each time step, the simulation identifies particles in contact and calculates the forces between them, which depend on their distance. The resulting force and torque acting on each particle is determined, except for when particle rotation is not permitted. Two sets of equations are then solved to achieve dynamic equilibrium of the particles. This leads to the calculation of the particles' translational and rotational movements, which are based on their inertia, acceleration, and out-of-balance forces. This iterative process is known as a discrete element analysis, even if the system appears nearly static, and is repeated until the simulation is complete. This procedure is shown in figure 3.1.

Figure 3.2 demonstrates that there are two primary sets of calculations within each time increment. To begin with, the analysis focuses on determining the equilibrium of individual particles, which is essential for computing their velocities and incremental displacements. Next, after updating the system's geometry, the forces at each contact point within the system are determined. The tangential component of these contact forces invariably generates rotational moments on the particles, while in certain instances, the normal contact force component may also produce a moment. The forces and moments are then allocated to the particles and used to modify their positions in the subsequent time increment.

Potyondy and Cundall (2004) identified key assumptions in particle-based DEM simulations. These assumptions include:

- The particles are rigid and have finite inertia that can be analytically described.
- They can move independently of each other and can translate and rotate.
- The program can identify new contacts between particles.

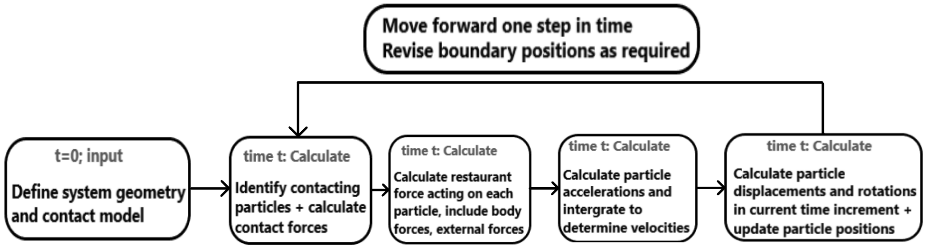


Figure 3.1: Schematic diagram of sequence of calculations in a DEM simulation, modified after (O'Sullivan, 2011)

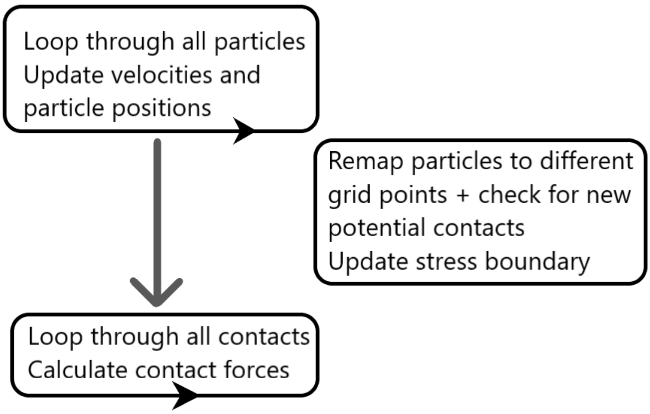


Figure 3.2: Calculation sequence within a time-step of DEM

- The contact between particles occurs over an infinitesimal area and involves only two particles.
- Particles are allowed to overlap slightly at contact points, analogous to the deformation that occurs between real particles, and the magnitude of the deformation is assumed to be small.
- Compressive inter-particle forces can be calculated from the magnitude of overlap.
- Particles can transmit tensile and compressive forces in the contact normal direction as well as a tangential force orthogonal to the normal contact force.

- Tensile inter-particle forces can be calculated based on the separation distance between two particles, and when the tensile force exceeds the maximum tensile force for that contact, the particles can move away from each other and the contact is deleted.

- The time increment chosen for the DEM simulation should be small enough that the motion of a particle over a given time step only influences its immediate neighboring particles.

- The use of agglomerates comprising rigid base particles presents a viable means of representing a physical particle as a whole, whereby the composite particles may undergo measurable deformation resulting from the relative motion of the base particles within the agglomerate.

In DEM, the equations of motion in each cycle are solved in time-steps. This method has a drawback in that its stability is conditional, requiring the use of small time-steps. In order to properly account for the complex non-linear nature of the problem, which encompasses dynamic changes in contact conditions and non-linear contact responses, it is necessary to minimize the changes in particle positions and contact forces between each time step. As a consequence, there is a constraint on the time increment, which must be kept small in order to accurately represent the non-linear behavior of the system. This insight was initially introduced by Cundall and Strack (1979). In a DEM simulation, the ideal time increment should be small enough that a particle's movement within a given time step affects only its immediate neighboring particles. According to Cundall and Strack (1979), a fundamental principle of DEM is that the time increment should be small enough that any disturbances caused by a particle cannot propagate beyond its closest neighboring particles in a single time step. The critical time-step is dependent on the smallest mass and stiffness of the system, as discussed by Cundall and Strack (1979):

$$\Delta T_{critical} \propto \sqrt{\frac{m}{K}} \tag{3.1}$$

where T is the time-step of the DEM simulation, m is the smallest mass of the system, and K is the stiffness in the mass-spring system. If the mass is smaller, the critical time-step will also be smaller. Consequently, having finer particles in the DEM simulation will result in a longer computational time due to the lower time-step.

