Discrete element simulation of elasto-plastic shock waves in high-velocity compaction

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Doctoral Thesis

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Abstract

Elasto-plastic shock waves in high-velocity compaction of spherical metal particles are the focus of this doctoral thesis consisting of an introduction and four appended papers (A-D). The compaction process is modeled by a discrete element method while using elastic and plastic loading, elastic unloading as well as adhesion and friction at contacts. 

**Paper A** investigates the dynamic compaction of a one-dimensional chain of homogeneous aluminum particles. The development of the elasto-plastic shock waves, their propagation and influence on the compaction process are examined. Simulations yield information on the contact behavior, velocity of the particle and its deformation during dynamic compaction. Furthermore, effects of changing loading parameters on the compaction process are discussed.

**Paper B** addresses the non-homogeneity in a chain having particles of different sizes and materials, voids between the particles and particles with/without adhesion between them. Simulations show transmission and reflection of elasto-plastic shock wave during the compaction process. The particle deformation during incident and reflected shocks and particle velocity fluctuations due to voids between particles are simulated. Finally, the effects of adhesion on particles separation during unloading stage are also discussed.

**Paper C** develops a simulation model for a high-velocity compaction process with auxiliary pistons, named relaxation assists, in a compaction assembly. The simulation results reveal that the relaxation assists offer smooth compaction during loading stage, prevention of the particle separation during unloading stage and conversion of higher kinetic energy of hammer into particles deformation. Furthermore, the influence of various loading elements on compaction process is investigated. These results support the findings of experimental work.

**Paper D** further extends the one-dimensional case of **Paper A** and **B** into a two-dimensional assembly of particles while adding friction between particles and between particles and container walls. Three special cases are investigated including closely packed hexagonal, loosely packed random and a non-homogenous assembly of particles of various sizes and materials. Consistent with the one-dimensional case, primary interest is the linking of particle deformation with the elasto-plastic shock wave propagation. Simulations yield information on particle deformation during shock propagation and overall particles compaction with the velocity of the hammer. Furthermore, the force exerted by particles on the container walls and rearrangement of the loosely packed particles during dynamic loading are investigated. Finally, the effects of presence of friction and adhesion on both overall particles deformation and compaction process are simulated.

The developed models in this doctoral thesis provide insights to understand various aspects of high-velocity compaction.
Dissertation

The doctoral thesis consists of this summary and four appended papers listed below and referred to as **Paper A** to **Paper D**. Leif Kari has acted as a supervisor for this thesis and Bruska Azhdar is co-supervisor.


Parts of work has been presented at the following two conferences:

M. Shoaib, L. Kari 2010 23rd Nordic Seminar on Computational Mechanics "High-velocity compaction simulation using the discrete element method"
M. Shoaib, L. Kari 2008 International Symposium on Non-Linear Acoustics "Elasto-plastic wave front propagation in non-linear particle systems"
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Part I

Overview and Summary
Chapter 1

Introduction

High-velocity compaction (HVC) of particulate material is a rapid production technique with the capacity to significantly improve the mechanical properties of the compact. HVC finds its applications in powder material structural parts and soft magnetic composites. In conventional compaction, powder is compacted by pressure in about one second, while in HVC particles are compacted with shock waves in less than 0.01 seconds. These shock waves are generated by giving the projectile or hammer a certain initial velocity, usually by a hydraulic press in the case of manufacturing process. This initial velocity along with the mass of the hammer results in a certain kinetic energy which controls the dynamic compaction process. During last years, high-velocity compaction of ferrous, ceramic and polymer powders have been investigated. The majority of these studies are restricted to the experimental work while mainly focusing on the gain in compact density and process parameters. In previous work at Department of Fibre and Polymer Technology at Royal Institute of Technology (KTH) [1, 2], various aspects of HVC process have been investigated including the pull-out phenomena, spring back and delay time. In order to minimize these problems, new technique has been developed by introducing the auxiliary pistons, named relaxation assists, in a compaction assembly. These experiments were performed on polymer powder.

The present work is on numerical simulation of high-velocity compaction process. Since the elasto-plastic shock waves are the main source of particle compaction during HVC, shock waves have been investigated in details in the present work. The main focus is to understand the generation, propagation and reflection of elasto-plastic shock waves and their effects on particle deformation and their movement during dynamic compaction. To investigate these and other issues, compaction model is reduced to a one and two-dimensional assemblies consist of one hundred to about one thousand particles. The reason for selecting spherical metal particles instead of polymer particles is the availability of contact models during compaction process. In the present work, well-established contact models for elastic and plastic loading and elastic unloading with and without adhesion and friction between contacts are used. When primary aspects of elasto-plastic shock wave are understood; then it is straightforward to extend the compaction model to any number of particles with 3-dimensions to address a more
realistic practical situation. The discrete element method (DEM) is used to model the compaction process. This numerical method has been widely used for simulating the large number of particles while studying granular matter and powder compaction.

