Numerical modeling of strain localization in granular materials using Cosserat theory enhanced with microfabric properties

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NUMERICAL MODELING OF STRAIN LOCALIZATION IN GRANULAR MATERIALS USING COSSEARAT THEORY ENHANCED WITH MICROFABRIC PROPERTIES

A Dissertation

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirement for the degree of Doctor of Philosophy

In

The Department of Civil and Environmental Engineering

By
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August, 2004
To my parents, Ibrahim and Fatima

To my Fiancée
ACKNOWLEDGMENTS

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ABSTRACT

Finite element solution in the updated Lagrangian frame is used to investigate the strain localization phenomenon “shear bands” in granular materials. The micro-polar theory was used as the mathematical foundation for the continuum formulations. A laboratory testing results are used for verification and comparison with the numerical simulation. Silica sand and glass beads with different shape indices, size and surface roughness were tested under biaxial and triaxial loading conditions to investigate the physics of the problem. The shape non-uniformity and the irregular surface roughness of the grains were studied carefully to evaluate their effect on shear band characteristics. To this end, attempts have been made to bring these additional micro-properties into the constitutive equations in this study. Elasto-plastic constitutive laws with a non-associated flow rule were used in order to capture the high deformations inside the localization zones. The Micropolar theory requires two independent kinematical fields; the first is the Cosserat objective strain tensor and the second is the curvature or the rotation gradient vector. The deviation in the kinematics is performed using the classical continuum with the incorporation of the couple stress effect.

A single hardening yielding model, (Lade’s model), with a different plastic potential function has been enhanced to account for the couple stresses and the rotations of the grains through the stress invariants. Finally, the finite element formulations in the updated Lagrangian frame were obtained. These formulations have been implemented into the finite element program ABAQUS using the user element subroutine utility (UEL). The study findings were consistent with the experimental results and the physical understanding of the phenomenon. The surface roughness of the particles was found to affect the shear band thickness and present model was able to feel such effects. The shape of the particles was found to significantly affect the shear
band thickness as well. The effect of the initial void ratio, confining pressure, particle size, surface roughness and shape of particles is discussed in this dissertation. At the end, the material properties spatial distribution was mapped into the finite element mesh and the material heterogeneity effect on strain localization is shown accordingly.
CHAPTER ONE

INTRODUCTION

1.1 Introduction

Granular materials exhibit a complex constitutive behavior. The complexity in the continuum behavior of the granular materials is essentially caused by the composition of the continuum and its micro-properties. The macro-composition of the continuum contains, in general, solids, liquid and gas. Each of these components has its own mechanical behavior and the mixture makes the continuum behavior complex that in some cases may not be adequately described by classical mechanics. The microstructure of the grains and how it affects the behavior is essentially justified by the non-uniformity in the shape and surface roughness at the micro or even at the nano-scale. The heterogeneity and anisotropy of the soil fabric due to the discreteness of the grains can also be considered. During the hardening regime, granular materials behave as a continuum until the failure or the instability point where deformations begin to localize into a small but finite shear zone, which is termed the shear band. Thicker shear bands indicate less shear strength, the angle inclination of such bands with respect to the minimum principal axis give an idea about the stability of the soil mass. In other words, this shear band which represents the failure zone can be treated as a failure surface in a given slope or soil mass under certain boundary conditions. The shear band is of interest to geotechnical engineers due to the fact that it appears in many real geotechnical structures (retaining walls, dams, foundations, highways, earth-fill embankments, slopes etc.) and it is the cause of major failures in these applications.

The present study is basically concentrated on the strain localization phenomenon in granular materials under plane strain conditions. It has been known that solutions for the strain
localization using classical continuum mechanics with numerical or analytical techniques suffer from ill-posed mathematics; therefore, non-classical methods are needed to rectify the problem. These methods should incorporate an internal length scale embedded in the formulation, which might be addressed using the gradient theory, Cosserat continua, or other non-local theories. In this study, the Cosserat continuum or the micro-polar theory was used to investigate the phenomenon of shear band formation considering the particle size as one of the internal length scales. However, this internal length scale might be adjusted to account for some micro-property effects such as the shape and the surface roughness of the particles.

Special attention was given to the material heterogeneity; this was done using, to some extent, real particle size distribution, real particle shape indices and real local void ratio distribution, all those distributions were obtained from SEM images. In this case the simulation will be more realistic in the sense that no localization zones will be forced to develop in a certain region or direction.

1.2 **Dissertation Objectives**

The main objective of this work is to model the behavior of granular materials using the Cosserat or the Micropolar theory. The main contributions of the current study are as follows:

1. Enhance the Lade’s yield function and plastic potential function to account for the effect of the couple stresses.
2. Incorporate the particle’s shape effect in the numerical solution to predict strain localization, certain shape indices and parameters at the micro-level will be used; the effect of the shape will be significant on the couple stress and angular momentums.
3. Study the effect of the particle surface roughness on the rotation and sliding resistance which will be explicitly formulated in the model.
4. Characterize the properties of natural silica sand and glass beads by developing shape and surface roughness indices using digital imaging techniques and utilizing the Scanning Electron Microscope (SEM) and the Optical Profiler (OP) (Alshibli and Alsaleh, 2004).

5. Study the effect of the surface roughness and shape of the grains on the shear banding under biaxial testing. The experiments were performed by (Alshibli (2004), Novoa (2003) and by the author).

6. Use the finite element program ABAQUS to implement the solution for the non-linear finite element system of equations. The implementation will be through user material and user element subroutines for ABAQUS.

7. Verify the numerical model using experimental data.

1.3 **Dissertation Outline**

The dissertation is organized as follows; the first Chapter is an introduction to the problem in hands showing the objectives of this study. In the second Chapter the author tried to show the literature survey that had been done to introduce and understand the problem. Chapter Three shows the materials and material characterization that were used in the study for the verification purposes. In Chapter Four, a detailed discussion was prepared for the constitutive model and the enhancement for that model to work in the Cosserat continuum. The finite element formulations are presented in Chapter Five; all the derivations in the updated Lagrangian frame have been shown. Chapter Six shows the finite element implementation using the User Element and User Material subroutines for ABAQUS. The results and discussions with verifications are presented in Chapter Seven and finally Chapter Eight lists the conclusions and the recommendations for future work.
CHAPTER TWO

LITERATURE REVIEW

2.1 Introduction to Strain Localization in Granular Materials

Many researchers have been working on strain localization in metals, composites and geomaterials since the early 1900’s. Coulomb’s equation for the shear strength was used by many researchers to describe the behavior of soils. It represents a single failure surface at a certain inclination with respect to one of the principal axes. Coulomb (1776) could observe the single failure surface behind a yielding wall when he introduced the active earth pressure coefficient. It was extended to the passive case (Gudehus and Konrad, 2002). Coulomb developed the well–known shear strength equation; Otto Mohr later came up with his known envelop that represents a limit for strength and stability. However, the Mohr-Coulomb theory or criterion has limitations when it comes to describing the constitutive behavior of granular materials (Rowe, 1962).

The granular assembly consists of discrete or discontinuous grains that have different shapes and sizes; therefore, the suggestion to treat it as a continuum is not correct and needs to be studied carefully. Rowe (1962) conducted experimental and theoretical study on ideal assemblies of rods and spheres to show that the shear strength and dilatancy depend on the surface friction, the way the particles packed and on the energy losses. Rowe’s findings support the fact that the strain localization will be affected by the shape of the particles “packing” and by the surface roughness which controls the friction.

Strain localization has been extensively investigated in the last two decades (e.g; Vardoulakis, 1979, 1980, 1981 and 1983; Vardoulakis and Aifantis 1989 and 1991; Vardoulakis and Sulem, 1995, Mühlhaus, and Vardoulakis, 1987; Mühlhaus, et. al., 2001 and 2002; Gudehus,

2.2 Theoretical Predictions of Shear Bands

As mentioned earlier there are several theoretical and numerical methods to study the shear bands or strain localization in granular materials. The following methods or theories are presented in this chapter.

2.2.1 Theory of Bifurcation

Bifurcation in a certain continuum implies that the deformations migrate from a continuous mode to both continuous and discontinuous modes. The theory of bifurcation has been used in the last three decades to investigate the splitting within the material continuum to capture the strain localization phenomenon that occurs in the post-bifurcation regime. When the localization begins to take place, the continuum will mostly split into three regions; the localization zone, and two new continua zones, one to the right and another to the left of this zone. The balance or equilibrium equations have a mathematical restriction; the acoustic tensor should vanish to have a non-trivial solution for the system of the differential equations that have a non-unique solution. The mathematical basis of this theory actually explains well the discontinuity that occurs in the continuum. Among the researchers who have pioneering contribution to this area, are Vardoulakis (1979, 1983), Sulem and Vardoulakis (1990), and Vardoulakis and Sulem (1995). In 1971, Cheng et al. investigated the necking and bulging phenomena in elasto-plastic cylindrical materials based on the theory of bifurcation. Their
findings were actually consistent with some findings in the literature in terms of the all-around hydrostatic pressure effect on the bifurcation limit. Once there is no volumetric change in the sample then the hydrostatic pressure will not improve the strength.

Vardoulakis (1979) investigated the bifurcation in triaxial tests and concluded that bifurcation might occur during the hardening stage and not only in the softening regime. In other words, strain localization begins to take place early in the triaxial tests. Vardoulakis (1983) extended his work by investigating the bifurcation in triaxial tests using rigid-granular dilative material and non-associated flow rule. He found that bulging occurs in the softening regime and necking occurs in the hardening regime. In the same article, Vardoulakis emphasized that the deformation discontinuity in triaxial test might take the shape of rigid cones at both ends of the specimen with shear bands in compression; and necking that localizes at the mid height of the specimen under tensile loading. In fact any of those localization zones are surrounded by discontinuity surface that have a significant jump in the velocity gradient. Based on the assumed continuity and compatibility laws one might be able to capture the localization zone.

Sulem and Vardoulakis (1990) distinguished between the two modes of bifurcations; one is the discontinuous or localized and the second is the continuous or the diffuse bifurcation. In the latter mode, tensile stresses might occur; leading to a vertical splitting in the sample as one type of the bifurcation modes. In triaxial test analysis for rock specimens, Sulem and Vardoulakis (1990) emphasized on the fact that the bifurcation will be initiated as the equations of axisymmetric motion have a non-unique solution. The bifurcation modes “diffuse and localization” provide sufficient information about failure progress in materials; diffuse mode might occur in the pre-peak regime where the strain localizations have more chances to occur in the post-peak regime of the stress-strain curve (Chau, 1992).
Extensive work has been reported by Vardoulakis and Sulem (1995) on the bifurcation phenomenon in triaxial and biaxial loading conditions. If one considers only the homogenous solution for the boundary value problem then no bifurcation will be observed and only homogenous stress and strain fields will be obtained. However, if the non-trivial solution is considered then the mathematical bifurcation will occur leading to one of the bifurcation modes. It is worth noting that the kinematics and the constitutive laws will highly control the results (Vardoulakis and Sulem, 1995).

Ikeda et al. (1997) have developed a technique to trace the bifurcation modes on the stress-strain curve. They introduced a mode switching phrase to avoid the assumption of the bifurcation uniqueness. Saada et al. (1999) studied the strain localization as one type of the bifurcation modes in thin long hollow cylinders of sands loaded by axial torsional and spherical (all-around) stresses.

Bauer (1999) used a rate-independent hypoplastic constitutive model to investigate the effect of the density and the pressure on the bifurcation. Instability type of failure happens in loose granular materials due to contractions and strain localization occurs in dense or dilative ones (Lade, 2002).

In summary the bifurcation theory can be applied to frictional and cohesive materials, metals as well as rocks to investigate failure modes such as necking, bulging, splitting and shear banding. The loading conditions, boundary conditions and the constitutive model of the material are factors that control the failure mode.

### 2.2.2 Cosserat “Micropolar” Continuum

The Cosserat theory can successfully separate the grain rotation from its translation adding other three additional degrees of freedom to any point in the 3D continuum. In classical
Continuum mechanics one has two different strain tensors, the Green-Lagrangian strain tensor and the Eulerian strain tensor. Either one of these tensors can be decomposed into symmetric part (stretch tensor) and antisymmetric part (spin tensor).

Granular materials undergo high rotational and translational deformations at failure. Therefore, the classical strain tensor fails to capture the real kinematics such as micro-rotation in granular materials and other alternative tensors need to be used instead (Vardoulakis and Sulem, 1995; Oda and Iwashita, 1999). Since the grains undergo rotational and translational deformations, then for a single grain one might have six degrees of freedom (three rotational and three translational) in the 3D space.

The Cosserat point has been found very reasonable to represent the individual grains in terms of kinematics (Kanatani, 1979 Mühlhaus and Vardoulakis 1987; Vardoulakis and Sulem 1995; and Oda and Iwashita 1999). According to Rubin (2000), the two Cosserat brothers (1909) were the first people who assigned directors for a point in any continua. In the Cosserat point, one might have translational and spinning (or rotational) deformation or velocity vectors. Researchers after Cosserat brothers made use of the Cosserat theory for points, shells and rods, and extended this theory for further applications in mechanics. Ever since researchers renamed the technique as micropolar theory, oriented continua, continuum theories with directors, non-local media, etc. (Vardoulakis and Sulem, 1995). In geomechanics, interests in Cosserat continuum began to increase in mid 1970’s where the links were made between Cosserat kinematics and strain localization phenomenon. In 1979, Kanatani used the micropolar theory to study the flow of granular materials; the grains were assumed to be homogenous rigid spheres with the same size. In his formulations the velocity ($v_i$) and the rotation ($\omega_{ij}$) of the grains are considered two independent variables that describe the deformation of the continua.
Making use of these independent kinematics in the macro conservation laws of mass, linear momentum and angular momentum, Kanatani was able to propose equations of motion for the granular materials. However, the assumption that grains have uniform contact distribution due to spherical shape of the particles is not correct and the non-uniformity of the shape should be accounted for instead.