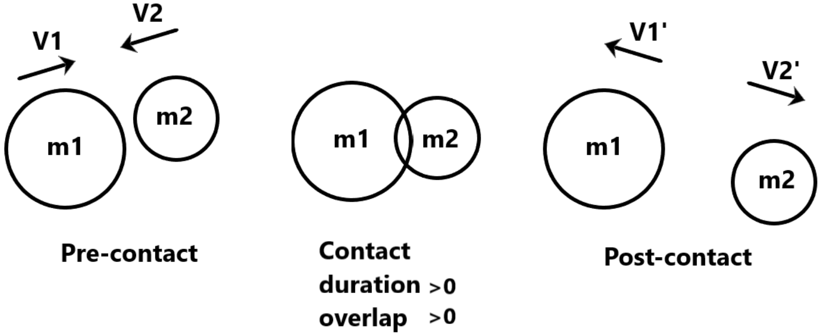
3.3.2 Particle size

The primary challenge when using DEM to model industrial problems, particularly railway granular materials, is the wide range of particle size present in the ballast and sub-ballast layers. According to the Swedish Transport Administration (Trafikverket), particle sizes in the sub-ballast layer range from 0.5 *mm* to 150 *mm*. Modeling such a broad range of particle sizes is exceedingly difficult given the limitations of current computational power. Thus, the first paper of this research explores particle up-scaling as a means of increasing the size of the smallest particle in the model while maintaining a high degree of simulation accuracy.

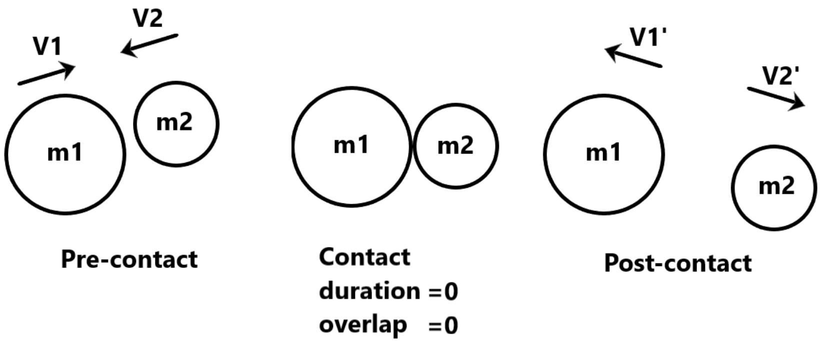
3.3.3 Contact models

According to Zhu et al. (2007), DEM can be categorized into two types of numerical techniques: soft models and hard models. The main difference between these categories is how the particles are approximated: "soft" particles allow for penetration at contact points, while "hard" particles do not allow for any deformation or penetration. Figure 3.3 provides a visual representation of both types of simulations. Both methods are time-dependent, meaning that the state of the particle assembly is analyzed at specific time intervals to observe its evolution over time.

In the current research, the soft approach was utilized. The soft sphere method involves solving equations that govern the linear and angular dynamic equilibrium of colliding or contacting particles in increments of discrete time. Despite the rigid nature of the particles in "soft sphere" simulations, they can still overlap at contact points, with friction and elastic restitution occurring only when there is penetration between spheres. The normal component of the inter-particle force is computed based on whether there is overlap or separation at the contact point for compressive and tensile forces, respectively, with the assumption that the overlap or separation is small. Shear or tangential forces are determined by the cumulative relative displacement at the contact points in a direction perpendicular to the contact normal orientation. Soft sphere models can handle systems with multiple simultaneous contacts, unlike the hard sphere approach that only considers a single collision at each time increment. This feature makes the soft sphere method particularly useful for static or quasi-static problems, such as those encountered in geomechanics applications (O'Sullivan, 2011; Cundall and Strack, 1979).



(a) Soft contact approach



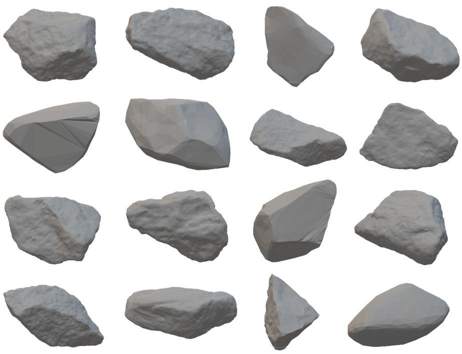
(b) Hard contact approach

Figure 3.3: Particle contact modeling approach, modified after (O'Sullivan, 2011)

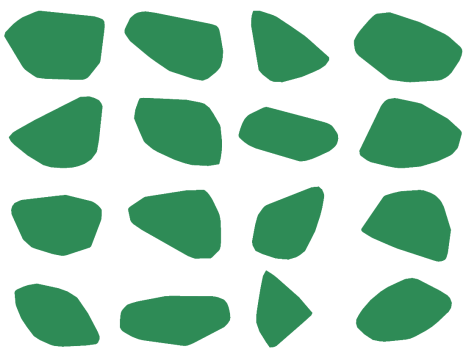
3.3.4 Particle shape

As discussed in section 2.1.2, simulating the real shape of particles is important for accurate DEM modeling. Therefore, the current study employed real sub-ballast particles for all the particle shapes, which were obtained by scanning them using the 3D laser scanner Artec Space Spider shown in figure 3.4a. A total of 16 sub-ballast particle shapes were scanned, as illustrated in figure 3.4b, and their scanned files were imported into PFC to generate the polygonal particles for the simulations which is shown in figure 3.4c.