The present work starts from the dynamic compaction of a one-dimensional chain of homogenous particles. Elasto-plastic shock wave generation, its propagation and influence on the compaction process are studied. Then non-homogeneity is introduced by considering the chain having particles of different sizes and materials, voids between the particles and particles with/without adhesion between them. Simulations reveal transmission and reflection of elasto-plastic shock wave; particle deformation during incident and reflected shocks and particle velocity fluctuations due to voids between particles. In addition, the effects of adhesion on particles separation during unloading stage are discussed. Furthermore, the effects of the presence of auxiliary pistons, known as relaxation assists, in a compaction assembly are investigated. It is shown that relaxation assists offer an increased locking of the particles during loading and unloading stages. These results support the findings of above mentioned experimental work. Finally, two-dimensional assembly of particles with friction between particles and between particles and container walls is investigated. The main focus is on the linking of particle deformation with the elasto-plastic shock wave.

1.1 Background

Considerable interest in the dynamic response of particulate and granular materials exists in the powder compaction, geomechanics and other branches of engineering. Quasi-static and dynamic compaction modeling of particulate material is studied in various domains. During compaction of particulate material; load is transferred almost equally to all the particles in quasi-static compaction, while during dynamic loading it propagates as shock wave. This shock wave propagation in discrete media differs considerably from the wave propagation in continues media. The granular matter shows discrete behavior when subjected to dynamic loading [3–5]. The dynamic wave propagation in granular media shows distinct behavior from the wave propagation in continues media [3]. Shukla and Damania [6] discuss the wave velocity in granular matter and shown experimentally that it depends upon elastic properties of the material and on geometric structure. Similarly, Shukla and Zhu [7] investigate explosive loading of a discs assembly and found that the force propagation through granular media depends on impact duration, arrangement of the discs and the diameter of discs. Tanaka et al. [8] investigate numerically and experimentally the dynamic behavior of a two-dimensional granular matter subjected to the impact of a spherical projectile.

To investigate dynamic response, many researchers [9–13] have modeled the granular matter as spherical particles using the micromechanical modeling of contact between particles. These studies focused on equivalent macro elastic constitutive constants during dynamic loading. Similarly, experimental work using dynamic photoelasticity and strain gage are performed to investigate contact loads between particles both under
static and dynamic loading [14, 15]. Saad et al. [14] perform numerical simulations to investigate the effects of the contact laws on wave propagation in granular matter. Similarly Saad et al. [15] use the discrete element method (DEM) to simulate wave propagation in granular materials. Results of that study show wave propagation speed and amplitude attenuation for two-dimensional assembly of spherical particles. However, that study is restricted to the elastic range only while the material stiffness and damping constants used in the model are determined by photoelasticity. The DEM was initially developed by Cundall and Strack [16] and this numerical method has been widely used for granular material simulations [17–19]. Different engineering approaches are discussed in Refs. [20, 21] to model the behavior of granular matter using DEM. Dynamic compaction of metal powder is also reported in the literature [22–26] and studies the distribution of stress, strain and wave propagation. However, these studies treat the powder as a continuum and determine the material constants experimentally.

Force transmission in spherical particles occurs in a chain of contacts, which is usually referred as the force chain. Force chains in granular matter have been widely investigated, experimentally [27, 28] and in simulations [29, 30]. However these studies do not consider wave propagation velocity during loading. Liu and Nagel [31] and Jia et al. [32] found experimentally that sound propagates in granular media along strong force chains. Somfai et al. [33] investigate the sound waves propagation in a confined granular system. Recently, Abd-Elhady et al. [34, 35] studied contact time and force transferred due to an incident particle impact while using the Thornton and Ning approach [36] and found a good agreement between DEM simulation and experimental measurements. However, these studies are restricted to the particle collision and are not modeling the shock wave propagation during dynamic loading of particles. Micromechanical modeling of powder compaction process is now well established. The pioneer work performed by Wilkinson and Ashby [37–40] and after that theoretical and experimental studies [41–44] resulted in a complete theory for static compaction. A detailed model of normal contact between viscoplastic particles is presented by Refs. [45] which relies on power law creep [46, 47], plastic flow theory [48, 49] and general viscoplasticity [48, 50]. The model proposes analytical equations which show the effects of the material and process parameters during powder compaction. The technique is used to analyze monolithic and composite powders compaction [51, 52].

Further progress in micromechanical modeling is achieved by numerical simulations based on the discrete element method. Recently, to investigate different aspects of powder compaction, DEM is used by Skrinjar and Larsson [53, 54] and also by Martin and Bouvard [55, 56]. Martin [57] models the powder compaction by introducing plastic loading, elastic unloading and decohesion at contacts using the formulation of Mesarovici and Johnson [58]. However, in these investigations, dynamic effects are included for numerical reasons only and their goal is to attain static equilibrium solutions during isostatic and die compaction. Quasi-static compaction models include the mechanical deformation mechanism of particles and do not analyze the mechanical energy transfer during shock propagation. During the last few years, high velocity compaction of ferrous, ceramic and polymers powders has been investigated in various domains [59–66].
However, most of these studies are restricted to the experimental work while mainly focusing on the gain in compact density. Wang et al. [59] determines experimentally the effects of impact velocity on green density and on the properties of the compacted body. Similarly, Refs. [60, 61] compare the conventional compaction and HVC to determine the conditions for attaining the maximum compact density. Doremus et al. [67] compare HVC and conventional compaction of metallic powders for different process parameters including the material densification and tooling strength. To understand the different aspects of powder compaction, comparison between numerical and experimental results is also reported in the literature [68–70].