Mühlhaus and Vardoulakis (1987) used the Cosserat kinematics for 2D space to investigate the thickness of shear bands in granular materials. Their work was one of the strongest links between the Cosserat continuum and strain localization in granular materials. In their approach, the continuum has an overall rotation ($\omega_{ij}$) which is different than the grain or the Cosserat rotation ($\omega_{ij}^c$). The deviation in the rotation would actually cause the non-symmetry in the strain and stress tensors and as a result those tensors will be different than the classical ones. Assuming infinitesimal deformation in the pre-banding regime, the following kinematics were proposed for plane strain case:

\begin{align}
\epsilon_{ij} &= \theta_{ij} + \omega_{ij} - \omega_{ij}^c \\
\kappa_i &= w_{3,i}^c \\
\end{align}

where;

\begin{align}
\theta_{ij} &= \frac{u_{i,j} + u_{j,i}}{2} ; \quad \omega_{ij} = \frac{u_{i,j} - u_{j,i}}{2} \\
\omega_{ij}^c &= -e_{ijk} w_{3}^c \\
\end{align}

where, $e_{ijk}$ is the Ricci permutation tensor. The curvature or the rotation gradient $\kappa_i$ is a measure of the relative rotation of a single grain with respect to the neighboring grain. If the rotation of the continuum coincides with the grain rotation then Equation (2.1) collapse into a classical
strain tensor. Following Kanatani (1981) and Nemat-Nasser & Oda (1982), a uniform distribution function for the contact normal was assumed over the perimeter of the sphere, \( f(\alpha) = \pi^2 \). Accordingly, Mühlhaus and Vardoulakis (1987) proposed a shear strain invariant that measures the slip at the contact between two neighboring grains as:

\[
\gamma = \left( g_1 e_{ij} e_{ij} + g_2 e_{ji} e_{ji} + g_3 R^2 \kappa_k \kappa_k \right)^{1/2}
\]  

(2.5)

where; \( g_1, g_2, \) and \( g_3 \) are weighting factors and the deviatoric strain tensor is defined as:

\[
e_{ij} = \varepsilon_{ij} - \frac{1}{2} \varepsilon_{kk} \delta_{ij}
\]  

(2.6)

Where, \( \delta_{ij} \) is the Kronecker delta. Equation (2.5) holds for continua that have translational and rotational degrees of freedom, however it might reduce to the classical one if the continuum rotation coincides with the grain rotation and the rotation of the grains is negligible. Therefore, one should be careful of making any assumptions that might lead to significant erroneous results. Vardoulakis and Sulem (1995) used the same arguments to represent the kinematics of the granular media with the Cosserat theory. Huang and Liang (1995) have used the micropolar theory to solve two-dimensional boundary element problems; they verified their work by solving problems of thermal stress in hollow cylinders. In (1996), Ristinmaa and Vecchi investigated the strain localization in materials using micropolar kinematics. Same concepts were used in their work to address the rotation and translation of any point in the continuum using the constrained Cosserat continua. Ristinmaa and Vecchi (1996) confirmed that in the Cosserat continuum, the thickness of the localization zone is a mesh independent due to the regularization of the deformations tackled by the rotational degrees of freedom.

Tejchman and Bauer (1996) polarized a hypoplastic constitutive model using the Cosserat rotation and the couple stress, their model was able to capture the shear banding in
biaxial type of testing. Oda et al. (1996) have investigated the phenomenon of strain localization in granular materials and supported the notion that the rotations of the grains are dominant at failure and must be taken into consideration with their couple stresses.

Ehlers and Volk (1997) developed coupled equations for a saturated cohesive-frictional porous media using micropolar kinematics. They distinguished between the continuum and the point rotation. Oda et al. (1997) emphasized on the fact that the grain rotations affect the behavior of the granular media at failure, in other words the dilatancy of the media is highly affected by the grain rotations. Adhikary and Dyskin (1997) developed a model for layered geomaterials based on the Cosserat theory to incorporate the rotations of the grains and the couple stresses that cause such rotations. The couple or moment stresses were found of high importance on the behavior of granular materials (Adhikary and Dyskin, 1997). Oda et al. (1997) studied the importance of the grain rotation on the behavior of the continua. Limat (1998) studied the elastic behavior of disks using micropolar elastic continua in which he confirmed that high rotations exist at failure and in the localized zone that need to be considered in the kinematics. Adhikary et al. (1999) emphasized that the couple stresses used in the Cosserat-type-of models are helpful in terms of overcoming the internal instabilities and interfaces interaction. The most rapid rotations were observed by Kuhn (1999) within and near micro-bands in the deforming granular materials. Oda and Iwashita (1999), emphasized that rotations and couple stresses should be considered in the modeling of granular materials. Those quantities are important and should be accounted for regardless of the type of the model or the solution technique.

The constitutive model should allow one to describe some phenomena inside the material, such as; slip system between the grains, strain localization and the grain rotations.
(Smolin et al., 2000). Bauer and Huang (2001) presented a numerical solution for the strain localization phenomenon in granular media under shearing; within the framework of the hypoplastic Cosserat continuum. The rotation of the grains at the boundaries and within the continua showed significant roles in controlling the results of shear banding. Pasternak and Mühlhaus (2001) derived a Cosserat continuum for granular materials in which they accounted for the relative rotations and the couple stresses at the contacts. In 2001, Tejchman and Gudehus and Tejchman and Poland have studied the shear banding or strain localization in a polar type-of-continua. Then Huang et al. (2002) extended the original hypoplastic model developed by co-workers (Gudehus 1996, Bauer 1996 and Tejchman 1997) to account for polar quantities and other internal variables. Antoinette and Walsh (2002) introduced the rolling resistance into a micropolar model; the importance of such resistance will definitely control the couple stresses at the contact and therefore affecting the behavior of the granular media. Pasternak and Mühlhaus (2002) extended their earlier work to investigate the large deformations in the granular media using the Cosserat continuum to account for the rotational degrees of freedom.

In summary, there is no doubt that the Cosserat or the micropolar theory is a powerful tool that accounts for the different types of deformations in granular continua.

### 2.2.3 Strain Gradient Theories

As mentioned earlier, the boundary value problem becomes ill-posed mathematically in the post-localization regime, moreover, the mesh-dependent solution might lead to a vanishing thickness as the mesh refined in the FE solution. These facts were actually supported by many researchers (e.g., Vardoulakis and Aifantis 1989 & 1991, Vardoulakis and Sulem 1995, Bauer and Huang 2001 and Voyiadjis and Song 2001). Strain homogenization or regularization technique is a good tool to overcome such phenomenon in large deformation problems,
Voyiadjis and Song (2001)). One alternative for such regularization is the Cosserat rotation and its’ gradient “the curvature”; the other effective approach is the use of high-order strain gradients. Among the researchers who contributed to this area, Vardoulakis and Aifantis (1989) who used the second-order gradient theory in studying the heterogeneous deformation in the granular media.

The dilatancy of the granular materials becomes gradient dependent and thereafter the Coulomb yield surface and the balance equations will be as well. In the same paper, Vardoulakis and Aifantis have modified a flow theory to incorporate high-order gradients and investigate the liquefaction problem in granular materials. Following this work, Vardoulakis and Aifantis (1991) have extended their findings to incorporate the second-order gradients into the flow rule and the yield function; therefore, with an appropriate length scale they were able to capture the shear band thickness.

For detailed formulations and better understanding for this application, interested readers are referred to Vardoulakis and Sulem (1995). Chambon et al. (2001) proposed local and Cosserat second-order gradient theories models to deal with the localization phenomena in geomaterials. Oka et al. (2001) used gradient dependent viscoplastic constitutive models to study the localizations in water saturated soils. In their study, they have used the second-order strain gradient in the hardening function and found that strain localization is highly dependent on the strain gradient. In 2001, Voyiadjis and Song have used the second-order gradient theory for the internal state variables of the porous media to capture the shear banding in such materials. The thermoelastic Helmholtz free energy function are dependent on those internal variables and their second-order gradients. Yang et. al. (2002) and Chen and Wang (2002) introduced a coupling between the use of the couple stresses and the high-order strain gradient theory through new
deformation theories. Borja (2002) proposed a finite element solution for the shear banding evolution using the deformation gradient to map between stress tensors. Song and Voyiadjis (2002) and Voyiadjis and Song (2002) used the gradient theory to account for the micro interaction between geomaterials’ grains to capture strain localizations. Voyiadjis and Dorgan (2002) used the second-order gradient theory in the kinematic hardening in order to introduce a material internal length scale.

In summary, that the gradient theory has been used as a very effective tool to homogenize the deformation and stress fields for the sake of studying the strain localization problems in geomaterials. Coupling between the micropolar theory and the gradient theory would really lead to more accurate assessment for strain localization.

2.2.4 **Couple Stresses**

Based on the fact that the grains are non-uniform in shape, they are neither spherical nor elliptical, then the interaction between such grains will generate a non-symmetric stress and couple stress tensors. The incorporation of the couple stresses into the simulation tools has not yet been addressed well. Kanatani (1979) was the first to propose micropolar formulations to study the effect of the couple stresses on the flow of granular materials. In his paper, Kanatani used duality between the couple stresses and the rate of the grain rotations; in other words, the link between the energy dissipation function and the couple stresses can be made through the rate of grain rotation. Mühlhaus and Vardoulakis (1987) and Vardoulakis and Sulem (1995) used the same argument to incorporate the effect of the couple stress into stress invariant. Ristinmaa and Vecchi (1996) have used the couple stress theory to capture the effect of the rotations on the localization of deformation in materials. Oda and Iwashita (1998, 1999, and 2000) and Oda et al. (1997, 1998), modified distinct element methods to incorporate the effect of the couple stresses
on the behavior of granular materials. Adhikary *et. al.* (1999) modeled the large strains using the micropolar theory and they assumed that the couple stress tensor to be conjugate in energy with the rate of rotation. Ehlers and Volk (1997, 1999) investigated the localization phenomena in the saturated porous media accounting for the effect of the couple stresses through the micropolar theory. Huang and Liang (1995) and Huang *et. al.* (2002), Bauer (1999) and Bauer and Huang (2001) extended a hypoplastic model to incorporate the couple stresses effect on the behavior of granular materials. Although the couple stress might be small if compared with the stress tensor but still it has an important effect on triggering the shear bands.

### 2.2.5 Constitutive Relations for Granular Materials

Many constitutive models have been proposed in the literature to describe the behavior of granular materials. However, most of the formulations within the framework of the theory of plasticity, hypoplasticity, hyperplasticity or the viscoplasticity have been developed to deal with a classical type of stresses and deformations. The problem in hands, however, requires non-classical equations to describe physical phenomena inside the continuum during loading-unloading conditions. Due to the discreteness of the granular continua and the nature of the grains, high irreversible deformations have been observed theoretically and experimentally.

Elasto-plastic behavior for such rate-independent materials was found sufficient to describe the high deformations that take place in granular materials. To describe the elastoplastic behavior of the materials one needs to have the theory of elasticity, yield criterion, plastic potential, hardening/softening rules and appropriate flow rule. Mühlhaus and Vardoulakis (1987) and Vardoulakis and Sulem (1995) used Mohr-Coulomb yield criterion and plastic potential with a non associated flow rule and modified invariants to describe the strain localizations in sands. Ristinmaa and Vecchi (1996) modified the von Mises yield function to incorporate the couple
stresses and they were able to capture the strain localization phenomenon. Bauer (1996, 1999), Bauer and Huang (2001), Huang et al. (2002), Tejchman and Wu(1996) and Tejchman and Poland (2001) used a modified polar hypoplastic type of model to investigate shear banding in granular materials. The major advantage of such model is; its capability to use a single function to describe the behavior of granular materials, the derivation of such function might not be easy to obtain, though.

In 1970’s Poul Lade began working on developing a constitutive model to describe the behavior of frictional/cohesive materials. Lade’s model accounts for the dilatancy effects which is missing in many models such as the Cam Clay model. After an extensive experimental work using triaxial, biaxial and true triaxial testing Kim and Lade later (1988) were able to modify their yield and plastic potential functions that can fairly describe the behavior of frictional/cohesive materials such as “clay and sand” within the elasto-plastic continuum. Lade’s model will be adopted in this dissertation.

2.2.6 Shear Band Inclination

The Mohr-Coulomb failure criterion has been widely considered in soils; where the rupture surface is dependent on the mobilized angle of internal friction (Equation 2.7). It does not account for the effects of volumetric changes and represents an upper bound solution for the failure surface in soils (Vardoulakis, 1980). The volumetric expansion “dilation” angle in soils was first introduced by Hansen (1958). The Roscoe solution (1970) (Equation 2.8) for the failure surface in soils is considered as a lower limit solution (Vardoulakis, 1980). Arthur et al. (1977) proposed a solution (Equation 2.9) based on experimental observations for the shear band inclination as a function of the friction and dilation angles. Vardoulakis (1980) verified Arthur solution using the bifurcation theory. Vermeer (1982) used compliance methods to reach a
solution that agreed with Arthur and Vardoulakis solutions. Published research in the last 10 years has shown that the inclination of the shear band will be within a range between the Roscoe and Coulomb solutions. In this section, some of the mentioned solutions are presented:

\[ \theta = 45 + \frac{\phi_p}{2} \]  
Mohr-Coulomb solution  \hspace{1cm} (2.7)

\[ \theta = 45 + \frac{\psi}{2} \]  
Roscoe Solution  \hspace{1cm} (2.8)

\[ \theta = 45 + \frac{\phi_p + \psi}{4} \]  
Arthur . and Vardoulakis \hspace{1cm} (2.9)

where, \( \theta \) is the shear band inclination angle, \( \phi_p \) is the peak friction angle and \( \psi \) is the dilatancy.