(a) 3D scanning of granular particles with scanner Artec Space Spider



(b) Scanned particles



(c) Simulated particles

Figure 3.4: 3D Scanner, all the scanned particles and their representative simulated particle in DEM, from (Ahmadi et al., 2023)

Chapter 4

Particle scaling

Chapter 2 highlights that one of the major challenges in detailed DEM modeling is the extensive simulation time required. To simulate a long railway embankment using DEM, thousands of particles of varying size distribution must be modeled in the ballast and sub-ballast layers, rendering it practically infeasible for DEM. Therefore, the first step of this research involved investigating the implementation of particle scalping on the sub-ballast material to decrease the overall number of particles in the model and increase the time-step value of the simulation to expedite the process. By reducing the number of particles, the number of contacts also reduces, resulting in faster simulations.

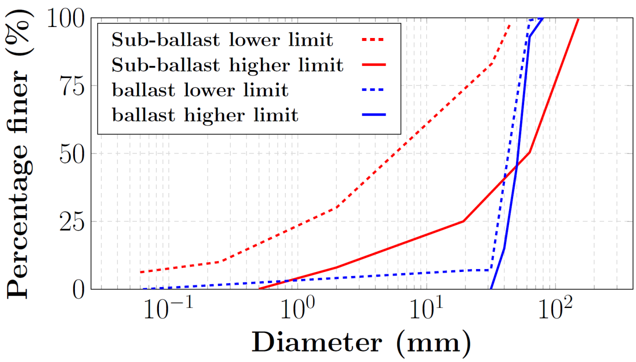
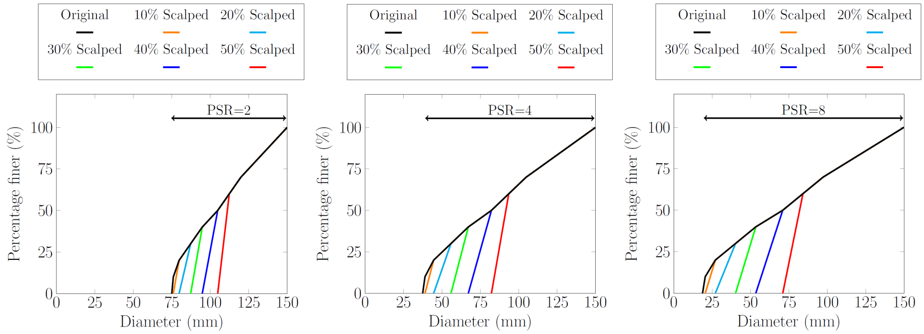


Figure 4.1: Particle size distribution according to Swedish Transport Administration



(a) PSR=2 (b) PSR=4 (c) PSR=8

Figure 4.2: Particle size distribution for the different percentage of scalping and different PSRs, from (Ahmadi et al., 2023)

4.1 Particle size distribution

According to the Swedish Transport Administration, ballast and sub-ballast particles should be chosen based on the limits shown in figure 4.1. As it is shown, sub-ballast material cover a wide range of size distribution. The present study demonstrates that sub-ballast materials have a diverse range of size distribution, making it difficult to model them accurately using DEM due to the presence of fine particles. The simulation time-step becomes exceedingly small with the inclusion of fine particles, and it is not practical to model the full range of particle sizes in this research. To overcome this challenge, paper "A" examines the particle scalping technique for sub-ballast material, which helps remove fine particles from the model without significantly affecting the results.

4.2 Scalping method

This study aimed to remove varying amounts of fine particles from a system without altering its total mass. To achieve this, larger particles were introduced to the system to replace the fine particles that had been removed, while maintaining the same total mass. Different particle size distributions were examined to gain insight into the efficacy of replacing finer particles with larger ones. This was important because some models only involve narrow particle size distributions, while others require the modeling of wider particle size distributions. Figure 4.2 displays the different particle size distributions that was investigated for particle scaling. These particle size distributions are categorized based on the particle size ratio (PSR), defined as follows:

$$PSR = \frac{D_{max}}{D_{min}} \tag{4.1}$$

where D_{max} is the largest particle size and D_{min} is the smallest particle size in the PSD. Since the largest particle in this study is 150 mm according to figure 4.1, D_{max} was chosen as 150 mm for all samples, but D_{min} was 75, 37.5, and 18.75 mm corresponding to PSR 2, 4, and 8, respectively. It is worth mentioning that these particle size distributions are comparable to each other through the percentage of the fine material which was scaled up, not the actual number of mass of these particles.

Tables 4.1 and 4.2 demonstrate the process of particle scalping, using an example of PSR=8 and a 30% scalping percentage. Table 4.1 displays the initial particle size distribution with a total sample weight of 1 kg and 100 grams of particles on each sieving diameter for better understanding. This data corresponds to the black line in figure 4.2c. To achieve 30% scalping, the first three rows, representing 30% of fine particles, are removed from the original sample. This amounts to a total of 300 grams of particles being removed. To maintain the total mass of the sample at its original value, 300 grams of particles with diameters equivalent to D40 are added to the sample. As a result, the fourth row in table 4.2 shows 400 grams of particles, while the first three rows display 0. The new particle size distribution is represented by the green line in figure 4.2c.