Recently, Bruska et al [1, 2] investigated the different aspects of HVC process and developed a new technique by introducing the projectile supports, known as relaxation assists. These metal pieces are of the same diameter and material as those of the piston. It is found that incorporation of the relaxation assists increases the material densification and compact properties including the reduction of pull-out phenomena — the top surface of the compact becomes uneven and the spring back — expansion of the compact during unloading stage. It has been suggested that above mentioned improvements are mainly due to the better locking of the powder during compaction process. Furthermore, the results of these studies suggest that HVC is not a continuous process but rather it includes several discontinuities which may effect differently the compact properties.

In the present work, discrete element method is used to simulate elasto-plastic shock wave propagation in a homogeneous, Paper A, and in non-homogeneous, Paper B, chains of spherical particles. The effects of shock wave on particle deformation and their movement and on the loading parameters are investigated. Paper C examines the significance of relaxation assists in a compaction assembly. It is shown that relaxation assists provide an increased locking of the particles during loading and unloading stages. Finally, high-velocity compaction of a two-dimensional assembly of spherical particles is examined in Paper D. Tightly packed, random and non-homogeneous particle assemblies are investigated while the main interest is to link particle deformation with elasto-plastic shock waves.
Chapter 2

Particles contact behavior

This section summaries the theories that describe the contact behavior between particles and between particles and container walls during loading-unloading-reloading stages. Here, the compact is modeled as a one and two-dimensional assembly of particles that indent each other. Both homogeneous and non-homogeneous particles assemblies are considered. Non-homogeneity is introduced by changing the size and material of the particles. The materials are assumed to be elastic, perfectly plastic while having no strain hardening. For two contacting particles \( p \) and \( q \) with radius \( R_p \) and \( R_q \); effective radius \( R_0 \), equivalent elastic modulus \( E^* \) and yield stress at contact \( \sigma_y \) are

\[
R_0 = \frac{R_p R_q}{R_p + R_q},
\]

\[
E^* = \frac{1}{E_p} \left[ 1 - \nu_p^2 \right]^{-1} \left[ 1 - \nu_q^2 \right]^{-1}
\]

and

\[
\sigma_y = \min (\sigma_p, \sigma_q),
\]

where \( E_p \) and \( E_q \) are the Young’s modulus; \( \nu_p \) and \( \nu_q \) are the Poisson’s ratio; \( \sigma_p \) and \( \sigma_q \) are the yielding stress; for the particles \( p \) and \( q \), respectively. The indentation or overlap between particles is denoted \( h \). The elastic normal contact force follows the Hertzian law [71] in the beginning of loading process

\[
F_e = \frac{4}{3} E^* \sqrt{R_0} h^{3/2}.
\]

In the plastic regime, normal contact force is [52, 57]

\[
F_p = 6\pi c^2 \sigma_y R_0 h,
\]

where the constant \( c^2 = 1.43 \) for ideally plastic material behavior. The contact radius \( a \) is given by

\[
a^2 = 2c^2 R_0 h
\]
and the contact stiffness is defined as

$$k = 6\pi c^2\sigma_y R_0.$$  \hspace{1cm} (2.7)\]

The parameters $F_0$, $a_0$ and $h_0$ denote normal contact force, contact radius and overlap, respectively, at the end of plastic loading stage. The uniform pressure at the contact is $p_0 = 3\sigma_y$ and $w$ is the work of adhesion. In the present case, it is set to $w = 0.5 \text{ J/m}^2$. During unloading of the contact, the distance between the centers of the particles $h_{pq}$ can be written as

$$h_{pq} = R_1 + R_2 - h_0 + h_u$$ \hspace{1cm} (2.8)\]

and the overlap is

$$h = h_0 - h_u,$$ \hspace{1cm} (2.9)\]

where $h_u$ denotes the indentation recovered during unloading of the contact, reading [56, 71]

$$h_u = \frac{2p_0a_0}{E^*} \sqrt{1 - \left(\frac{a}{a_0}\right)^2}.$$ \hspace{1cm} (2.10)\]

The contact radius $a_0$ during unloading of the contact can readily be determined from Eq. (2.10). The normal contact force $F_u$ during unloading is [56, 71]

$$F_u = 2p_0a_0^2 \left[ \arcsin\left(\frac{a}{a_0}\right) - \frac{a}{a_0} \sqrt{1 - \left(\frac{a}{a_0}\right)^2} \right] - 2\sqrt{2\pi w E^* a_0^3}.$$ \hspace{1cm} (2.11)\]

In Eq. (2.11), the term $-2\sqrt{2\pi w E^* a_0^3}$ is the force due to adhesion traction between particles [57, 58]. This term should be included in loading equations when adhesion between particles is considered. Furthermore, the friction between particles and between

---

**Figure 2.1:** Schematic of two particles in contact, here $h$ is the overlap between particles.
particles and container walls is considered in this work. Thus, a Coulomb-type friction law is incorporated as

\[ F_f = \mu_f F_n, \]  

(2.12)

where \( F_f \) is the friction force perpendicular to the normal force \( F_n \). Friction force opposes the relative motion between the contacting surfaces. In the present case, the coefficient of friction is set to \( \mu_f = 0.1 \).
Chapter 3