### 2.2.7 Factors Affecting the Shear Band Evolution

As will be shown below in the experimental observations, some work has been done to investigate the effects of the confining pressure, grain size, density and some micro-properties on the thickness and evolution of the shear bands. Yet, no well formulated equations has been developed to quantify the effect of the surface roughness and grain shape on the thickness or/and the inclination of the shear band. Gudehus and Nübel (2002) emphasized on the fact that the angularity of the grains will control to some extent the polar friction which will affect the rotational resistance of the grains.

The same notion was supported by Oda and Iwashita (1999). Vardoulakis and Sulem (1995) emphasized that the surface roughness will affect the interparticle slipping in granular materials. Huang et al. (2002) attempted to bring the surface roughness and shape of the grains into a hypoplastic model to study their effect on the strain localization in granular materials. The latter authors have put solid theoretical efforts in their work; however, these theories suffer from linking the theoretical parameters to physical quantities.
2.3 Experimental Observations for Shear Bands in Granular Materials

The experimental characterization of the mechanical behavior of soils actively began in the second half of the 20th century. This effort was lead by many researchers such as Roscoe (1970) at Cambridge who conducted many experiments in this field and tried to relate the results to the theory. Rowe (1962) has shown, experimentally, the effect of the inter-particle friction on the strength for an assembly of grains using different materials. In the simple shear and triaxial tests, he observed a narrow failure zone within the sample found to be distorted at failure. This zone is called the shear band. In the early 1970’s the x-ray and γ-ray techniques were employed as non-destructive testing tools to enable one to study the fabric of the material at any strain level.

In soil mechanics, different destructive or/and non-destructive techniques can be employed to define the mechanical properties of a certain soil. However, many factors might play a significant role in controlling the behavior and the outcomes of the test. Namely, they are the boundary conditions, loading mode, initial properties and composition of the specimen, and the equipment accuracy and capabilities.

Roscoe (1970) observed the localization phenomenon in different soils using test walls and the centrifuge technique. He reached several conclusions from his experimental work regarding the failure surface. Roscoe (1970) introduced the dilatancy (kinematic basis) effect on the inclination of the failure surface.

The recent experimental work on strain localization showed that the shear band inclination and thickness depend on the micro-structural properties (size, shape and roughness) of the materials, and the boundary and loading conditions. In other words one can force the shear band to develop in a certain direction.
2.3.1 Void Ratio Observations

In a series of publications, Oda and co-workers (1972, 1982, 1996, 1998, and 1999) have conducted extensive experimental program on granular materials to investigate the fabric and shear banding. X-ray technique was used in order to study the phenomenon. In their tests, the void ratio inside the shear band was found to exceed the maximum value for the macro assembly. Oda et al. (1982) concluded that the grain rotation is dominant at failure and what mainly causes the high void ratio inside the shear band is the rotation due to the bucking of column-like structure. The void ratio inside the shear band has values of about 120% the maximum macro or global void ratio (Oda et al. 1982). Nemat-Nasser and Okada (1998) found that the shear strain around the center of the shear band reaches a value of 500% compared to 10% outside the shear band which leads to a very high void ratio in that zone. Alshibli and Sture, (1999) observed values of the void ratio inside the shear band to be greater than the maximum macro ones.

2.3.2 Observations on Shear Band Inclination

Shear strain inside the shear band tends to increase and at the same time the inclination of the shear band tends to decrease as the confining pressure increases; these observations were obtained from a series of bi-axial tests on dry coarse sand conducted in 1993 by Han and Drescher. In their tests the inclination of the shear band was found to deviate highly from the Mohr-Coulomb solution at high confining pressure which is questionable. Mokni and Desrues (1998) found that the inclination of shear band in sand with respect to the minimum principal stress decreases with increasing the mean stress level and the specimen density. One important observation in their result was that the inclination of the shear band in the loose sand is close to that obtained by the Coulomb solution, (i.e no dilation effect). In a series of biaxial testing on
three different sands, the shear band inclination was found to increase with density, and decrease with increasing the confining pressure and mean grain size (Alshibli and Sture, 2000). In 1987, Mühlhaus and Vardoulakis reported shear band inclination of 62.5° and 60.1° for fine and medium sands respectively.

### 2.3.3 Observations on Shear Band Thickness

The thickness of the shear band was found in the range of 7.5 to 9.6 times the mean grain size and it tends to increase with decreasing the density (Mokni and Desrues, 1998). Alshibli and Sture, (1999) found that the shear band thickness increases as the mean grain size increases and increases with density. They also found that the shear band thickness ranges from 10.63 to 13.86 times the mean grain size which is consistent with Vardoulakis (1978) who reported values of 10 to 15 times the mean grain size. In 1987, Mühlhaus and Vardoulakis reported shear band thickness of 18.5 and 13 times the mean grain size. DeJong and Frost (2002) have shown that the shear band can be clearly identified with increasing the grain angularity but that will not affect the thickness, on the other hand, the thickness decreases as the confining stress increases. Oda et al. (1997) showed that the shear band doesn’t have a straight boundaries where the thickness will vary along the failure surface.

### 2.3.4 Observations on Shear Band Occurrence

Lade and Wang (2001) and Wang and Lade (2001) found that the shear band begins to take place during the hardening regime and thus localization affect the peak stress value; its inclination was found to increase slightly with the density for sand loaded under the true triaxial apparatus. Gudehus and Nübel (2002) used a biaxial approach and model wall to study the localization patterns in granular materials. They observed a reflection of the shear band when it
hits the rigid boundary in the biaxial test. A set of complicated shear bands tend to develop behind the wall when the wall moves outwards; where a less complicated sets develop once the wall is pushed against the fill material. Beneath the foundation, the localization phenomenon is much more complicated. Experiments by Vesic (1973) and Tatsuoka et al. (1990) show some related observations.

Some researchers were interested in the behavior of the saturated sand, testing under drained and undrained condition was conducted to study the possible localization phenomenon in the saturated soils, (e.g. Mokni and Desrues, 1998; Finno et al. 1997).

Shear band can develop in both drained and undrained conditions, its thickness decreases as the confining pressure increases. Shear band boundaries experience high jumps in strains and excess pore water pressure, thus the phenomenon can tell some information about the liquefaction phenomenon in saturated loose sands. Desrues (1998) and Desrues et al. (1996) have used the sterophotogrammetry and the computed tomography techniques to study the strain localization in sands and clays. In their study they observed, besides the shear banding, cracks to grow during shearing in ductile materials such as clays. In the specimens tested under plane strain conditions with short lengths; a complex pattern of shear bands was observed and that might be due to the boundary effects.

In results obtained by Desrues and Hammad (1989) the measured shear band inclination angle agrees fairly with the Mohr-Coulomb solution in loose samples and deviate significantly from the same solution in the dense specimens. This might explain the effect of the dilation on the inclination of the failure surface which was introduced by Roscoe solution.

To this end the current literature in the field of the geomechanics leads the interested researchers to be careful when dealing with the localization phenomena in granular materials.
Such material has a microstructure and internal variables such as grain size distribution; shape of the grains, surface roughness if one is interested to look at the micro-scale, density “porosity” and existence of pore fluids. Other variables should be involved such as the geometry of the problem, how the external loads are applied and how the boundary conditions, if exist, constrain the deformations and loads. In fact all the variables mentioned lately are significant and play important roles, observed in experiments, in determining the amount and type of the deformation that such materials exhibit.
CHAPTER THREE

MATERIALS MICROSTRUCTURAL CHARACTERIZATION

3.1 Introduction

Shape, surface roughness, and gradation of particles have a significant influence on strength and deformation properties of granular materials. Sands with a predominance of angular particles possess greater friction than those consisting mainly of rounded particles. Koerner (1968) investigated the effects of angularity, gradation and mineralogy on shear strength of cohesionless soils and found that the angle of internal friction increases with increasing angularity of particles, and decreases with increasing effective size. Sedimentologists generally express particle shape in terms of surface texture, roundness and sphericity. Surface texture is used to describe the surface of particles (e.g. polished, greasy, frosted, etc.) that are too small to affect the overall shape. Roundness refers to those aspects of grain surface (sharpness of corners and edges) that are on a larger scale than those classed as surface texture, but that are smaller than the overall dimensions of the grain. Sphericity is used to describe the overall form of the particle irrespective of the sharpness of edges and corners. It is a measure of the degree of conformity of particle shape to that of a sphere.

Wadell (1932) was the first to point out that the terms shape and roundness were not synonymous, but rather include two geometrically distinct concepts. He defined roundness as the ratio of the average of radii of corners of the grain image and the maximum radius of the inscribed circle. There are also many other scale definitions for the roundness (e.g., Russel and Taylor 1937; Pettijohn 1949; Powers 1953, 1982). Wadell (1932) was also the first to choose the sphere as a standard. Ideally, the property of sphericity may be defined as the ratio of the surface
area of a sphere of the same volume as the fragment in question to the actual surface area of the grain.

Recently, Masad et al. (2001) introduced the surface Texture Index (TI) in which they referred to the fast Fourier transform, a good correlation between TI and the rutting resistance for hot-mix asphalt was found in their study. In 1998, Grigoriev et al. studied the surface texture at the nano-scale level and concluded that it affects the contact behavior between two surfaces. James and Vallejo (1997) defined the roughness as the general shape and surface irregularity, they emphasized that roughness is an important characteristic that affects the mass behavior of the soil. A definition of particle shape in terms of sphericity and roundness is widely accepted. However, methods have not been standardized because of the tedious task of making numerous readings. Analysis of sphericity and roundness are often made visually. Pettijohn (1949) supplemented his roundness classes with detailed descriptions so that the particle can be classified visually. Referring to Russell and Taylor (1937) and Pettijohn (1949) work, Powers (1953) introduced a new roundness scale for sedimentary particles. Powers (1953) emphasized that roundness does not depended on particle’s shape instead it depends on the sharpness of edges. In his work, Powers introduced the sphericity terminology to describe the shape as well as the roundness index. In 1982 Powers modified his chart to include more classes for sphericity and he assigned index numbers for the different roundness and sphericity classes. In this chapter, the results of particle surface measurements using optical interferometry are presented. The measurements were performed on three silica sands and two glass sizes of beads. This work also presents a literature summary of particle roundness/sphericity quantification along with introducing new roundness and sphericity indices (Figure 3-1). Table 3-1 shows the roundness grades proposed by Russell and Taylor (1937) and Pettijohn (1949) and Table 3-2 shows the
grades introduced by Powers (1953). The surface roughness has been studied lately using more accurate and complicated methods such as Fractal Geometry (ASME, 2000), fuzzy uncertainty texture spectrum (Lee et al. 1998), Structural 3-D approaches (Hong et al. 1999), SURFASCAN 3D (Content & Ville 1995) and photometric stereo acquisition and gradient space domain mapping (Smith 1999).

Figure 3-1 Modified Visual Comparison Chart for Estimating Roundness and Sphericity (Powers 1982) and (Alshibli and Alsaleh 2004).
In this chapter, the results of particle surface measurements using optical interferometry are presented. The measurements were performed on three silica sands and two glass sizes of beads. This work also presents a literature summary of particle roundness/sphericity quantification along with introducing new roundness and sphericity indices.

Table 3-1 Roundness Grades according to Russell & Taylor and Pettijohn Classifications (Powers 1953)

<table>
<thead>
<tr>
<th>CLASSIFICATION</th>
<th>RUSSELL AND TAYLOR</th>
<th>PETTIJOHN</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Class Limit</td>
<td>Arithmetic Mid-Point</td>
</tr>
<tr>
<td>Angular</td>
<td>0 – 0.15</td>
<td>0.075</td>
</tr>
<tr>
<td>Subangular</td>
<td>0.15 – 0.3</td>
<td>0.225</td>
</tr>
<tr>
<td>Subrounded</td>
<td>0.30 – 0.50</td>
<td>0.40</td>
</tr>
<tr>
<td>Rounded</td>
<td>0.50 – 0.70</td>
<td>0.60</td>
</tr>
<tr>
<td>Well rounded</td>
<td>0.70 – 1.0</td>
<td>0.85</td>
</tr>
</tbody>
</table>

Table 3-2 Power Roundness Classification (Powers 1953)

<table>
<thead>
<tr>
<th>CLASSIFICATION</th>
<th>CLASS INTERVALS</th>
<th>GEOMETRIC MEAN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Very angular</td>
<td>0.12 – 0.17</td>
<td>0.14</td>
</tr>
<tr>
<td>Angular</td>
<td>0.17 – 0.25</td>
<td>0.21</td>
</tr>
<tr>
<td>Subangular</td>
<td>0.25 – 0.35</td>
<td>0.30</td>
</tr>
<tr>
<td>Subrounded</td>
<td>0.35 – 0.49</td>
<td>0.41</td>
</tr>
<tr>
<td>Rounded</td>
<td>0.49 – 0.70</td>
<td>0.59</td>
</tr>
<tr>
<td>Well rounded</td>
<td>0.70 – 1.0</td>
<td>0.84</td>
</tr>
</tbody>
</table>
3.2 Surface Roughness Measurements

3.2.1 Methodology and Materials.

The surface roughness of three different sizes of silica sand was measured using an optical surface profiler called Wyko Optical Interferometer (WOI) manufactured by Veeco Metrology Group. It is a none-contact optical profiler that uses two technologies to measure a wide range of surface heights (roughness). Figure 3-2 and Figure 3-3 show schematic and digital photographs of WOI, respectively. It has two operating phase; Phase Shifting Interferometry (PSI) mode allows measuring smooth surfaces and steps, while the Vertical Scanning Interferometry (VSI) measures rough surfaces and steps up to millimeters high. In this study, the VSI mode was used since it gives better resolution for the three sands used in the investigation. In the VSI mode, a white light source is used since it works best for vertical scanning interferometry. The height of the surface at a specific coordination is measured based on the phase data (i.e., pixel value) and the wavelength of the source light.