The selection of the scalping target diameter relies on the intended use of the simulation and the available computational resources. Increasing the scalping diameter results in more particles being eliminated from the model, leading to a larger time-step. In complex models that contain numerous fine particles, the process of scalping can be beneficial as it removes a significant amount of fine particles and their associated contacts.

To investigate the efficacy of the scalping method, a calibrated direct shear test model was employed and detailed in Paper A. Various particle shapes and size distributions were tested as illustrated in figure 4.2. The findings, depicted in figure 4.3, demonstrate that augmenting the percentage of scalping significantly reduces the number of particles in the model and increases the critical time-step of the simulation. Additionally, the impact of particle scalping is more pronounced for wider particle size distributions, as evidenced by comparing the results for PSR=2 to PSR=8.

Sieve diameter (mm)	Mass retained on sieve (gr)	Percentage of mass retained	Percentage of finer particles
18.75	100	10	0
20.51	100	10	10
27.09	100	10	20
40.26	100	10	30
53.43	100	10	40
70.99	100	10	50
84.16	100	10	60
97.32	100	10	70
114.88	100	10	80
132.44	100	10	90
150.00	0	0	100
Sum	1000	-	-

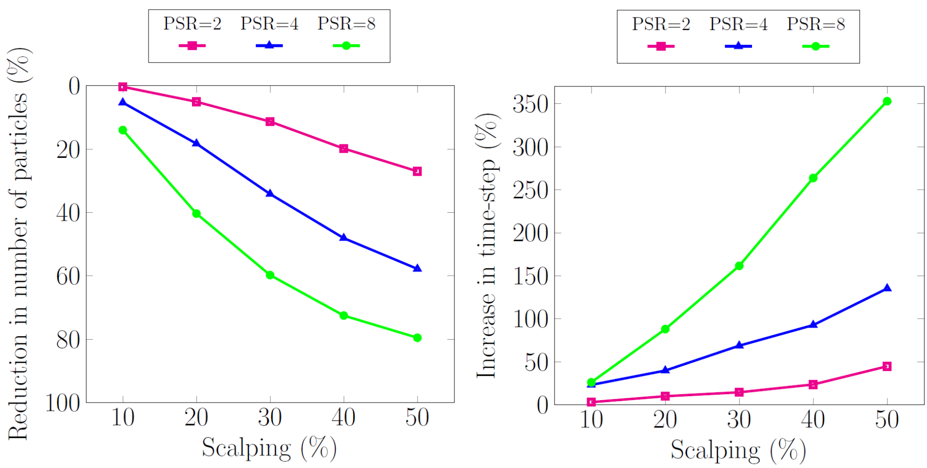
Table 4.1: Original sample

4.3 Summary

It was demonstrated that the scalping method effectively reduces the particle count and enhances the time-step of the simulation. Consequently, this method was implemented on the initial particle size distribution, displayed in Figure 4.1, to expedite the simulations in this investigation. The scalped particle size distribution was utilized to construct the granular layer of the railway embankment, which is elaborated on in Chapter 5.

Sieve diameter (mm)	Mass retained on sieve (gr)	Percentage of mass retained	Percentage of finer particles
18.75	0	0	0
20.51	0	0	0
27.09	0	0	0
40.26	400	40	0
53.43	100	10	40
70.99	100	10	50
84.16	100	10	60
97.32	100	10	70
114.88	100	10	80
132.44	100	10	90
150.00	0	0	100
Sum	1000	-	-

Table 4.2: 30% scalped sample



(a) Scanned particles (b) Simulated particles

Figure 4.3: Changes in the number of particles and time-step with scalping, from (Ahmadi et al., 2023)

Chapter 5

Railway model

In this chapter, the challenges and procedure of modeling a railway track in discrete element method is presented.

5.1 Particle size distribution

The railway track contains layers of granular material under the super-structure. The main layers that can be modeled in discrete element method are ballast and sub-ballast layers.

The ballast layer is a vital constituent of railway tracks as it is responsible for providing support and stability to the rail tracks by distributing the load from the rails and sleepers to the underlying subgrade soil. Moreover, it contributes to maintaining the track's alignment and level, decreasing vibrations and noise, and promoting drainage. Typically, the ballast layer is composed of crushed stone, gravel, or other robust materials placed between the railway sleepers and the subgrade, designed to be porous to allow water to drain through and avoid water accumulation that can cause instability and erosion. Additionally, the particle size and grading are carefully considered to resist the lateral and vertical movement of the railway tracks caused by train traffic's dynamic forces.

The subballast layer is a layer of material that is inserted between the ballast layer and the subgrade layer in the construction of railway tracks. Its primary purpose is to create a stable and uniform base that supports the ballast layer, which in turn supports the trains and track. The subballast layer has several functions, including distributing the load of the trains evenly across the subgrade layer, which helps prevent differential settlement of the ballast layer and enhances the overall stability of the track. It also provides drainage by allowing water to flow

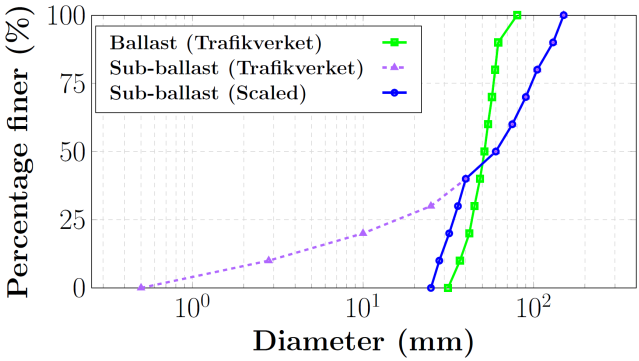


Figure 5.1: Particle size distribution used in railway models

away from the ballast layer, preventing it from becoming saturated, which can lead to ballast degradation and instability of the track. Additionally, the subballast layer offers extra strength to the track structure, which helps resist the lateral forces created by trains and lowers the possibility of track failure. Materials like crushed stone, gravel, or sand are commonly used in the subballast layer because of their stability, drainage properties, and ability to resist deformation under load.