Model

3.1 Discrete element method

The dynamic compaction process is simulated by DEM. This numerical method is used by Martin and Bouvard [56] and other researchers to simulate static compaction. In the present work, DEM is extended to simulate shock wave propagation in a chain of spherical particles using established contact models. Here each particle is modeled independently and the interaction between neighboring particles is governed by contact laws as described in the previous section. This contact response plays an important role in the use of DEM to simulate shock wave propagation through the particles. During calculations at time $t + \Delta t$, where $t$ is previous time and $\Delta t$ is the time step, contact force between particles is calculated which determines the net force or compaction force $\overline{F}$ acting on each particle. By using Newton’s second law, these resultant forces enable new acceleration, velocity and position of each particle. At time $t = 0$, force, velocity and position of each particle are known because it is the moment of the first hit. The velocity $\overline{v}_{i}^{(t+\Delta t)}$ of a particle $i$ at a time $t + \Delta t$, is determined by adopting a central difference scheme as

$$\overline{v}_{i}^{(t+\Delta t)} = \overline{v}_{i}^{(t+\Delta t/2)} + \overline{F}_{i} \frac{\Delta t}{m_{i}}$$

(3.1)

where the position $x_{i}$ is given by

$$x_{i}^{(t+\Delta t)} = x_{i}^{t} + \overline{v}_{i}^{(t+\Delta t/2)} \Delta t.$$  

(3.2)

During iterative calculations, the size of time step $\Delta t$ plays an important role to ensure numerical stability. For problems of a similar nature, Cundall and Strack [16] have proposed a relationship to calculate the time step which is further developed by O’Sullivan and Bray [72] for the central difference time integration scheme as

$$\max (\Delta t) = f_{t} \sqrt{\frac{m}{k}}.$$  

(3.3)

where correction factor $f_{t} = 0.01$ for the present case, $m$ is the mass of the lightest particle and $k$ is the approximate contact stiffness given by expression Eq. (2.7). This
value of the time step is shown to be sufficient to ensure numerical stability during calculations.

During the compaction process, particle contact goes through several loading, unloading and reloading sequences. In the beginning of compaction, contact force is initially elastic for small values of contact radius \( a \) and it is given by Eq. (2.4). The contact force follows the same curve during unloading and reloading in the elastic regime. At larger contact radius, the contact becomes plastic and contact force follows Eq. (2.5). The term relating the adhesion \( -2\sqrt{2\pi wE^*a^2} \) is added in elastic and plastic equations when considering adhesion traction. If the contact is unloaded, normal force follows elastic unloading Eq. (2.11). When contact is reloaded during unloading then it follows the same equation up to the value of the contact radius on which it was unloaded. Beyond this point, plasticity is reactivated and Eq. (2.5) applies.

The compaction models used in the dynamic loading of particles in Papers A-D are explained in the following sections.

### 3.2 Compaction model for one-dimensional chains of particles

The dynamic compaction models for homogeneous (in Paper A) and non-homogeneous (in Paper B) chains of particles are shown in the Figure 3.1 and 3.2, respectively. In Figure 3.1, there is a chain of micron-sized identical, spherical particles aligned in a container with one end open and the other blocked. At the open end, these particles are in contact with a compaction tool which has the same diameter as those of the particles. Friction between the particles and the container walls is not considered. In Figure 3.2, there are chains of spherical particles with different arrangements. These particles are in contact with compaction tool at one end and with the rigid wall on the opposite end. The model is confined to the one-dimensional motion of the particles. In both cases, hammer and compaction tool form the dynamic load which is given a certain initial velocity by a hydraulic pressure supply. The impact velocity along with the loading mass determines the compaction energy.
Figure 3.2: One-dimensional compaction model. (a) Homogenous particles, (b) particles of different materials, (c) particles with different sizes, (d) particles with voids between them, (e) considering adhesion/no adhesion between the particles, (f) combination of particles with different materials, sizes and gaps.
3.3 Compaction model for piston-die assembly with relaxation assists

The equipment used in experimental work of Bruska et al. [1, 2] is shown in the Figure 3.3. In those investigations, two new metal pieces, named relaxation assists are introduced in the piston-die assembly. These parts are of identical material and diameter as those of the piston but of different lengths. By using the setup of Figure 3.3, they performed experiments for high-velocity compaction and compared the results obtained with and without relaxation assists. The one-dimensional compaction model used for numerical simulation in Paper C is shown in the Figure 3.4. There is a chain of spherical particles aligned in a container. These particles are in contact with one of the loading elements – hammer, piston or relaxation assist – at front end and with relax assist RA2 or die wall at the rear end. Friction between the particles and container walls is assumed small and, therefore, not taken into account. The number of particles is identical in all the cases. The case B and E correspond to the experimental work [1, 2]. However, more cases i.e., A to E, are simulated in this paper to explain the effects of individual elements in detail. To start the compaction process, the hammer is given a certain initial velocity. The impact velocity along with hammer mass determines the compaction energy. The first case uses the hammer only as excitation and then piston and relaxation assists are incorporated into the model, as illustrated in Figure 3.4.

The variables describing the dynamic loading process are explained subsequently. The sum of ends displacement (SED) is the sum of net displacement of the compaction ends and the sum of particle deformation (SPD) is defined as the sum of the deformations of
all the particles, see Figure 3.5. The net displacement of a loading element is the change of its position during compaction process. As compaction proceeds, front compaction end moves forward with the loading element and particles are deformed resulting in an increase of SED and SPD. These two quantities change almost identically during the loading stage. However, this is not generally the case during the unloading stage. The reason for the difference between SED and SPD is that the loading elements move back to a longer distance compared to the total expansion of the particles (due to elastic unloading). This situation creates some space for particles to move freely and become separated. Here it is referred as room for separation and it can be interpreted as: Room for separation = SPD − SED.