Based on the white light reflection at the surface and on the reflected wavelength, the height of every single point (pixel) on the sand particle surface can be measured using WOI at the VSI mode. The resolution of the system at the VSI mode was 3 nm, the system was calibrated using known standards traceable by the National Institute of Standards and Technology (NIST). Three sands were used in this study to represent fine-, medium-, and coarse-grained silica sands with different surface roughness and shapes. The fine-grained sand is uniform silica (quartz) sand with mean particle size ($d_{50}$) of 0.22 mm. It was obtained from the Ottawa Industrial Silica Company and commonly denoted as F-75 Ottawa sand (Banding Sand, herein labeled as F-sand).
Figure 3-2 Schematic of the Wyko Optical Interferometer (WOI)

Figure 3-3 The LSU Wyko Optical Interferometer (WOI)
The medium-grained sand (herein labeled as M-sand) was obtained from Unimin Corporation. It is industrial uniform white quartz sand termed grade No. 30 with 0.55 mm mean particle size. The third sand is crushed silica sand obtained from the Connecticut Silica Company (herein labeled as C-sand) with mean particle size of 1.6 mm. Figure 3-4 shows the particle size distributions for those silica sands.

The small glass beads have a size range of 0.75 – 1.0 mm whereas the large ones were in the range of 3.30 – 3.6 mm; (Figure 3-5). Samples of the three sands and the two glass beads were randomly mounted on thin glass slides and then gold-coated. Particle Gold coating is essential in Scanning Electron Microscopy (SEM) and VSI because it causes electron beam and light reflection for better image viewing in both systems.

A total of 120 particles for each of the sands were scanned. They were arbitrarily selected among each slide. To avoid errors due to particle’s surface curvature and edges only the center part of particle is used in roughness calculations as illustrated in Figure 3-6a. The WOI is supplemented with computer software called Vision 32 (Figure 3-6b) in which a series of mathematical algorithms are executed for each scan to estimate different roughness indices. The reference mean line is taken automatically and the overall roughness is given according to the image taken for each particle. This approach was not used in our study since particle edges are included in the calculations and thus sharp edges will show up causing sudden drop or rise in the height (represented by the pixel value).

To avoid such problem, after the scans were completed, an ASCII file for each image was generated using Vision 32 software. Then, MathCAD software was used to process the generated ASCII files and to calculate the following roughness indices for the three sands. Figure 3-7 summarizes the sequence of processes used to quantify particles’ surface roughness.
Figure 3-4 Grain Size Distribution for the Three Silica Sands (Alshibli, 1995)

Figure 3-5 Grain Size Distribution for the Glass Beads (Novoa, 2003).
Figure 3-6 (a) Illustrative Image of Sand Particle Captured Using WOI Method; (b) Particle Surface Roughness Measurements were acquired using Vision 32 software.
The following parameters are calculated.

- **Average roughness** ($R_a$): is the arithmetic mean of the absolute values of the surface departure from the mean plane.

\[
R_a = \frac{1}{MN} \sum_{i=1}^{M} \sum_{j=1}^{N} |Z_{ij}|
\]  

(3.1)

Where $M$ and $N$ are the number of pixels in $X$ and $Y$ direction, $Z$ is the surface height at a specific pixel relative to the reference mean plane and $Z_{ij}$ is defined as:

\[
Z_{ij} = \lambda L_{ij}
\]  

(3.2)

Where $\lambda$ is the wavelength used in the scan and $L$ is the wave value for specific coordinates at the particle surface. $R_a$ is usually used to describe the roughness of a finished

---

Figure 3-7Flow Chart of Processes Used to Calculate Particles’ Surface Roughness
surface, so it can be used to describe the roughness of the sand particle surface. The main disadvantage that might be encountered here is, with average roughness, the effect of a single spurious, non-typical peak or valley will be averaged out and have only small influence on the overall roughness. So this index or the average will give no information about the shape of the irregularities or the surface of the particle. For granular materials and particle–to–particle friction, $R_a$ represents, to some extent, the overall roughness used for friction calculations.

- Root mean square roughness ($R_q$): is calculated as follows:

$$R_q = \sqrt{\frac{1}{MN} \sum_{i=1}^{M} \sum_{j=1}^{N} Z_{ij}^2} \quad (3.3)$$

It represents the standard deviation of the surface heights. $R_q$ has the same disadvantage as the $R_a$ does. The only advantage that $R_q$ compared to the $R_a$ is due to the fact that the heights are squared here and thus the valleys and peaks will have more significance in $R_q$.

- The maximum profile peak height ($R_p$) is the distance between the highest point of the surface and the mean surface for the entire dataset. Therefore, it represents the peak value for the surface.

- The maximum profile valley depth ($R_v$) is the distance between the lowest point of surface and the mean surface for the entire dataset (i.e., it measures the depth of the valley of a given surface).

- The maximum height of the surface ($R_t$) is the vertical distance between the lowest and highest point on the surface.

$$R_t = R_p + R_v \quad (3.4)$$

- Skewness ($R_{SK}$) measures the asymmetry of the surface about the mean plane, it is mean-cubed roughness.

$$R_{SK} = \frac{1}{MNR_q^3} \sum_{i=1}^{M} \sum_{j=1}^{N} Z_{ij}^3 \quad (3.5)$$
The advantage of this index that if the two different surfaces have the same $R_a$ and $R_q$ values one can distinguish between them using the skewness. Valleys in the surface will yield negative $R_{SK}$ whereas peaks will give positive ones.

- **Kurtosis ($R_{KU}$):** measures the peakedness of the surface about the mean plane, $R_{KU}$ is calculated using the following expression:

$$R_{KU} = \frac{1}{MNR_q^4} \sum_{i=1}^{M} \sum_{j=1}^{N} Z_{ij}^4$$ \hspace{1cm} (3.6)

It is mostly used for the machined surfaces. $R_{KU}$ will register high values when a high proportion of the surface falls within a narrow range of heights. In addition, Scanning Electron Microscope (SEM) images were taken for the same sands and the glass beads to look at the surface at high magnification and see the roughness of the grain surface (Figure 3-8 and Figure 3-9). To some extent, the SEM images showed good uniformity in the surface roughness for each of the three sands and the two glass beads.

### 3.2.2 Surface Roughness Results

As mentioned earlier, 120 particles were randomly selected and analyzed to quantify surface roughness. The ASCII files that contain the scan results were exported to MathCad software for further analysis and calculations which includes calculating roughness indices defined in the previous sub-section and generating 3D renderings of particles’ surface profile (Figure 3-10 and Figure 3-11). Table 3-3 through Table 3-7 list a statistical summary of analysis conducted on F-, M-, and C-sands, respectively.

Furthermore, Figure 3-12 shows frequency distribution of average surface roughness ($R_a$) and Root mean square roughness ($R_q$) for the three sands and the glass beads used in the investigation. Comparing the statistical summaries of the three sands and the glass beads, one can
notice that statistical parameters for $R_q$ are slightly higher than those for $R_d$ for each of the three sands.

Figure 3-8 SEM Images of the Three Sands at Different Magnification Levels.
Figure 3-9 SEM Images of the Two Glass Beads at Different Magnification Levels.

Furthermore, the mean values for \( R_a \) and \( R_q \) are 0.8487 \( \mu m \) and 0.9815 \( \mu m \) for the F-sand, respectively, compared to 0.9460 \( \mu m \) and 1.0822 \( \mu m \) for M-sand and 1.1169 \( \mu m \) and 1.2383 \( \mu m \) for C-sand. For the glass beads those values were 0.3365 \( \mu m \) and 0.3941 \( \mu m \) for the small size and 0.2135 \( \mu m \) and 0.2573 \( \mu m \) for the large beads.

Figure 3-12 shows that frequency distributions for \( R_a \) and \( R_q \) differ slightly from each other for the same sand and their standard deviations are \(-0.55-0.61 \mu m\) for F-sand to \(-0.61-0.67 \mu m\) for M-sand and \(-0.50-0.52 \mu m\) for C-sand. Those values were \(-0.825-0.813 \mu m\) for small glass beads and \(-0.845-0.842 \mu m\) for the large glass beads. The frequency distribution was skewed to the right for the sand and the glass beads.
Figure 3-10 Typical Optical Microscope Profiler Images for the Sands Used in this Study.
Figure 3-11 Typical Optical Microscope Profiler Images for the Glass Beads Used in the Investigation.

Table 3-3 Statistical Summary of Roughness parameters for F sand

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>$R_a$ (µM)</th>
<th>$R_z$ (µM)</th>
<th>$R_p$ (µM)</th>
<th>$R_y$ (µM)</th>
<th>$R_T$ (µM)</th>
<th>$R_{SK}$</th>
<th>$R_{KU}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum</td>
<td>0.2620</td>
<td>0.3168</td>
<td>0.6149</td>
<td>0.6149</td>
<td>1.2298</td>
<td>-1.1334</td>
<td>1.2102</td>
</tr>
<tr>
<td>Mean</td>
<td>0.8487</td>
<td>0.9815</td>
<td>1.9631</td>
<td>1.9631</td>
<td>3.9263</td>
<td>-0.1539</td>
<td>2.0603</td>
</tr>
<tr>
<td>Median</td>
<td>0.7075</td>
<td>0.8316</td>
<td>1.7691</td>
<td>1.7691</td>
<td>3.5383</td>
<td>-0.1275</td>
<td>2.0012</td>
</tr>
<tr>
<td>RMS$^a$</td>
<td>1.0105</td>
<td>1.1569</td>
<td>2.2466</td>
<td>2.2466</td>
<td>4.4932</td>
<td>0.6096</td>
<td>2.1047</td>
</tr>
<tr>
<td>Std. Dev.</td>
<td>0.5510</td>
<td>0.6153</td>
<td>1.0977</td>
<td>1.0977</td>
<td>2.1953</td>
<td>0.5927</td>
<td>0.4322</td>
</tr>
<tr>
<td>Standard Error.</td>
<td>0.0538</td>
<td>0.0600</td>
<td>0.1071</td>
<td>0.1071</td>
<td>0.2142</td>
<td>0.0578</td>
<td>0.0422</td>
</tr>
</tbody>
</table>

$^a$ RMS is the root mean square
Table 3-4 Statistical Summary of Roughness parameters for M sand

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>$R_a$ (µM)</th>
<th>$R_q$ (µM)</th>
<th>$R_p$ (µM)</th>
<th>$R_y$ (µM)</th>
<th>$R_z$ (µM)</th>
<th>$R_{SK}$</th>
<th>$R_{KU}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum</td>
<td>0.3538</td>
<td>0.3997</td>
<td>0.5387</td>
<td>0.5387</td>
<td>1.0774</td>
<td>-1.3663</td>
<td>1.1555</td>
</tr>
<tr>
<td>Maximum</td>
<td>2.8653</td>
<td>3.1205</td>
<td>5.8650</td>
<td>5.8650</td>
<td>11.7299</td>
<td>1.1276</td>
<td>2.9372</td>
</tr>
<tr>
<td>Mean</td>
<td>0.9460</td>
<td>1.0822</td>
<td>1.9176</td>
<td>1.9176</td>
<td>3.8351</td>
<td>-0.2900</td>
<td>1.9272</td>
</tr>
<tr>
<td>Median</td>
<td>0.7165</td>
<td>0.8130</td>
<td>1.6201</td>
<td>1.6201</td>
<td>3.2403</td>
<td>-0.3910</td>
<td>1.9149</td>
</tr>
<tr>
<td>RMS$^a$</td>
<td>1.1259</td>
<td>1.2685</td>
<td>2.1404</td>
<td>2.1404</td>
<td>4.2808</td>
<td>0.7315</td>
<td>1.9666</td>
</tr>
<tr>
<td>Std. Dev.</td>
<td>0.6141</td>
<td>0.6657</td>
<td>0.9563</td>
<td>0.9563</td>
<td>1.9127</td>
<td>0.6754</td>
<td>0.3938</td>
</tr>
<tr>
<td>Standard Error</td>
<td>0.0655</td>
<td>0.0710</td>
<td>0.1019</td>
<td>0.1019</td>
<td>0.2039</td>
<td>0.0720</td>
<td>0.0420</td>
</tr>
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</table>