Figure 4.1 shows the particle size distribution of these layers according to Swedish Transport Administration. Since the subballast layer contains of a wide range of particle sizes, it is not practical to model its actual size in the railway DEM. Therefore, its particle size distribution is scaled up based on particle scalping discussed in chapter 4. The particle size distribution of these two layers which is used for railway models in DEM is presented in figure 5.1.

5.2 Modeling structural elements

When it comes to modeling the rail beam and other structural elements of railway tracks using the DEM, it presents a difficult challenge. This is due to the DEM's representation of materials as discrete particles interacting through contact forces, making it challenging to capture the smooth deformation and continuous stresses that occur in a railway beam under applied loads. Consequently, previous research that employed DEM to model railways excluded the rail beam. For instance, studies conducted by Chen et al. (2023); de Frias Lopez et al. (2021) and Feng et al. (2019) excluded the rail beam from their models. Some researchers tried to address this challenge by performing cyclic loading tests on ballast without the rail beam, examining the behavior of granular material buildup. These include studies by Indraratna et al. (2020); de Frias Lopez et al. (2019) and McDowell and Li (2016). However, Bian et al. (2020) revealed that the cyclic modeling of granular material buildup is insufficient in accurately representing the principal stress rotation phenomena resulting from the movement of train loads.

To address the challenge of modeling the rail beam in DEM, researchers such as Shi et al. (2021b) and Zhang et al. (2017) utilized a linear parallel bond contact model to connect disc particles. This approach simulates the flexural and axial stiffness of a continuum beam. Parallel bond contact stiffness parameters are calculated as:

$$k_{pn} = \frac{E}{2\lambda R} \tag{5.1}$$

$$k_{ps} = \frac{G}{2\lambda R} \tag{5.2}$$

where k_{pn} and k_{ps} are parallel bond normal and shear contact stiffness, respectively, E and G are elastic and shear modulus of physical rail, respectively, λ is the parallel bond radius multiplier, and R is the rail disc radius.

In this part of the research projects, the influence of ignoring a rail beam in the discrete element model is explored. Two models are constructed and compared: First a model with rail beam and other structural elements of ballasted track. Second a model without the rail beam of a ballasted track.

Standard 60E1 (UIC60, 60 kg/m) rail profile is chosen to be simulated in this research. Figure 5.2 shows the railway model and structural elements.

To model the railpads that connect rails to sleepers, disc particles are employed, similar to the rail particles. Meanwhile, rectangular particles are used to simulate the sleepers between the railpads and ballast material. In this approach, all contacts between the structural materials are modeled using the parallel bond contact model, as suggested by Zhang and Thornton (2007).

5.3 Track length

To model a long railway embankment using discrete element method, a significant number of particles are required to accurately simulate the granular material behavior. However, this leads to a high computational cost, making the simulation impractical and time-consuming. Additionally, the interactions between particles are complex and nonlinear, involving various forces such as friction that are challenging to model accurately. Moreover, the boundary conditions of a railway embankment are difficult to model, as it is typically supported by a complex system of retaining walls, bridges, and other structures. To accurately model a long

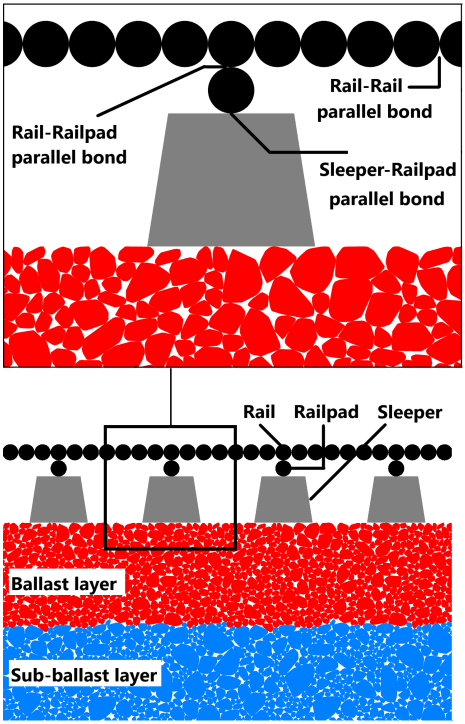


Figure 5.2: Railway model consisting structural elements

railway track, it is crucial to include critical parts such as transition zones. These zones experience a significant differential settlement over a long distance and must be accurately simulated. However, modeling such long railway tracks using discrete element modeling can be challenging and requires sophisticated techniques to achieve practical results within a reasonable time frame. In this research, a ballasted track railway model is constructed and calibrated. Afterwards, the model will be extended to include transition zone in the second phase of this research project.