### 3.4 Compaction model for two-dimensional assembly of particles

The two-dimensional dynamic compaction model used in *Paper D* is shown in the Figure 3.6. Three particular assemblies of micron-sized spherical particles are
investigated. These include a closely packed hexagonal assembly (case A), loosely packed random assembly (case B) and a non-homogenous assembly of particles with different sizes and material (case C). To start the compaction process, the hammer is given a certain initial velocity applying a hydraulic pressure supply. The impact velocity along with the hammer mass mainly determine the compaction energy. During the compaction process, particles deform, change their position and have velocities both in $x$ and $y$-directions. Particle rotation is neglected in this study. A particle may make several contacts with other particles and container walls at a time and its contacting partners may change as compaction proceeds. When a new contact between two particles is made, it is assumed to be in virgin state and then its history is maintained. If particles are separated and then make contact again, contact is resumed from the last unloading stage.

Figure 3.5: Sum of ends displacement (SED) and sum of particle deformation (SPD) are used to explain the compaction process.
Figure 3.6: Two-dimensional compaction model. (A) Tightly packed hexagonal, (B) loosely packed random, (C) non-homogeneous assembly. In model A and C, container having width of 32 normal particle radii is used.
Chapter 4

Dynamic compaction of spherical particles

This section describes the main results of simulation of dynamic loading of one and two-dimensional assemblies of spherical particles and effects of relaxation assists in a compaction assembly. The time step used is $\Delta t = 2.3$ ns which is estimated as explained in the Section 3.1. The most frequent particles are of aluminum of density 2700 kg/m$^3$, yielding stress 146 MPa, Young’s modulus 70 GPa and Poisson’s ratio 0.30. The material properties of the steel particles are: density 7800 kg/m$^3$, yielding stress 400 MPa, Young’s modulus 210 GPa and Poisson’s ratio 0.35.

4.1 Compaction of a one-dimensional chain of particles

Dynamic loading of a homogenous and non-homogenous particles are simulated in Paper A and B respectively. In both cases, one hundred particles are used. In first case, particles are of aluminum having diameter 100 $\mu$m while in second case heterogeneity is introduced by changing the material and size of the particles, voids between the particles and considering adhesion/no adhesion between them. Dynamic compression load is applied on the particles by supplying hydraulic pressure of 13.5 MPa which gives the hammer an impact velocity of 10 m/s. This impact velocity along with the different choices of loading mass results in a compaction energy of 1 J/g to 6.5 J/g. These loading parameters correspond to a typical high-velocity compaction process.

Dynamic effects during particle compaction like elasto-plastic shock wave propagation, particle contact behavior and their velocity along with loading parameters are investigated in Paper A. The dynamic load transferred in particles is described using elasto-plastic shock wave propagation variables like shock wave front velocity. The shock wave front is interpreted as the maximum absolute compaction force at a particular time while shock wave velocity is defined as the velocity of wave front. The movement of the shock wave from compaction to dead end and then back to the compaction end is described as one compaction cycle. The shock completes its one compaction cycle in the following
Figure 4.1: Dynamic loading of homogenous particles. (a) Propagation and reflection of elasto-plastic shock wave, (b) particle velocity, (c) particle deformation.
way; it starts from the compaction end, passes through the particles, reflected from the
dead end and then moves back from the last particle to the first particle. During forward
part of the cycle, as shock passes through a particle, net force on the particle increases
which results in the particle motion. This net force decreases to zero as particle gains
approximately the hammer velocity. The shock amplitude becomes negative as wave
moves back from the last particle to the first particle. It decreases the particle velocity
which eventually becomes zero. Shock wave propagation and velocity of particles are
shown in Figure 4.1a and b, respectively. As shock wave passes through the chain, it
results in particle plastic deformation. During one compaction cycle, deformation of all
the particles remains almost the same as in Figure 4.1c.

Effects of non-homogeneity on elasto-plastic shock propagation are examined in Paper
B. The results of the compaction of a mixture in which half of the aluminum particles
(particles 51 to 100) are replaced by steel particles are shown in the Figure 4.2. In the
beginning of the compaction process, aluminum particles are compacted in a normal
way. They are compacted and start moving approximately with the hammer velocity
as can be seen in Figure 4.2a. When the shock hits the steel particles, they are less
compacted and gain less velocity, due to their large contact stiffness and more mass.
It results in lowering the velocity of the aluminum particles while creating a reflected
shock in the aluminum particles. As incident shock wave proceeds in steel particles
(particles 51 to 100), a reflected wave moves back in aluminum particles towards the
compaction end. As the shock propagates in steel particles, they start moving while
velocity of aluminum particles decreases by reflected wave. Due to symmetric particles
arrangement, incident shock and reflected shock hit the compaction end and dead end,
respectively, almost at the same time. At this moment all the particles have almost
the same velocity which is nearly half the velocity of hammer. The incident shock is
then reflected back from the dead end while a reflected shock from the compaction
end goes through the aluminum particles. In this way, during one compaction cycle,
there are two extra reflected waves in the aluminum particles. Beside the incident
shock, aluminum particles are also compacted during these reflected waves as shown in
Figure 4.2b. This result in more deformation of aluminum particles compared to the
deformation of aluminum particles in a normal chain while having the same loading
conditions. Wave propagation velocity of the reflected shock is approximately equal to
that of incident shock in aluminum but the shock amplitude decreases considerably. The
average shock propagation velocity during first compaction cycle; for a chain consisting
of only aluminum particles is approximately 827 m/s, chain of only steel particles 803
m/s and for the symmetric case of aluminum and steel is 816 m/s. During the simulation
of these velocities, adhesion between particles is not taken into account. The wave
propagation velocity reduces due to adhesion between particles; for instance, in only
aluminum case it becomes approximately 763 m/s. In a random population of steel
particles in an aluminum chain, it is hard to distinguish between incident and reflected
shocks. However, it is possible to visualize easily the velocity of particles and their
deformation. Like a different material particle, changing the size of a particle effects
the shock propagation and deformation of particles during the compaction process.
Figure 4.2: Compaction of different material particles, Particles 1-50 are of aluminum and 51-100 are of steel. (a) Particle velocity, (b) particle deformation.
Generally, mixtures of particles with different sizes and materials depict similar behavior during the compaction.