Table 3-5 Statistical Summary of Roughness parameters for C sand

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>$R_a$ (µM)</th>
<th>$R_q$ (µM)</th>
<th>$R_p$ (µM)</th>
<th>$R_y$ (µM)</th>
<th>$R_z$ (µM)</th>
<th>$R_{SK}$</th>
<th>$R_{KU}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum</td>
<td>0.6515</td>
<td>0.7737</td>
<td>1.1823</td>
<td>1.1823</td>
<td>2.3646</td>
<td>-1.2507</td>
<td>1.1416</td>
</tr>
<tr>
<td>Maximum</td>
<td>2.6958</td>
<td>2.9494</td>
<td>4.2120</td>
<td>4.2120</td>
<td>8.4239</td>
<td>1.0594</td>
<td>2.5140</td>
</tr>
<tr>
<td>Mean</td>
<td>1.1169</td>
<td>1.2383</td>
<td>2.0519</td>
<td>2.0519</td>
<td>4.1037</td>
<td>-0.3373</td>
<td>1.6537</td>
</tr>
<tr>
<td>Median</td>
<td>0.9639</td>
<td>1.0414</td>
<td>1.9138</td>
<td>1.9138</td>
<td>3.8276</td>
<td>-0.4367</td>
<td>1.6619</td>
</tr>
<tr>
<td>RMS$^a$</td>
<td>1.2227</td>
<td>1.3423</td>
<td>2.1663</td>
<td>2.1663</td>
<td>4.3325</td>
<td>0.7790</td>
<td>1.6805</td>
</tr>
<tr>
<td>Std. Dev.</td>
<td>0.5033</td>
<td>0.5241</td>
<td>0.7029</td>
<td>0.7029</td>
<td>1.4058</td>
<td>0.7105</td>
<td>0.3023</td>
</tr>
<tr>
<td>Standard Error</td>
<td>0.0768</td>
<td>0.0799</td>
<td>0.1072</td>
<td>0.1072</td>
<td>0.2144</td>
<td>0.1084</td>
<td>0.0461</td>
</tr>
</tbody>
</table>

Table 3-6 Statistical Summary of Roughness parameters for small glass beads

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>$R_a$ (µM)</th>
<th>$R_q$ (µM)</th>
<th>$R_p$ (µM)</th>
<th>$R_y$ (µM)</th>
<th>$R_z$ (µM)</th>
<th>$R_{SK}$</th>
<th>$R_{KU}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum</td>
<td>0.0949</td>
<td>0.124</td>
<td>0.346</td>
<td>0.346</td>
<td>0.69199</td>
<td>-1440000</td>
<td>1060000</td>
</tr>
<tr>
<td>Maximum</td>
<td>1.66</td>
<td>1.68</td>
<td>2.64</td>
<td>2.64</td>
<td>5.27</td>
<td>1170000</td>
<td>6450000</td>
</tr>
<tr>
<td>Mean</td>
<td>0.33649</td>
<td>0.39409</td>
<td>0.9884</td>
<td>0.9884</td>
<td>1.9768</td>
<td>162845</td>
<td>2755300</td>
</tr>
<tr>
<td>Median</td>
<td>0.258</td>
<td>0.3095</td>
<td>0.958</td>
<td>0.958</td>
<td>1.915</td>
<td>318500</td>
<td>2625000</td>
</tr>
<tr>
<td>RMS$^a$</td>
<td>0.40831</td>
<td>0.46287</td>
<td>1.06385</td>
<td>1.06385</td>
<td>2.12776</td>
<td>820962.9</td>
<td>2964624</td>
</tr>
<tr>
<td>Std. Dev.</td>
<td>0.23244</td>
<td>0.24400</td>
<td>0.39548</td>
<td>0.39548</td>
<td>0.79101</td>
<td>808703.6</td>
<td>1099732</td>
</tr>
<tr>
<td>Standard Error</td>
<td>0.02324</td>
<td>0.02440</td>
<td>0.03954</td>
<td>0.0399</td>
<td>0.07910</td>
<td>808703.6</td>
<td>109973.</td>
</tr>
</tbody>
</table>
Table 3-7 Statistical Summary of Roughness parameters for large glass bead

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>( R_a (\mu m) )</th>
<th>( R_q (\mu m) )</th>
<th>( R_p (\mu m) )</th>
<th>( R_f (\mu m) )</th>
<th>( R_T (\mu m) )</th>
<th>( R_{SK} )</th>
<th>( R_{KU} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum</td>
<td>0.0581</td>
<td>0.0829</td>
<td>0.245</td>
<td>0.245</td>
<td>0.49000</td>
<td>-1500000</td>
<td>1300000</td>
</tr>
<tr>
<td>Maximum</td>
<td>0.569</td>
<td>0.68</td>
<td>1.56</td>
<td>1.56</td>
<td>3.11999999</td>
<td>1240000</td>
<td>7650000</td>
</tr>
<tr>
<td>Mean</td>
<td>0.213536</td>
<td>0.257343</td>
<td>0.69745</td>
<td>0.69745</td>
<td>1.3953</td>
<td>-232676</td>
<td>2907100</td>
</tr>
<tr>
<td>Median</td>
<td>0.193</td>
<td>0.2435</td>
<td>0.6885</td>
<td>0.6885</td>
<td>1.38</td>
<td>-434000</td>
<td>2765000</td>
</tr>
<tr>
<td>RMS(^a)</td>
<td>0.236783</td>
<td>0.280603</td>
<td>0.743836</td>
<td>0.743836</td>
<td>1.48814999</td>
<td>840775</td>
<td>3091758</td>
</tr>
<tr>
<td>Std. Dev.</td>
<td>0.10283</td>
<td>0.112423</td>
<td>0.259866</td>
<td>0.259866</td>
<td>0.5200309</td>
<td>812008.7</td>
<td>1057793</td>
</tr>
<tr>
<td>Standard Error.</td>
<td>0.010283</td>
<td>0.011242</td>
<td>0.025987</td>
<td>0.025987</td>
<td>0.0520030</td>
<td>812008.7</td>
<td>105779.3</td>
</tr>
</tbody>
</table>

Figure 3-12 Frequency Distribution of \( R_a \) and \( R_q \) for the Sands and the Glass Beads Used in the Study.
Continue Figure 3-12
3.3 **Particles’ Roundness and Sphericity**

The shape/roundness of granular particles can be evaluated using different indices such as the Form Factor ($FF$), which is widely used in the literature and defined as:

$$ FF = \frac{4\pi A}{P^2} \quad (3.7) $$

Where $A$ is the projected area of the particle and $P$ is the perimeter of this area.

Masad *et al.* (2001) proposed the following definitions to quantify the aggregates shape characteristics.

- **Sphericity Parameter ($SP$)** is used in literature to define the angularity of particles:

$$ SP = \sqrt[3]{\frac{d_s d_i}{d_L^2}} \quad (3.8) $$

where $d_L$ = the longest particle dimension,

$d_i$ = the intermediate particle dimension, and;

$d_s$ = the shortest particle dimension

- **Shape Factor ($SF$):**

$$ SF = \frac{d_s}{\sqrt{d_L d_i}} \quad (3.9) $$

Furthermore Masad *et al.* (2001) introduced the Form Index ($FI$), Angularity indices ($AI$) which are defined as follows:

$$ FI = \sum_{\theta=5}^{355} \frac{|R_{\theta+5} - R_{\theta}|}{R_0} \quad (3.10) $$

$$ AI = \sum_{\theta=5}^{355} \frac{|R_{\theta} - R_{EE\theta}|}{R_{EE\theta}} \quad (3.11) $$
Where $R$ is the radius of the particle at a directional angle $\theta$, $R_{EE\theta}$ is the radius of an equivalent ellipse at a directional angle $\theta$. Masad et al. (2001) proposed correlations for the rutting resistance of the asphalt with $FI$, $AI$ and $TI$. The rutting resistance was measured using the Purdue Wheel-tracking device (PURWheel), strong correlation was found between those indices and the resistance. Matsushima and Konagai (2001) studied the grain-shape effect on peak strength of granular materials using Discrete Element Method (DEM). In their study they concluded that the shape doesn’t affect the strength at the same void ratio where the surface roughness is dominant here, they verified that using real sands. Brezezicki and Kasperkiewicz (1999) proposed a method for an automatic characterization of the shape of the coarse particles based on image analysis technique. Ghalib & Hryciw (1999) proposed an imaging and watershed analysis method to determine the soil particle distribution. Yudhbir and Abedinzadeh (1991) used an image analyzer to quantify the shape of particles. They used Equation (3.8) to measure particle sphericity.

In this chapter, two new indices were introduced to define sphericity and roundness of particles. The sphericity index ($I_{sp\theta}$) is defined as:

$$I_{sp\theta} = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{D_{eq}(i)}{d_{s(i)}} - \frac{D_{eq}(i)}{d_{L(i)}} \right|$$

(3.12)

Where $D_{eq}$ is the equivalent particle diameter (perimeter/$\pi$) and $d_{s}$ and $d_{L}$ are as defined before. The roundness index ($I_{R}$) is defined as follows:

$$I_{R} = \frac{1}{N} \sum_{i=1}^{N} \frac{P_{wad(i)}}{\pi \left( \frac{d_{s(i)} + d_{L(i)}}{2} \right)}$$

(3.13)
Where $P_{arc(i)}$ is the actual perimeter of the particle. Particles listed in Power’s chart (Figure 3-1) were scanned and converted to image format. Scion Image Analysis Software (SIAS) has drawing tools that enable one to manually measure the parameters in Equations (3.12 and 3.13) by simply choosing the proper tool (i.e., line, polygon, circle, cross hair, etc.) and performing the measurement on the selected particles. Then $I_{qph}$ and $I_{R}$ values were calculated and the results of the analysis are shown in Figure 3-1, which shows that $I_{R}$ ranges from 1.0 for well-rounded particles to >1.5 for very angular particles and $I_{qph}$ ranges from 0.0 for discoidal particles to >1.0 for prismoidal particles.

Scion image analysis software was also used to measure the areas, perimeter, the shortest and longest axes of 25 particles of each of the three sands. High-resolution SEM images were used to do the measurements. The equivalent circular diameter for each particle was then calculated. The equivalent diameter was considered to be the mean axis length as well. Due to the fact that the SEM images were taken for the particles as is, no flushing was done, more than 5 particles were available in the image and it wasn’t easy to separate the inter-particle. Then a free-hand drawing tool of SIAS was used to trace the perimeter of each particle and then the measurements were done based on the features available in this software (Figure 3-13). The shape/roundness factors discussed and defined above are calculated and Table 3-8 through Table 3-12 list statistical summarizes of the analysis.

Based on the classification proposed by the author ($I_{R}$ and $I_{qph}$) the F sand mainly consists of spherical well-rounded particles whereas M- and C-sands consist of sub-prismoidal rounded particles. The same shape indices for the glass beads were obtained and the values indicated that the small beads, referring to the modified chart (Figure 3-1) one can easily
conclude that the glass beads have pretty much a well rounded discodial shape. The fact the glass beads have a uniform shape

Table 3-8 Shape Factor Results for the F sand

<table>
<thead>
<tr>
<th>STATISTICAL PARAMETER</th>
<th>AREA (µm²)</th>
<th>DS (µm)</th>
<th>DL (µm)</th>
<th>P (µm)</th>
<th>DEQU (µm)</th>
<th>FF</th>
<th>SP</th>
<th>SF</th>
<th>IR</th>
<th>ISPH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>18124.1</td>
<td>127.6</td>
<td>168.16</td>
<td>507.60</td>
<td>161.66</td>
<td>0.8215</td>
<td>0.9334</td>
<td>0.7703</td>
<td>1.0953</td>
<td>0.3364</td>
</tr>
<tr>
<td>Median</td>
<td>15588.0</td>
<td>126.0</td>
<td>156.00</td>
<td>484.00</td>
<td>154.14</td>
<td>0.8222</td>
<td>0.9335</td>
<td>0.7503</td>
<td>1.0969</td>
<td>0.3411</td>
</tr>
<tr>
<td>RMS</td>
<td>20688.7</td>
<td>134.6</td>
<td>175.04</td>
<td>529.29</td>
<td>168.57</td>
<td>0.8238</td>
<td>0.9342</td>
<td>0.7796</td>
<td>1.097</td>
<td>0.4032</td>
</tr>
<tr>
<td>Std. Dev.</td>
<td>10182.7</td>
<td>43.85</td>
<td>49.59</td>
<td>153.08</td>
<td>48.75</td>
<td>0.0622</td>
<td>0.0381</td>
<td>0.1224</td>
<td>0.0619</td>
<td>0.2269</td>
</tr>
</tbody>
</table>

Table 3-9 Shape Factor Results for the M sand

<table>
<thead>
<tr>
<th>STATISTICAL PARAMETER</th>
<th>AREA (µm²)</th>
<th>DS (µm)</th>
<th>DL (µm)</th>
<th>P (µm)</th>
<th>DEQU (µm)</th>
<th>FF</th>
<th>SP</th>
<th>SF</th>
<th>IR</th>
<th>ISPH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>275247.6</td>
<td>454.52</td>
<td>753.5</td>
<td>2076.52</td>
<td>661.31</td>
<td>3.5608</td>
<td>1.023</td>
<td>0.6902</td>
<td>1.087</td>
<td>0.6565</td>
</tr>
<tr>
<td>Median</td>
<td>239205</td>
<td>430.00</td>
<td>727.0</td>
<td>1973.00</td>
<td>628.34</td>
<td>0.7573</td>
<td>0.899</td>
<td>0.6376</td>
<td>1.120</td>
<td>0.6038</td>
</tr>
<tr>
<td>RMS</td>
<td>291080.7</td>
<td>473.61</td>
<td>766.7</td>
<td>2140.23</td>
<td>681.60</td>
<td>14.235</td>
<td>1.198</td>
<td>0.7398</td>
<td>1.107</td>
<td>0.8645</td>
</tr>
<tr>
<td>Std. Dev.</td>
<td>96645.44</td>
<td>135.86</td>
<td>144.4</td>
<td>529.905</td>
<td>168.47</td>
<td>14.067</td>
<td>0.635</td>
<td>0.2717</td>
<td>0.212</td>
<td>0.5741</td>
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</tbody>
</table>