5.4 Train load

Applying a train load to the track is a fundamental step in railway modeling using DEM due to its strong correlation with the structural elements of the track.

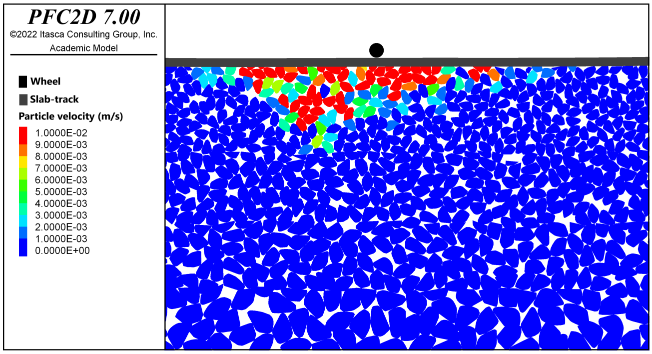
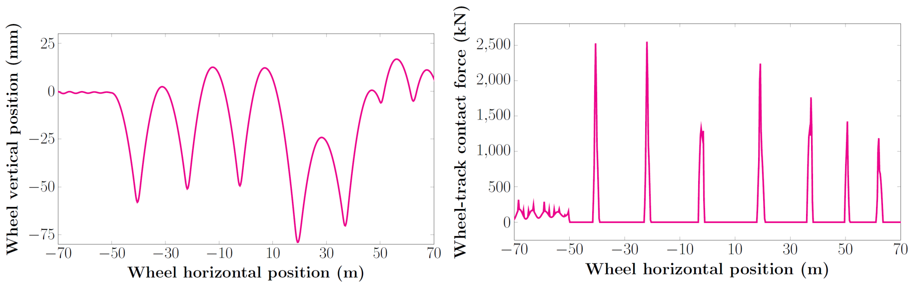


Figure 5.3: Moving wheel model



(a) Wheelset position

(b) Wheelset contact force

Figure 5.4: Wheelset position and contact force in the moving wheel model

This section discusses various strategies for applying train loads, each of which was modeled and tested with different parameters, and the resulting data was compared to existing literature to assess its reliability.

5.4.1 Moving wheel

The first approach of applying the train load on the track is moving wheel. In this method, the weight of an axle of a train is applied as mass of a wheelset which travels on the track. The Hertz contact model was adopted for the wheel-track contact. Then the wheel was rotated and moved along the track to apply the train load on the track. The model is shown in figure 5.3.

Despite its convenience, this model yielded poor performance results. Due to track irregularities, the wheelset lost contact with the track while traveling

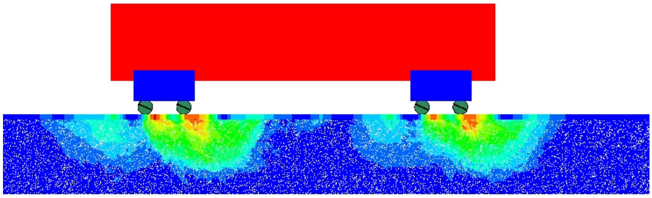
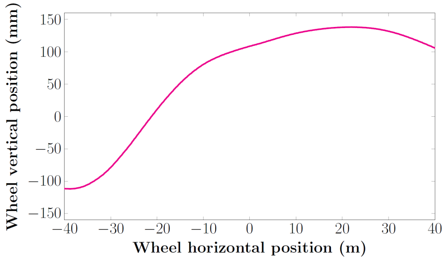
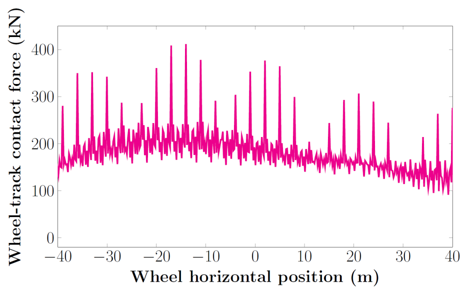


Figure 5.5: Vehicle model



(a) wheelset position



(b) wheelset contact force

Figure 5.6: wheelset position and contact force in the vehicle model

on it, causing it to bounce and generate high-impact magnitudes on the track. This phenomenon persisted across different damping and restitution coefficients. Figure 5.4 depicts the wheelset passage position and its contact force with the track.

5.4.2 Vehicle model

In the event that the rail beam is reliable, it becomes feasible to construct a vehicle model comprised of bogies and wheelsets, which can travel on the track at the desired train speed. Nevertheless, as the interactions between structural elements are limited in DEM, regulating the vibration frequency of the wheelset is not a straightforward task. Furthermore, incorporating distinct contact models for each vehicle component can lead to a slower contact detection mechanism. Figure 5.5 shows a vehicle model on the track. This vehicle consists of two bogies and four wheelsets.

Figure 5.6 illustrates the position of the wheelset and its corresponding contact force with the track. This data is just one of the many models constructed to examine the performance of the vehicle model. Despite the wheelset's smooth path, the contact force between the wheelset and track shows significant impacts, which can be attributed to the segments of the track. The drawback with this vehicle model lies in its inability to control the vibration and loading frequency, which ultimately led to its abandonment for this research.