In a chain of particles, voids or gap between particles affect shock propagation and their deformation during compaction. The results of a chain of homogenous aluminum particles with two voids before particles 56 and 57 are shown in the Figure 4.3. At the start of the compaction, shock travels from particle 1 to 55 in a normal way and the particles start to move with almost the hammer velocity. Due to void after particle 55, net force on it increases and results in a higher particles velocity, See Figure 4.3a. Particle 56 undergoes the same motion. When shock hits the particle 57, which is stationary before voids are covered, it starts to move. However, velocity of the particles behind it reduces. This fluctuation, caused by the sudden decrease in velocity of particles before voids, goes back to hammer, meanwhile the velocity of the particles after the voids increases. Fluctuation is reflected from the hammer and it moves in particles just before the main shock passes a particle. This fluctuation is reflected from the compaction ends and travels in particles distorting the motion of main shock. Since there is no continuous source behind this wave, it decreases and disappears practically after the third cycle. Particles are also compacted when this distortion passes through them. After the fluctuation dies out, particles are compacted in the normal way which is shown in Figure 4.3.

Heterogeneity due to change in sizes or material of particles have different influence than voids between particles. Disturbance caused by the voids between the particles decreases in strength and dies out after a few compaction cycles. However, disturbance due to change in size or material remains throughout the compaction process. It is possible to visualize and trace the effects of a single disturbance, even of a small magnitude, in normal chain of particles. However in the case of more disturbances, usually the effect of disturbances with lower strength is suppressed by those of the stronger disturbances.

4.2 Incorporating the relaxation assists in the piston-die assembly

The significance of relaxation assists in a piston-die assembly is investigated in Paper C. In the compaction model, the hammer mass is set to $1300 \times \text{particle mass}$ while the piston mass and relaxation assist mass are one half and one quarter of the hammer mass, respectively. The piston side in contact with the hammer has a radius of $18 \times \text{particle radius}$. The hammer is given an initial velocity of $3 \text{ m/s}$. In all the cases one hundred aluminum particles of diameter $2R = 100 \mu \text{m}$ are used. All the loading elements are made of steel with a high yielding stress, therefore, during loading, these elements deform only elastically. The density, Young’s modulus and Poisson’s ratio for piston and relaxation assists material are same as those for steel particles. The compaction process for various compaction systems (A to E in Figure 3.4) is simulated. The movement of the compaction ends, particle deformation and change in the energy of the loading elements are investigated. Furthermore, it is explained how relaxation...
Figure 4.3: Compaction of particles with voids of 0.1 radius between particles 55–56 and particles 56–57. (a) Particle velocity, (b) particle deformation.
Figure 4.4: Compaction process for case B. (a) Loading elements velocity, (b) net displacement and compact deformation.
Figure 4.5: Compaction process for case D. (a) Loading elements velocity, (b) net displacement and compact deformation.
assists offer a smooth compaction — where the particles are compacted more evenly at several compaction rounds — during the loading stage while reducing the particle separation during the unloading stage.

To explain the working of dynamic compaction system, two particular cases B and D (Figure 3.4) are discussed below. The loading elements in case B are the hammer and a piston. In the beginning of the compaction process, the hammer strikes the piston at the velocity of 3 m/s. As a result, the piston velocity increases from zero to around 4 m/s while the hammer velocity decreases to around 1 m/s, point P0 in Figure 4.4a. The piston compacts the particles until its velocity becomes zero at point P1. Then particles expand due to elastic unloading energy and push the piston back from point P1 to P2. Thereafter, the piston which moves freely until it is again struck by the hammer at P3. The piston velocity increases and particles are again compacted mostly plastically during the second loading to point P4. The second elastic unloading stage ends at P5 after which there is no change in SPD, see Figure 4.4b. However, the piston moves freely until it is again struck by the hammer at P6. Beyond the point P6 the velocity of the piston is negligible.