Table 3-10 Shape Factor Results for the C sand

<table>
<thead>
<tr>
<th>STATISTICAL PARAMETER</th>
<th>AREA (mm²)</th>
<th>DS (mm)</th>
<th>DL (mm)</th>
<th>P (mm)</th>
<th>DEQU (mm)</th>
<th>FF</th>
<th>SP</th>
<th>SF</th>
<th>IR</th>
<th>ISPH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>2.6772</td>
<td>1.4068</td>
<td>2.2556</td>
<td>6.482</td>
<td>2.064</td>
<td>0.7711</td>
<td>0.9036</td>
<td>0.6628</td>
<td>1.126</td>
<td>0.593</td>
</tr>
<tr>
<td>Median</td>
<td>2.2600</td>
<td>1.3400</td>
<td>2.2300</td>
<td>6.440</td>
<td>2.0510</td>
<td>0.7887</td>
<td>0.9124</td>
<td>0.6708</td>
<td>1.126</td>
<td>0.512</td>
</tr>
<tr>
<td>RMS</td>
<td>2.903</td>
<td>1.4529</td>
<td>2.3088</td>
<td>6.623</td>
<td>2.1092</td>
<td>0.7734</td>
<td>0.9049</td>
<td>0.6793</td>
<td>1.128</td>
<td>0.703</td>
</tr>
<tr>
<td>Std. Dev.</td>
<td>1.1455</td>
<td>0.3707</td>
<td>0.5031</td>
<td>1.386</td>
<td>0.4414</td>
<td>0.0618</td>
<td>0.0476</td>
<td>0.1519</td>
<td>0.0617</td>
<td>0.384</td>
</tr>
</tbody>
</table>
Table 3-11 Shape Factor Results for the Small Glass Beads

<table>
<thead>
<tr>
<th>STATISTICAL PARAMETER</th>
<th>AREA (µm²)</th>
<th>DS (µm)</th>
<th>DL (µm)</th>
<th>P (µm)</th>
<th>DEQU (µm)</th>
<th>FF</th>
<th>SP</th>
<th>SF</th>
<th>IR</th>
<th>ISPH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>490785</td>
<td>2522.7</td>
<td>794.2</td>
<td>786.4</td>
<td>250.45</td>
<td>9.8807</td>
<td>3.1728</td>
<td>5.6567</td>
<td>1.0151</td>
<td>0.216</td>
</tr>
<tr>
<td>Median</td>
<td>449400.</td>
<td>2419.2</td>
<td>766</td>
<td>750</td>
<td>238.9</td>
<td>9.8768</td>
<td>3.1675</td>
<td>5.6558</td>
<td>1.0151</td>
<td>0.216</td>
</tr>
<tr>
<td>RMS</td>
<td>498947</td>
<td>2532.3</td>
<td>797.3</td>
<td>789.4</td>
<td>251.4</td>
<td>9.8818</td>
<td>3.1729</td>
<td>5.6568</td>
<td>1.0150</td>
<td>0.216</td>
</tr>
<tr>
<td>Std. Dev.</td>
<td>100490</td>
<td>246.02</td>
<td>78.248</td>
<td>77.118</td>
<td>24.560</td>
<td>0.1589</td>
<td>0.0112</td>
<td>0.0095</td>
<td>0.0007</td>
<td>0.001</td>
</tr>
</tbody>
</table>

Table 3-12 Shape Factor Results for the Large Glass Beads

<table>
<thead>
<tr>
<th>STATISTICAL PARAMETER</th>
<th>AREA (mm²)</th>
<th>DS (mm)</th>
<th>DL (mm)</th>
<th>P (mm)</th>
<th>DEQU (mm)</th>
<th>FF</th>
<th>SP</th>
<th>SF</th>
<th>IR</th>
<th>ISPH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>6.6625</td>
<td>9.3425</td>
<td>2.9225</td>
<td>2.94</td>
<td>0.9363</td>
<td>9.7040</td>
<td>3.1478</td>
<td>5.6499</td>
<td>1.0153</td>
<td>0.220</td>
</tr>
<tr>
<td>Median</td>
<td>6.72</td>
<td>9.37</td>
<td>2.94</td>
<td>2.925</td>
<td>0.9315</td>
<td>9.6824</td>
<td>3.1637</td>
<td>5.6350</td>
<td>1.0152</td>
<td>0.215</td>
</tr>
<tr>
<td>RMS</td>
<td>6.66343</td>
<td>9.3427</td>
<td>2.9235</td>
<td>2.9411</td>
<td>0.9367</td>
<td>9.7205</td>
<td>3.1490</td>
<td>5.6500</td>
<td>1.0153</td>
<td>0.221</td>
</tr>
<tr>
<td>Std. Dev.</td>
<td>0.12868</td>
<td>0.0624</td>
<td>0.0866</td>
<td>0.0955</td>
<td>0.0304</td>
<td>0.6537</td>
<td>0.0970</td>
<td>0.0445</td>
<td>0.0061</td>
<td>0.016</td>
</tr>
</tbody>
</table>

Figure 3-13 Scion Image Analysis Window Showing Particles Analysis.
The SEM images shown above for the three sands and the glass beads were used to estimate the shape indices ($I_R$ and $I_{sph}$) over the domain to incorporate the real distribution of such parameters in the numerical model. Figure 3-1 shows the frequency distribution for those shape indices; based on those distributions spatial distributions were generated for the shape indices, surface roughness and grain size.

![Frequency Distribution of $I_R$ and $I_{sph}$ for the Sands and the Glass Beads Used in the Study.](image)

Figure 3-14 Frequency Distribution of $I_R$ and $I_{spH}$ for the Sands and the Glass Beads Used in the Study.
Continue Figure 3-14.
CHAPTER FOUR
CONSTITUTIVE MODEL AND MODEL PARAMETERS
CALIBRATION

4.1 Introduction

Many constitutive models have been developed in the literature to describe the mechanical behavior of granular materials. However, most of the formulations have been developed within the framework of the theories of plasticity, hypoplasticity, hyperplasticity or viscoplasticity to deal with a classical type of stresses and deformations. The problem here, however, requires non-classical equations to describe physical phenomena inside the continuum during loading-unloading conditions. Due to the discreteness of the granular continua and the nature of the grains, high irreversible deformations have been observed theoretically and experimentally. Elasto-plastic behavior for such rate-independent materials was found reasonable to describe the high deformations that take place in granular materials. To describe the elasto-plastic behavior of such material one need a proper elasticity law, yield criterion, plastic potential, hardening rules and appropriate flow rule.

In this chapter, a single hardening constitutive model that was developed by Lade and co-workers with a non-linear elasticity function is presented. This model assumes non-associative flow rule and high non-linear plastic work-based hardening function.

4.2 Model Description

4.2.1 Non-Linear Elasticity Modulus

Lade and Nelson (1987) developed an isotropic model for the nonlinear elastic behavior of granular materials. In their model they proposed a non-linear elasticity modulus described by Equations (4.1). The derivation of this formula was based on the principle of conservation of energy (i.e. energy neither generated nor dissipated along a stress closed-path).
\[
E = M_L P_a \left[ \left( \frac{I_I}{P_a} \right)^2 + R_L \frac{J'_{2}}{P_a^2} \right]^{\lambda}
\] (4.1)

Where;

\( P_a \) = the atmospheric pressure

\( I_I \) = the first invariant of the stress tensor, which reads:

\[
I_I = \sigma_{ii}, \quad i = 1, 2, 3
\] (4.2)

\( J'_{2} \) = the second invariant of the deviatoric stress tensor, this invariant is enhanced to account for the couple stress and it reads:

\[
J'_{2} = \frac{1}{6} \left[ (\sigma_{11} - \sigma_{22})^2 + (\sigma_{33} - \sigma_{22})^2 + (\sigma_{11} - \sigma_{33})^2 \right] + \sigma_{12}^2
\] (4.3)

\( R_L = \frac{6(1 + \nu)}{1 - 2\nu} \) and \( \nu \) is the constant Poisson’s ratio and;

\( M_L \) and \( \lambda \) are dimensionless material parameters to be determined from a series of simple experiment that have loading-unloading-reloading cycles.

4.2.2 The Yield Function

The theory of plasticity assumes that any material would behave elastically within some loading limit and once the stresses or the strains reaches this limit the material will yield and plastic deformation begins.

There are many yield criteria available for different types of materials. Granular materials yield at a very early stages of the loading processes because of the nature of the particles and the cohesionless properties. The stresses needed to yield the granular materials under isotropic or hydrostatic loading are very high and can’t be easily achieved in the laboratory. Lade and Kim (1988) developed a yield function to deal with frictional/cohesive materials. The model is
powerful to simulate the constitutive behavior of granular materials. Lade-Kim yield function reads:

\[ f_p = f_p'(\sigma) - f_p''(W_p) = 0 \] (4.5)

Where;

\( f_p'(\sigma) \) is the driving yield function and \( f_p''(W_p) \) is the plastic work hardening function during hardening regime and it switches into softening function during the softening regime.

\[ f_p'(\sigma) = \left[ \Psi_1 \frac{I_1^3}{I_{III}^2} - \frac{I_1^2}{I_{II}} \frac{I_1}{P_a} \right] e^q \] (4.6)

\( \Psi_1 \) is a weighting factor counts for the shape of the yield surface between triangular to circular. This factor can be determined easily using the following expression:

\[ \Psi_1 = 0.00155m^{-1.27} \] (4.7)

Where; \( m \) is a failure criterion parameter that can be determined from experiment as will be shown later in this Chapter. \( I_{II} \) and \( I_{III} \) are the second and the third stress invariants defined in Equation (4.8), the second invariant will be enhanced later in Chapter Five to incorporate the effect of the couple stresses (\( m_i \)).

\[ I_{II} = \left[ \sigma_{12}\sigma_{21} - \sigma_{11}\sigma_{22} - \sigma_{11}\sigma_{33} - \sigma_{22}\sigma_{33} \right] \] (4.8a)

\[ I_{III} = \left[ \sigma_{11}\sigma_{22}\sigma_{33} - \sigma_{33}\sigma_{12}\sigma_{21} \right] \] (4.8b)

The parameter \( h \) is a material yield parameter which can be determined from experimental data and \( q \) is a model parameter (Equation (4.9a)) that ranges from zero at the hydrostatic condition to unity at failure.

\[ q = \frac{\alpha S}{1 - (1 - \alpha)S} \] (4.9a)

Where, \( \alpha \) is a material parameter and \( S \) is a stress level defined as:
\[ S = \frac{1}{\eta_l} \left( \frac{I_1^3}{I_{III}} - 27 \right) \left( \frac{I_1}{P_a} \right)^m \] (4.9b)

where; \( \eta_l \) is another failure criterion parameter and can be estimated from experiment. Lade’s yield surface takes the shape of an eye drop (Figure 4-1); each yield surface represents a contour for the plastic work.

### 4.2.3 Plastic Work Hardening/Softening Functions

The plastic work function is a non-linear function defined as:

\[ W_p = CP_a \left( \frac{I_1}{P_a} \right)^p \] (4.10)

It can be used only during isotropic loading and as any other preferred stress path starts; a certain integration scheme is needed to update this state variable, this technique will be discussed later in this Chapter.

Parameters \( C \) and \( p \) are estimated from isotropic loading data as will be explained in the following Section. During the hardening regime, Equation (4.11) is used to describe the non-linear hardening component defined in Equation (4.5).

\[ f_p^m = \left( \frac{1}{D} \right)^{m_{\rho_{ls}}} \left( \frac{W_p}{P_a} \right)^{1\rho_{ls}} \] (4.11)

Where;

\[ \rho_{ls} = \frac{p}{h} \] (4.12a)
As the material fails or reaches the instability point; the hardening regime is terminated and softening takes place. At this point Equation (4.13) will be used to describe the exponential decay or softening in the material.

\[ D = \frac{C}{(27\psi_1 + 3)^{\alpha}} \]  

(4.12b)
\[ f_p'' = A e^{-b \left( \frac{w_p}{\tau_p} \right)} \] (4.13)

Where; \( A \) and \( B \) are material constants that can be estimated at the failure point, and (i.e. when \( S = q = 1.0 \)) and :

\[ B = \left( b \frac{\partial f_p^*}{\partial \left( \frac{W_p}{P_a} \right)} \right)_{S=1} \quad 0 \leq b \leq 1.0 \] (4.14a)

\[ A = \left( f_p^* e^{B \frac{W_p}{P_a}} \right)_{S=1} \] (4.14b)

The above constants \( A \) and \( B \) need to be estimated once at failure and \( b \) is a material constant. Figure 4-2 illustrates the hardening and softening regimes for any material.

Figure 4-2: Hardening-Softening Regimes.
4.2.4 Plastic Potential Function.

In general, granular materials exhibit volumetric and shear strains. The data available in the literature supports the notion that the shear strains are always larger than the volumetric strains. Therefore, an associative flow rule is not acceptable to describe the plastic deformations. The flow rule suggests that the directions of the principal stress axes will always coincide with the principal plastic strain increments. This suggestion allows the estimation of the plastic strain increments from:

\[ \dot{\varepsilon}_{ij}^p = \dot{\lambda}_p \frac{\partial g_p}{\partial \sigma_{ij}} \]  

(4.15)

Where, \( \dot{\lambda}_p \) is a scalar proportionality factor and it should be a positive definite; and \( g_p \) is the plastic potential function defined as:

\[ g_p = \left[ \psi_1 \frac{I_1^2}{I_{III}} - \frac{I_1^2}{I_{II}} + \psi_2 \left( \frac{I_1}{P_a} \right)^\mu \right] \]  

(4.16)

Where; \( \psi_2 \) and \( \mu \) are plastic potential parameters that can be estimated from experiment as will be discussed later in his Chapter. The other parameters were defined earlier.