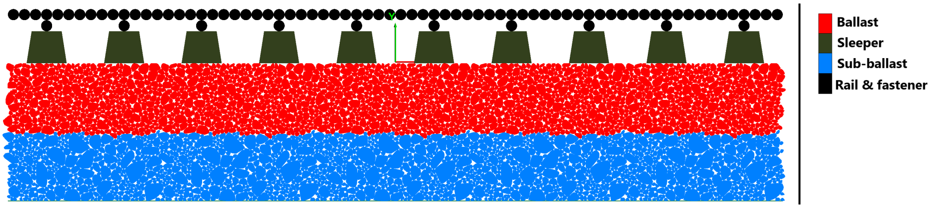
5.4.3 Moving load

Another method for applying the train load on the track involves directly applying the desired loading pattern onto the track structure and moving it along the track. The benefit of this approach is the ability to directly control and modify the loading magnitude and frequency as input to the model. However, because the loading pattern must be updated at every step and position of the track, this method is more time-consuming than previous approaches.

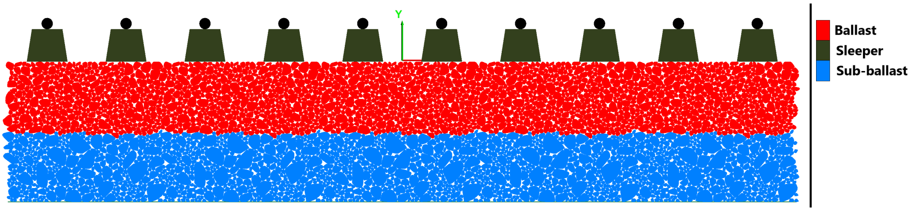
Directly applying a moving load on the rail particles is feasible, but it can cause wave propagation along the rail which presents a significant challenge. Because the structural element and damping mechanism are limited in DEM, this approach was abandoned after multiple attempts. As a result, the moving load was instead applied directly to the railpads of the ballasted track. This involved adopting a loading pattern for a railpad as a function of time, shifting it with respect to the travel time between two adjacent railpads, and then applying all these loading patterns to the railpads. A more detailed explanation of this method can be found in Paper B and in Bian et al. (2020).

5.5 Railway model

Using the information discussed in the previous sections, a railway model was constructed. During this stage of the research, the impact of the absence of the rail beam in the ballasted tracks was examined. This is because in many cases, the rail beam is disregarded in DEM simulations to avoid complications with the structural elements in DEM, as in the studies by Chen et al. (2023) and Bian et al. (2020). Figure 5.7 shows the two models for this exploration. The results of this investigation are presented in detail in Paper B.



(a) Model with rail beam



(b) Model without rail beam

Figure 5.7: Railway model with and without rail beam

5.6 Summary

This chapter has covered the methods and obstacles involved in modeling railways using the discrete element method. This portion of the research serves as a groundwork for the upcoming phase, which focuses on examining high-speed railway transition zones. The chapter began by establishing the particle size distribution and structural elements of the model, followed by the implementation of the train load. Lastly, an exploration was conducted to evaluate the impact of the rail beam in the discrete element model of the railway track.

Chapter 6

Summary of appended papers

6.1 Paper A

Scaling granular material with polygonal particles in discrete element modeling

Alireza Ahmadi, Stefan Larsson, Carl Wersäll.

Particuology 75 (2023): 151-164.

The primary challenge in using DEM to model granular materials is the significant computational time required, which can impact the efficiency and objectives of the models. To address this issue, researchers may need to sacrifice certain details to improve simulation time. In this study, the authors explored the use of particle scaling techniques to determine how much scaling could be employed while still retaining sufficient accuracy, leading to a meaningful reduction in computational time.

The impact of particle angularity and particle size range on the accuracy of the scalping method was investigated. The direct shear test was selected as a representative test for granular material shearing behavior, based on the recommendations of previous studies by Alabbasi and Hussein (2021); Wu et al. (2020); Jing et al. (2020), and Coetzee (2016). The model was first calibrated against experimental and numerical studies by Ngo et al. (2016); Ngo and Indraratna (2016); Indraratna et al. (2014), and Ngo et al. (2014). Three different particle size distributions (PSDs) were then considered to evaluate the effect of PSD on the results, following the suggestion of Guo et al. (2020a). For each PSD, particle scalping was performed on various particle size ranges to investigate the impact of removing fine particles from the granular system. In addition, to examine the influence of particle angularity on the effectiveness of the scalping method, polygonal particle shapes derived from scanning real sub-ballast particle shapes were used in simulations with different types of particle angularities. The main conclusions are:

- The effectiveness of the particle scalping method increases as the particle size distribution becomes wider.
- The particle scalping method increased the time-step of the model by removing the smallest particles, resulting in a significant decrease in computational time of up to 90%.
- When the particle angularity decreases, the difference in shear strength and volumetric strain between the scalped models and the original models increases.
- More angular particles lead to a decrease in particle rotation and an increase in coordination numbers, resulting in better interlocking and contact force transmission and showing more shear strength and volumetric strain in the samples.
- The difference between the shear strength and volumetric strain of the scalped models and original models increases with an increase in the scalping percentage.
- An increase in the coordination number resulting from an increase in the scalping percentage causes a reduction in the average particle rotation.