In case D, the loading elements are the hammer, the piston and relaxation assist #1 (RA1). In the beginning of the compaction process, the hammer strikes the piston which hits the RA1 and, as a consequence, the hammer velocity decreases to 1 m/s while the piston and RA1 gain velocity to around 1.5 m/s and 5 m/s, respectively (Figure 4.5a). RA1 compacts the particles until its velocity becomes zero, point P1 in the Figure 4.5. Then the particles expand and push the RA1 back from P1 to P2. RA1 moves freely from P2 to P3 where it is again struck by the piston. During this collision piston velocity decreases. However, it regains energy at the collision with the hammer at P5. This sequence of operations is repeated in the next two compaction rounds after which the absolute velocity of the loading elements becomes small. The introduction of RA1 makes the compaction process smooth with the less particles expansion during unloading stage as can be seen in Figure 4.5. Finally, the presence of RA1 reduces the room for particles separation, and thus, is improving the compaction process.

Figure 4.6 illustrates the improvements of incorporating different loading elements; piston, RA1 and RA2 to the simple hammer die system (case A). Figure 4.6a shows that the compaction takes place more evenly from case A to E. Similarly, SPD increases in the same sequence, see Figure 4.6b. In addition, the room for separation reduces accordingly. Finally the hammer velocity for different cases are shown in the Figure 4.6c. At the end of the compaction process, case E has minimum absolute velocity which indicates that most of the the hammer kinetic energy is transferred to the compact deformation (including piston, RA1 and RA2).

Adhesion between particles plays an important role during the unloading stage. As unloading stage proceeds, particles expand due to elastic unloading energy and push back the loading element. The contact force between the particles decreases and these particles start to move with different velocities depending upon their position from the loading element. In case of without adhesion, most of the particles are separated as the
Figure 4.6: Comparison between all the compaction models. (a) Displacement of compaction ends, (b) compact deformation, (c) hammer velocity.
Figure 4.7: Particles separation when adhesion is taken into account. (a) Separation of a particle from its predecessor, (b) total separation.
contact force between them becomes zero. However, in case of with adhesion, additional tensile force is required to separate the particles. Therefore, only a few particles are separated.

Figure 4.7a shows particle separation — the separation between two adjacent surfaces of a particle and its predecessor — in case of adhesion between the particles. The results shown are at the end of final particle expansion. Obviously, the more loading elements (A to E), the less number particles are separated and the less are separation between the particles. Figure 4.7b shows the total separation between all the particles for these cases.

4.3 Compaction of a two-dimensional assembly of particles

The dynamic loading of two-dimensional assembly of particles is investigated in Paper D. Three different cases, as shown in the Figure 3.6, are investigated. In case A and C, 992 particles and in case B 100 particles are taken into account. Fewer particles are considered in case B since it is hard to visualize the position of more than, say, one hundred particles. The hammer impact velocity is 5 m/s which along with different choices of loading mass results in a compaction energy of 0.1 J/g to 0.6 J/g. In the present study, net force, particle velocity and displacement are taken positive along positive $x$ and $y$-axes, otherwise negative. Similarly, compression particle deformation is positive. The sum of all the contact deformations of a particle is named particle deformation and the sum of all the particle deformation is named compact deformation. In simulation, aluminum particles with the radius of 50 $\mu$m are used. In the following, the dynamic loading of loosely packed random particle assembly, with the same initial position as shown in the case B in Figure 3.6 is explained. The positions of the particles during compaction process are visualized in Figure 4.8 along with the hammer velocity at corresponding times in Figure 4.9a. In the beginning of the compaction process, particles move to fill the cavities in the container. Then particles rearrange their positions to fill the gap between particles and finally make almost the hexagonal shape with a fully packed assembly, positions at P0, P1 and P2 in Figure 4.8. The hammer kinetic energy decrease at a slow rate during filling of the cavities and rearrangement of the particles, as can be seen in Figure 4.9a. During the rearrangement period, particles deformation mainly depends upon their location in the assembly, see bar graphs in Figure 4.9. Up till rearrangement point, P2 in Figure 4.8, particles which fill the cavity are mainly elastically compacted while mostly recover their original dimensions by unloading. After densely packed, particles are heavily compacted. As particles are deformed at higher rate, therefore, hammer velocity decreases sharply, point P2 to P3 in Figure 4.9a. Similarly, there is less change in particles positions; compare positions P2 and P3 in Figure 4.8.

The effects of friction and adhesion between particles and between particles and
Figure 4.8: Particles positions at different stages of hammer velocity, see Figure 4.9a.
Figure 4.9: Dynamic compaction of random particles assembly. (a) Hammer velocity, while bar graphs are particle deformation at corresponding points mentioned in (a).
Figure 4.10: Effects of friction and adhesion on compaction process. (a) Hammer velocity, (b) compact deformation.
container walls are examined. The assembly consists of loosely packed random particles of the same material and size, see case B in Figure 3.6. The effect of the frictional force at a particular contact between two particles is to oppose the relative motion of the contacting surfaces. During dynamic compaction, each particle makes several contacts with other particles. In the current scenario of loosely packed assembly, friction resists the particles rearrangement in the beginning of the compaction process, see stage S1 in Figure 4.10. Therefore, more kinetic energy of the hammer is used during rearrangement of particles which affects its velocity, Figure 4.10a. In the normal case without friction and adhesion, particles rearrange their positions easier, earlier and velocity of hammer decreases slower. However, at the end of compaction stage, S2 in Figure 4.10a, the particles without friction move more readily into a dense, hexagonal like assembly, and are therefore resisting the hammer displacement strongly, resulting in a sharp hammer velocity reduction. On the other hand, the particles with friction move more slowly into the dense, hexagonal like assembly, thus resulting in a later and slower hammer velocity decrease, see S2 in Figure 4.10a. In the present situation, there is more compact deformation at the end of loading stage in friction case compared to the normal case, see Figure 4.10b. This compaction also includes small amount of recoverable elastic unloading deformation. Finally, adhesion between particles effects on the compaction process in a similar fashion as that of friction, Figure 4.10.
Chapter 5