The origin of the plastic potential function can go beyond the origin of the principal axes if the material has some cohesion. Figure 4-3 shows schematic illustration for the plastic potential surface in the principal stress plane, which has the shape of a bullet.

The extension of the plastic potential surface beyond the origin of the principal axes is explained by the fact that cohesive materials will have an additional component to the strength at zero normal stresses as:

\[ \bar{\sigma}_{ij} = \sigma_{ij} + aP_a \delta_{ij} \]  

(4.17)
where; \( a \), is a material constant equals to zero for granular materials and a non-zero value for cohesive materials and \( \delta \) is the kroncker’s delta.

Figure 4-3: Plastic Potential Surface in the Principal Axes Space.

### 4.3 Model Parameters Estimation

#### 4.3.1 Non-Linear Elastic Modulus Parameters.

As shown above this model has three material parameters that need to be estimated \((M_L, \lambda, \text{ and } \nu)\). The fact that this model depends on the stress invariants would allow us to use any type of experiment such conventional triaxial, biaxial, true triaxial or any combination of these
tests. Using Hook’s law, one might compute $E$ form any of the tests mentioned above with loading-unloading and reloading cycles. Moreover, Poisson’s ratio can be estimated from the same data. Once Poisson’s ratio is estimated for a certain material, the quantity

$$\left[ \frac{I_1}{P_a} \right]^2 + R_z \frac{J'}{P_a^2}$$

can be plotted versus $\frac{E}{P_a}$ on a log-log scale and therefore the values of $M_L$ and $\lambda$ can be estimated accordingly. In this section, the very dense F-75 sand is used as an example to show how to estimate the three non-linear elasticity parameters. Poisson’s ratio for any material can be defined as;

$$\nu = -\frac{\varepsilon_{lateral}}{\varepsilon_{axial}}$$

(4.18)

Values of about 0.13 were reported by Alshibli (1995) for the Silica sands used in this study. The variation of the Possion’s ratio does not affect the numerical results of the present model. The initial elasticity modulus is misleading most of the times and therefore it is preferred to estimate it from the unloading-reloading cycles; Figure 4-4 shows the unloading-reloading cycles for the F-75 sand under axisymmetric triaxial conditions.

It is worth noting here that an experimental data using any stress path will be good enough to estimate the non-linear elastic modulus due to the fact that the model is stress invariants dependent.

For the estimation of the remaining elasticity parameters; Figure 4-5 should be prepared and from linear regression one can estimate those parameters. In linear regression analysis three data points are the minimum needed to estimate the linear model parameters. Therefore, at least three tests with different confining pressures will be required to estimate the model parameters. It is worth noting that the three elasticity parameters depend on the density and the microstructural properties of the material.
4.3.2 Yield Function and Failure Parameters.

As shown in the previous subsection, the material parameters that need to be estimated are $\Psi_1$, $\alpha$, $h$, $\eta_1$ and $m$. Starting with the failure criterion parameters the following failure criterion was proposed and accordingly the failure parameters can be estimated from simple testing:

$$S = 1.0 = \frac{f_N}{\eta_1} = \frac{1}{\eta_1} \left( \frac{I_1^3}{I_{III}} - 27 \right) \left( \frac{I_1}{P_o} \right)^m$$  \hspace{1cm} (4.19)
Based on this failure criterion, one can plot $\frac{P_c}{I_1}$ versus $\left(\frac{I_3^3}{I_{III}} - 27\right)$ at failure on log-log scale (Figure 4-6) and thereafter these failure parameters can be estimated.

![Figure 4-5: Estimation of Non-Linear Elasticity Model Parameters for the Very Dense F-75 Sand.](image)

The plastic work has a unique value along the yield surface (Figure 4-1) which means that the value of the driving stress is unique as well. If one considers two stress paths (Figure 4-1) $OA$ along the hydrostatic axis and $OB$ another arbitrary stress path then the following equity holds:

$$f'_{pA} = f'_{pB}$$

(4.20)
Accordingly;

\[
    h = \ln \left( \frac{\left( \frac{I^3_{IB} - I^2_{IB}}{27\psi_1} \right) e}{\frac{I_{III}}{I_{IB}}} \right)
\]

Where \( e \) is the base of the natural logarithm.

Figure 4-6: Estimation of Material Failure Parameters for the Very Dense F-75 Sand.
It is worth noting here that loading the material under hydrostatic conditions would require very high pressure that can not be achieved by most of the available testing machines. A numerical extrapolation is used here to obtain the value of the $I_{IIa}$, this is achieved by plotting the plastic work versus the first stress invariant during isotropic compression. For the same material and the same density one can obtain, for any stress path, the plastic work at failure, ($W_{pB}$), which is the same as the plastic work at failure during isotropic loading, $W_{pA}$ (i.e. $W_{pA} = W_{pB}$). Knowing that one can extrapolate the plastic work versus the first stress invariant (Figure 4-7) to obtain $I_{IIa}$. Using this argument and applying Equation (4.21) one can calculate $h$.

![Figure 4-7: Plastic Work during Isotropic Compression (F-75 Sand).](image)
4.3.3 Estimation of Material Hardening and Softening Parameters

The parameters $C$ and $p$ need to be estimated before the numerical simulation stage. Data from isotropic compression test should be used to estimate those material parameters. Once the data is available a plot of \( \frac{W_p}{P_a} \) versus \( \frac{I_i}{P_a} \) on log-log scale will be needed to obtain Figure 4-8 that provides the values of those two parameters for the very dense F-75 sand.

All the above parameters that have been estimated to this end will enable us to obtain the values of the stress level parameters, $S$ and $q$:

$$ S = \frac{1}{\eta_1} \left( \frac{I_i^3}{I_{III}} - 27 \right) \left( \frac{I_i}{P_a} \right)^m $$

\[ (4.22a) \]

$$ q = \ln \left( \frac{W_p}{DP_a} \right)^{\frac{1}{\eta_1}} \left( \frac{I_i^3}{I_{III}} - \frac{I_i^2}{I_2} \right) \left( \frac{I_i}{P_a} \right)^n $$

\[ (4.22b) \]

Using an experimental data set one can plot $S$ versus $q$ will produce (Figure 4-9) which will be used to obtain the value of $\alpha$.

4.3.4 Estimation of Material Parameters for the Plastic Potential Function

Two material parameters need to be estimated for the plastic potential function. These parameters are $\Psi_2$ and $\mu$. To be able to estimate those two parameters one needs to evaluate the following quantities:

$$ \xi_s = \frac{1}{1 + \nu} \left[ \frac{I_i^3}{I_2} \left( \sigma_1 + \sigma_3 + 2\nu \sigma_3 \right) + \psi_1 \frac{I_i^4}{I_3} \left( \sigma_1 \sigma_3 + \nu \sigma_3^2 \right) \right] - 3\psi_1 \frac{I_i^3}{I_{III}} + 2 \frac{I_i^2}{I_2} $$

\[ (4.23a) \]
Figure 4-8: Plastic Work during Isotropic Compression for the Very Dense F-75 Sand.

\[\xi_y = \frac{I_1}{I_{III}} - \frac{I_2}{I_2}\]  

(4.23b)

These two quantities can be estimated for a given data set at failure and then plotting \(\xi_y\) versus \(\xi_x\) on arithmetic scale and Figure 4-10 can be produced.

To this end, all the material parameters have been estimated and the next stage will be the implementation for all the equations shown above in a numerical algorithm that can predict the constitutive behavior for a material with known parameters.
Figure 4-9: Stress Level Parameters from Experimental Data for the Very Dense F-75 Sand.

Figure 4-10: Determination of the plastic Potential Function Parameters for the F-75 Sand.
4.4 **Numerical Implementation of Lade’s Model with Cosserat Rotation**

The constitutive equations discussed earlier need to be incrementalized before any numerical implementation. This incrementalization will need a proper integration scheme and a correction technique for crossing the yield surface.

### 4.4.1 Derivatives and Incremental Form of the Constitutive Equations

In this subsection, the constitutive equations will be shown in an incremental form to be able to implement them numerically. Lade and Jakobsen (2002) have proposed the incremental form of the single hardening Lade’s model for granular materials. In this work the same form will be used with modifications on the stress invariants to account for the couple stresses and the Cosserat rotation as will be shown later in Chapter Five.

As stated in the theory of plasticity the total strain increments can be decomposed into two parts, elastic and plastic components as:

\[ \dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^e + \dot{\varepsilon}_{ij}^p \]  

Applying the non-associative flow rule will produce:

\[ \dot{\varepsilon}_{ij}^p = \dot{\lambda}_p \frac{\partial g_p}{\partial \sigma_{ij}} \]

The proportionality multiplier can be expressed as:

\[ \dot{\lambda}_p = \frac{\begin{bmatrix} \partial f_p' \\ \partial \sigma \end{bmatrix}^T \begin{bmatrix} D_e \end{bmatrix} \{\dot{\gamma}\} + \frac{\partial f_p^*}{\partial W_p} \mu g_p}{\begin{bmatrix} \partial f_p' \\ \partial \sigma \end{bmatrix} D' \begin{bmatrix} \partial g_p \\ \partial \sigma \end{bmatrix} + \frac{\partial f_p^*}{\partial W_p} \mu g_p} \]

The partial derivative of the yield and plastic potential functions can be obtained using the chain rule as:
\[
\frac{\partial f_p}{\partial \sigma} = \frac{\partial f_p}{\partial I_I} \frac{\partial I_I}{\partial \sigma} + \frac{\partial f_p}{\partial I_{II}} \frac{\partial I_{II}}{\partial \sigma} + \frac{\partial f_p}{\partial I_{III}} \frac{\partial I_{III}}{\partial \sigma} \quad (4.27a) \\
\frac{\partial g_p}{\partial \sigma} = \frac{\partial g_p}{\partial I_I} \frac{\partial I_I}{\partial \sigma} + \frac{\partial g_p}{\partial I_{II}} \frac{\partial I_{II}}{\partial \sigma} + \frac{\partial g_p}{\partial I_{III}} \frac{\partial I_{III}}{\partial \sigma} \quad (4.27b)
\]

The problem in hand is a plane strain problem (Figure 4-11); the stress and strain tensors are defined as such:

\[
\{\sigma\} = \begin{bmatrix} \sigma_{11} & \sigma_{22} & \sigma_{33} & \sigma_{13} & \sigma_{31} \end{bmatrix} \quad (4.28a)
\]

\[
\{\gamma\} = \begin{bmatrix} \gamma_{11} & \gamma_{22} & \gamma_{33} & \gamma_{13} & \gamma_{31} \end{bmatrix} \quad (4.28b)
\]

As will be discussed later in Chapter Five; \(\gamma\) is a new objective strain tensor.

Figure 4-11 Illustration for the Plane Strain Problem in Hand.
The partial derivatives of the stress invariants with respect to the stresses can be expressed as:

\[
\frac{\partial I_I}{\partial \sigma} = \begin{bmatrix}
1 \\
1 \\
0 \\
0 \\
\end{bmatrix}
\]  
(4.29a)

\[
\frac{\partial I_{II}}{\partial \sigma} = \begin{bmatrix}
-(\sigma_{22} + \sigma_{33}) \\
-(\sigma_{11} + \sigma_{33}) \\
-(\sigma_{11} + \sigma_{22}) \\
\sigma_{21} \\
\sigma_{12} \\
\end{bmatrix}
\]  
(4.29b)

\[
\frac{\partial I_{III}}{\partial \sigma} = \begin{bmatrix}
(\sigma_{22}\sigma_{33}) \\
(\sigma_{11}\sigma_{33}) \\
(\sigma_{22}\sigma_{11} - \sigma_{12}\sigma_{12}) \\
-\sigma_{33}\sigma_{21} \\
-\sigma_{33}\sigma_{12} \\
\end{bmatrix}
\]  
(4.29c)

The derivative of the yield and the plastic potential functions with respect to the stress invariants are:

\[
\frac{\partial f_p'}{\partial I_I} = \left[3 + h \frac{\partial q}{\partial I_I}\right] f_p' + \frac{I_I}{I_{II}} \left( \frac{I_I}{P_a} \right)^h e^q
\]  
(4.30a)

\[
\frac{\partial f_p'}{\partial I_{II}} = \frac{I_I^2}{I_{II}^2} \left( \frac{I_I}{P_a} \right)^h e^q
\]  
(4.30b)

\[
\frac{\partial f_p'}{\partial I_{III}} = f_p' \frac{\partial q}{\partial I_{III}} - \psi \left( \frac{I_I^3}{I_{III}^2} \left( \frac{I_I}{P_a} \right)^h \right) e^q
\]  
(4.30c)
\[\frac{\partial g_p}{\partial I_1} = \left[ \psi_1 (\mu + 3) \frac{I_1^2}{I_{III}} - (\mu + 2) \frac{I_1}{I_{II}} + \frac{\mu \psi_2}{I_1} \right] \left( \frac{I_1}{P_a} \right)^\mu \]  \hspace{1cm} (4.31a)

\[\frac{\partial g_p}{\partial I_{II}} = \frac{I_1^2}{I_{II}^2} \left( \frac{I_1}{P_a} \right)^\mu \]  \hspace{1cm} (4.31b)

\[\frac{\partial g_p}{\partial I_{III}} = -\psi_1 \frac{I_1^3}{I_{III}^3} \left( \frac{I_1}{P_a} \right)^\mu \]  \hspace{1cm} (4.31c)