CRediT author statement

Alireza Ahmadi: Methodology, Software, Formal analysis, Investigation, Writing - Original Draft, Writing - Review and Editing, Visualization

Stefan Larsson: Conceptualization, Validation, Writing - Review, Resources, Supervision, Funding acquisition

Carl Wersäll: Conceptualization, Validation, Writing - Review, Resources, Supervision, Project administration, Funding acquisition

6.2 Paper B

The influence of rail beam on the settlement of high-speed railway track: A discrete element study

Alireza Ahmadi, Carl Wersäll, Karl Norberg, Sacha Emam, Stefan Larsson
Submitted to Transportation Geotechnics

The modeling of structural elements like the rail beam in railway tracks using DEM is challenging due to the discrete particle representation and contact forces used in DEM. This makes it difficult to capture the smooth deformation and continuous stresses that occur in the rail beam under load. Therefore, many studies using DEM exclude the rail beam (e.g. Chen et al. (2023); de Frias Lopez et al. (2021); Feng et al. (2019)). Some researchers have tried cyclic loading tests on ballast without the rail beam to study the behavior of the build-up of granular materials (Indraratna et al., 2020; de Frias Lopez et al., 2019; McDowell and Li, 2016). However, according to Bian et al. (2020), this approach is insufficient to accurately represent the principal stress rotation phenomena caused by moving loads of the train.

The objective of this research is to evaluate the effects of not considering the rail beam in the ballasted track of high-speed railways in both short and long term. A DEM model is used, which is calibrated against measurements of a full-scale physical ballasted track. The model is then expanded to include the rail beam and rail-pads on sleepers. A moving load pattern resembling a 300 km/h high-speed train is applied to the track for up to 2000 loading axles. Results indicate that not including the rail beam has minimal impact on the initial loading axles, but its effect becomes more significant after several hundred axle passages. For long-term analysis of tracks, it is essential to incorporate the rail beam, as its absence leads to higher principal stress rotation, greater settlement, unrealistic displacement of the sleepers, and increased sleeper vibration.

Here are the summarized findings and recommendations based on the study:

- Initially, the absence of the rail beam in a ballasted track model may not cause a significant effect on the track's vertical displacement. However, as the number of axle passages increases, the difference in settlement between a model with and without a rail beam becomes more apparent.

- The absence of a rail beam in a ballasted track model leads to a greater differential vertical displacement among the sleepers, which results in a non-realistic settlement of the track.

- The permanent settlement and vibration velocity of sleepers in a ballasted track are considerably higher in a model without a rail beam than in a model with a rail beam. In a model without a rail beam, there is a larger particle rearrangement under the sleepers due to the increased vibration velocity of the sleepers. This particle rearrangement leads to a more irregular settlement of the track.

- A model without a rail beam experiences more principal stress rotation than a model with a rail beam. As a result, it is recommended to include the rail beam in DEM models when simulating the long-term behavior of high-speed railway tracks. Additionally, the presence of the rail beam is critical in large-scale models of the tracks, such as the study of transition zones, where accurately simulating track settlement is crucial.

CRediT author statement

Alireza Ahmadi: Methodology, Software, Formal analysis, Investigation, Writing - Original Draft, Writing - Review and Editing, Visualization

Carl Wersäll: Conceptualization, Validation, Writing - Review, Resources, Supervision, Funding acquisition

Karl Norberg: Conceptualization, Validation, Writing - Review

Sacha Emam: Software, Writing - Review

Stefan Larsson: Conceptualization, Validation, Writing - Review, Resources, Supervision, Project administration, Funding acquisition

Chapter 7

Conclusion and Future Work

In this thesis, the computational time of the discrete element method has been improved through particle scaling. Then, the resultant particle size distribution was used in a railway model to simulate the granular layers of the high-speed track. Structural elements of the railway track were modeled in discrete element method. Then, the influence of rail beam has been investigated in a ballasted track.

Up to this point, a discrete element method has been utilized to model a ballasted track for high-speed railways. One crucial aspect that needs to be studied in future work is the transition zones. Transition zones are the areas where the track changes from one type of structure to another, such as from a ballasted track to a slab-track or from embankment to the bridge. Studying these zones is important because they can cause differential settlement, which is when one part of the track settles more than another. Differential settlement can lead to track irregularities, such as bumps and dips, which can be hazardous for high-speed trains. Differential settlement is particularly destructive for high-speed railways because the trains travel at very high speeds, which can create dynamic forces on the track. These forces can cause the track to deform, leading to track irregularities and potential derailments. Therefore, it is crucial to study differential settlement and find ways to minimize it.

Another crucial factor that needs to be studied in future work is particle breakage in the granular material of the railway track. Modeling particle breakage of railway ballast is also important for settlement calculation. The ballast layer is the layer of stones and rocks that sits between the railway ties and provides support for the track. Over time, the ballast can break down and become compacted, which can lead to settlement. By modeling particle breakage, researchers can better understand how the ballast layer behaves over time and predict settlement more accurately. This information is crucial for maintaining the track and preventing derailments.

Therefore, as the next step of this research, this model will be further developed to incorporate the breakage mechanism to simulate particle breakage in the granular layer of the track. The model will be applied to a long railway section, including a bridge transition zone, to examine the long-term and differential settlement of the track. Finally, potential solutions to reduce the differential settlement of high-speed railway tracks in transition zones will be explored and discussed.

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Appendix A

Appended Papers