Conclusions and outlook

In this study, discrete element method is used to investigate the dynamic loading of a one and two-dimensional assembly of spherical particles. The elasto-plastic shock propagation, particle velocity and deformation are simulated in a homogenous and non-homogenous chains of particles. In the case of a two-dimensional hexagonal close packing, simulation shows particles deformation when shock propagates through the particles during different cycles. Results show the force exerted by the particles on the container walls and effects of the incident shock which travels in the direction of dynamic load. The change in compact deformation with the hammer movement are plotted. In addition, the compaction of a loosely packed random particles assembly is simulated. Results show how particles rearrange their positions to become closely packed in the end the compaction process. Furthermore, changes in particles positions and their deformation with the load movement are shown. In addition, the effects of friction and adhesion between particles are discussed. It is shown that both friction and adhesion increase the overall particles deformation resulting in less hammer kinetic energy during unloading.

Furthermore, the discrete element method is used in this study to investigate numerically the significance of relaxation assists in a one-dimensional model of a compaction assembly. It is shown that by using the relaxation assists, the locking of particles is improved during the compaction process. Simulation results show the displacement of the compaction ends and particle deformation during the whole compaction process. It is found that particles are more compacted and the room for particle separation is reduced by using relaxation assists in the compaction assembly. The movement of the relaxation assists during the compaction process is also plotted which is difficult to acquire experimentally. It is shown that the presence of relaxation assist offers; smooth compaction during loading stage, prevention of particles separation during unloading stage and conversion of the higher kinetic energy of the hammer into particle deformation.
The present study is believed to enlighten several new aspects of elasto-plastic shock waves in high-velocity compaction. Nevertheless, it would be interesting to expand this work in several directions including:

- Extension of the one and two-dimensional analysis to three-dimensions
- Examine the effects of each relaxation assistant separately
- Investigation of complex die geometries including the more realistic objects such as gears, bearings and tools
- To investigate multi-stage high-velocity compaction including double acting compaction
- To model more complex particles such as non-spherical particles and nano-particles
Chapter 6

Summary of Appended Papers

6.1 Paper A

Discrete element simulation of elasto-plastic shock wave propagation in spherical particles

M. Shoaib and L. Kari

Elasto-plastic shock wave propagation in a one-dimensional assembly of spherical metal particles is presented by extending well established quasi-static compaction models. The compaction process is modeled by a discrete element method while using elastic and plastic loading, elastic unloading and adhesion at contacts with typical dynamic loading parameters. Of particular interest is to study the development of the elasto-plastic shock wave, its propagation and reflection during entire loading process. Simulation results yield information on contact behavior, velocity and deformation of particles during dynamic loading. Effects of shock wave propagation on loading parameters are also discussed. The elasto-plastic shock propagation in granular material has many practical applications including the high-velocity compaction of particulate material.

6.2 Paper B

Simulating the dynamic loading of non-homogenous spherical particles using discrete element method

M. Shoaib and L. Kari

Dynamic loading of a chain of non-homogenous spherical particles is presented by using the discrete element method. The dynamic response of particles is modeled by using
elastic and plastic loading, elastic unloading and adhesion at contacts. Of particular interest is to study the transmission and reflection of elasto-plastic shock wave through a chain having; particles of different sizes and materials, voids between the particles and particles with/without adhesion at contacts. Simulation yields information on shock propagation, particles velocity and their deformation during dynamic compaction. Furthermore, particles deformation during incident and reflected shocks, particle velocity fluctuations due to voids between particles and effects of adhesion on particles separation during unloading stage are simulated. Although the developed model is confined to one-dimensional studies, nevertheless useful for simulating high-velocity compaction processes.

6.3 Paper C

Simulation of high-velocity compaction process with relaxation assists using the discrete element method

M. Shoaib, L. Kari and B. Azhdar

The discrete element method is used to investigate the high-velocity compaction process with additional piston supports known as relaxation assists. It is shown that by incorporating the relaxation assists in the piston-die assembly, particles can be better locked during the compaction process. The simulation results reveal that relaxation assists offer; smooth compaction during loading stage, prevention of the particle separation during unloading stage and conversion of higher kinetic energy of hammer into particle deformation. Finally, the influences of various loading elements on compaction process and effects of presence of adhesion during unloading stage are investigated. The results support the findings of experimental work.

6.4 Paper D

High-velocity compaction simulation of a two-dimensional assembly of spherical particles using the discrete element method

M. Shoaib and L. Kari

High-velocity compaction of a two-dimensional assembly of spherical particles is numerically studied using the discrete element simulation technique. Three particular cases are investigated including closely packed hexagonal, loosely packed random and a non-homogenous assembly of particles of various sizes and materials. Of primary interest is the linking of particles deformation with the elasto-plastic shock wave propagation.
Simulation yields information on particle deformation during shock propagation and change in overall particles compaction with the velocity of the hammer. Moreover, the force exerted by particles on the container walls and rearrangement of the loosely packed particles during dynamic loading are also investigated. Finally, effects of presence of friction and adhesion on overall particles deformation and compaction process are simulated.
Bibliography