Where;

\[\frac{\partial q}{\partial I_1} = \frac{\partial q}{\partial S} \frac{\partial S}{\partial I_1} = \frac{\alpha}{\eta_1 (1 - (1 - \alpha)S)} \left[ \frac{m S \eta_1}{I_1} + \frac{3 I_1^2}{I_3} \left( \frac{I_1}{P_a} \right)^m \right] \]  \hspace{1cm} (4.32a)

\[\frac{\partial q}{\partial I_{III}} = \frac{\partial q}{\partial S} \frac{\partial S}{\partial I_{III}} = \frac{\alpha}{\eta_1 (1 - (1 - \alpha)S)} \left[ \frac{I_1^3}{I_3^3} \left( \frac{I_1}{P_a} \right)^m \right] \]  \hspace{1cm} (4.32b)

The derivatives of the yield function with respect to the plastic work for both hardening and softening regimes, respectively, will be:

\[\frac{\partial f_p}{\partial W_p} = \frac{1}{\rho (DP_a)^{1/\rho}} W_p^{1/\rho - 1} \]  \hspace{1cm} (4.33a)

\[\frac{\partial f_p}{\partial W_p} = -\frac{AB}{P_a} \exp \left( - \frac{B W_p}{P_a} \right) \]  \hspace{1cm} (4.33b)

### 4.4.2 Numerical Implementation of Lade’s Model

The constitutive relations proposed above have been implemented into a FORTRAN code used later in the USER ELEMENT and USER MATERIAL (UEL and UMAT) subroutines for the finite element program (ABAQUS). In this Chapter the FORTRAN code used to predict
the constitutive behavior of materials will be discussed and verified. Equation (4.34) represents the incremental constitutive relations for an elasto-plastic material:

\[
\{\sigma\} = [D]\{\gamma\} 
\]

(4.34a)

\[
[D] = \left[ D^c \right] - \frac{1}{\left[ D^c \right]} \left[ \begin{array}{c} \partial f_p' \cr \partial \sigma \end{array} \right]^T \left[ D^c \right] \left[ \begin{array}{c} \partial g_p \cr \partial \sigma \end{array} \right] + \frac{\partial f_p'}{\partial W_p} \mu g_p
\]

(4.34b)

\[
\begin{bmatrix} K + G & K - G & K - G & 0 & 0 \\ K - G & K + G & K - G & 0 & 0 \\ K - G & K - G & K + G & 0 & 0 \\ 0 & 0 & 0 & 2G & 0 \\ 0 & 0 & 0 & 0 & 2G \end{bmatrix}
\]

(4.34c)

Where G and K are the shear and bulk moduli.

### 4.4.2.1 Structure of the Constitutive Code

The FORTRAN code used in this work has a general structure as shown in Figure 4-12. For more details interested readers are referred to Jakobsen and Lade (2002).

### 4.4.2.2 Correcting for Crossing the Yield Surface

Using an explicit integration scheme to update the stresses and the other state variables will cause a drift from the yield surface. This drift will very much depends on the integration scheme and the size of the strain increment and needs to be corrected accordingly. Several methods have been proposed in the literature to correct for crossing the yield surface using any
plasticity model. In this dissertation, a method proposed by Potts and Gens (1985) and verified by Jakobsen and Lade (2002) will be used. This method assumes that the total strain increment will be constant, however, the decomposed components (elastic and plastic) will be balanced to bring the stress back to the new yield surface within certain tolerance. Figure 4-13 shows an illustration for the correction technique, which will basically require the stress and the plastic work to be corrected.

The correction technique will require changing the stresses and the plastic work at point “C” to the following values at point “B”:

\[
\sigma^{(B)} = \sigma^{(C)} - \chi \mathbf{D}^f \frac{\partial g_p}{\partial \sigma^{(C)}} \quad \text{(4.35a)}
\]

\[
W_p^{(B)} = W_p^{(C)} + \chi \frac{\partial g_p}{\partial \sigma} \quad \text{(4.35b)}
\]

\[
\chi = \frac{f(\sigma^{(C)}, W_p^{(C)})}{\left\{ \frac{\partial f}{\partial \sigma^{(C)}} \right\}^T \mathbf{D}^f \left\{ \frac{\partial g_p}{\partial \sigma^{(C)}} \right\} - \left\{ \frac{\partial f}{\partial W_p^{(C)}} \right\} \left\{ \frac{\partial g_p}{\partial \sigma^{(C)}} \right\}^T \sigma^{(C)}} \quad \text{(4.35c)}
\]

4.4.2.3 Integration Scheme

Jakobsen and Lade (2002) have discussed different explicit integration schemes to update the model state variables. The Forward Euler Scheme was found to be good enough to be used to predict the elasto-plastic behavior of granular materials because of the implementation simplicity and the good accuracy. In this subsection, the forward Euler integration scheme will be discussed with some details.

The forward Euler method suggests that the strain increment to be subdivided into subincrements, one disadvantage in this method is that this subincrementation should be defined upfront manually as:
Figure 4-12 Schematic Flow Chart Describes the Structure for the Constitutive Numerical Code.

Start with Confining Stresses, Initial Strain Increment and Initial Plastic Work

Compute the Elastic Stress Tensor,
\[ \{ \sigma \} = [D \gamma] \]

Check the Consistency Condition, \( f_p \)
\[ f_p(\sigma, W_{pl}) \]

If \( f_p(\sigma, W_{pl}) \leq 0 \)

No

Yes

If \( f_p(\sigma_0, W_{pl}) = 0 \)

No

Yes

\( \delta = 0 \)

Determine the Ratio, \( \delta \)

Compute the stress for the first crossing the yield surface as:
\[ \sigma_c = \sigma_c + \delta \sigma_{\varepsilon} \text{ and } \Delta \gamma = (1 - \delta) \Delta \gamma \]

Update the Stresses, Plastic Work and Elasto-Plastic Matrix Using the Forward Euler Integration Scheme

If \( f_p(\sigma, W_{pl}) \leq \varepsilon \)

No

Yes

Correct for crossing the yield surface

Return with Updated Stresses, Plastic Work and Elasto-Plastic Stiffness Matrix
Figure 4-13 Illustration shows the Drift from the Yield Surface and the Correction Technique.

\[ \delta \gamma = \frac{\dot{\gamma}}{n} \]  \hspace{1cm} (4.36)

Where; \( n \) is an integer represents the number of subincrements. The stress components are updated according to:

\[ \sigma^{(i)} = \sigma^{(i-1)} + \dot{\sigma}^{(i)} \]  \hspace{1cm} (4.37a)

\[ \dot{\sigma} = \sum_{j=1}^{n} \delta \sigma_j \]  \hspace{1cm} (4.37b)

\[ \delta \sigma_j = D(\sigma_{j-1}, W_{p,i-1}, \delta \gamma) \cdot \delta \gamma \]  \hspace{1cm} (4.37c)

While the plastic work component is updated using:

\[ W_p^{(i)} = W_p^{(i-1)} + \dot{W}_p^{(i)} \]  \hspace{1cm} (4.38a)

\[ \dot{W}_p^j = \sum_{j=1}^{n} \delta W_p^j \]  \hspace{1cm} (4.38b)

\[ \delta W_p^j = \dot{\lambda}(\sigma_{j-1}, W_{p,i-1}, \delta \gamma) \sigma_{j-1} \frac{\partial g_p}{\partial \sigma_{j-1}} \]  \hspace{1cm} (4.38c)
4.5 Applications of the Code to Predict the Stress-Strain Behavior of Different Granular Materials

4.5.1 Fine Graded Silica Sand

The numerical model has been used to predict the constitutive behavior of the fine silica sand, which had been described earlier in Chapter Three. Stress-strain results were compared for both dense and very dense states. Table 4-1 and Table 4-2 show the values of the material parameters used in the numerical prediction for both dense and very dense states respectively. Figure 4-14 and Figure 4-15 show the comparison between prediction and experimental results under triaxial testing.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$M_L$</th>
<th>$\lambda$</th>
<th>$\nu$</th>
<th>$m$</th>
<th>$\eta_1$</th>
<th>$\Psi_2$</th>
<th>$\mu$</th>
<th>$h$</th>
<th>$\alpha$</th>
<th>$C$</th>
<th>$P$</th>
<th>$b$</th>
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<tbody>
<tr>
<td>Value</td>
<td>292.6</td>
<td>0.25</td>
<td>0.13</td>
<td>0.37</td>
<td>84.1</td>
<td>-3.06</td>
<td>2.2</td>
<td>0.95</td>
<td>0.30</td>
<td>7</td>
<td>-5</td>
<td>2.6</td>
</tr>
</tbody>
</table>

Table 4-2: Very Dense Fine Silica Sand Constitutive Parameters for Lade’s Model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$M_L$</th>
<th>$\lambda$</th>
<th>$\nu$</th>
<th>$m$</th>
<th>$\eta_1$</th>
<th>$\Psi_2$</th>
<th>$\mu$</th>
<th>$h$</th>
<th>$\alpha$</th>
<th>$C$</th>
<th>$P$</th>
<th>$b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>292.6</td>
<td>0.26</td>
<td>0.13</td>
<td>0.40</td>
<td>103.2</td>
<td>-3.06</td>
<td>2.18</td>
<td>0.565</td>
<td>0.62</td>
<td>7</td>
<td>-5</td>
<td>1.64</td>
</tr>
</tbody>
</table>

Plane strain results are available for the very dense F-75 sand (Alshibli (1995)); the numerical model is capable to predict the stress-strain behavior of the granular material under triaxial, true triaxial and biaxial tests. Using the material parameters shown in Table 4-2 for the very dense F-75 sand; the numerical model was used to predict the stress-strain and the volumetric strain curves for this material under plane strain condition (Figure 4-16). It is shown in Figure 4-16 that the model predicted the stress-strain behavior fairly good where the volumetric strains were poorly predicted.
Figure 4-14 Comparison between Experimental Results and Numerical Predictions for Dense F-sand (Axisymmetric Triaxial Tests).

(a) Deviatoric Stress versus Axial Strain

(b) Volumetric Strain versus Axial Strain
Figure 4-15: Comparison between Experimental Results and Numerical Predictions for the Very Dense F-sand (Axisymmetric Triaxial Tests).

(a) Deviatoric Stress versus Axial Strain

(b) Volumetric Strain versus Axial Strain
Figure 4-16 Comparison between Experimental Results and Numerical Predictions for the Very Dense F-sand (Plane Strain Test).

(a) Deviatoric Stress versus Axial Strain

(b) Volumetric Strain versus Axial Strain
4.5.2 **Coarse Graded Silica Sand**

The coarse graded silica sand that has been characterized in Chapter Three is used here with triaxial tests results to show the ability of the constitutive model in predicting the stress-strain behavior of such materials. Table 4-3 shows the material parameters used in the predictions and Figure 4-17 shows a comparison between predicted and measured stress-strain curves under different confining pressures using plane strain conditions.

Table 4-3: Coarse Silica Sand Constitutive Parameters for Lade’s Model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$M_L$</th>
<th>$\lambda$</th>
<th>$\nu$</th>
<th>$m$</th>
<th>$\eta_1$</th>
<th>$\Psi_2$</th>
<th>$\mu$</th>
<th>$h$</th>
<th>$\alpha$</th>
<th>$C$</th>
<th>$P$</th>
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<tbody>
<tr>
<td>Value</td>
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<td>0.32</td>
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<td>0.30</td>
<td>90.1</td>
<td>-3.10</td>
<td>2.09</td>
<td>0.58</td>
<td>0.50</td>
<td>2</td>
<td>4</td>
<td>1.52</td>
</tr>
</tbody>
</table>

4.5.3 **Small and Large Glass Beads**

The glass beads which had been discussed in chapter three are used in this section for verification purposes. Table 4-4 and Table 4-5 shows the material parameters; Figure 4-18 and Figure 4-19 show the comparisons between measurement and predictions.

Table 4-4: Small Glass Beads Constitutive Parameters for Lade’s Model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$M_L$</th>
<th>$\lambda$</th>
<th>$\nu$</th>
<th>$m$</th>
<th>$\eta_1$</th>
<th>$\Psi_2$</th>
<th>$\mu$</th>
<th>$h$</th>
<th>$\alpha$</th>
<th>$C$</th>
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</thead>
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<td>Value</td>
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<td>0.2</td>
<td>0.2</td>
<td>14.82</td>
<td>-3.09</td>
<td>1.05</td>
<td>0.70</td>
<td>0.52</td>
<td>6</td>
<td>5</td>
<td>2.3</td>
</tr>
</tbody>
</table>

Table 4-5: Large Glass Beads Constitutive Parameters for Lade’s Model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$M_L$</th>
<th>$\lambda$</th>
<th>$\nu$</th>
<th>$m$</th>
<th>$\eta_1$</th>
<th>$\Psi_2$</th>
<th>$\mu$</th>
<th>$h$</th>
<th>$\alpha$</th>
<th>$C$</th>
<th>$P$</th>
<th>$b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>192</td>
<td>0.35</td>
<td>0.19</td>
<td>0.28</td>
<td>18.81</td>
<td>-3.2</td>
<td>1.5</td>
<td>0.65</td>
<td>0.66</td>
<td>1.2</td>
<td>4</td>
<td>1.9</td>
</tr>
</tbody>
</table>

4.6 **Sensitivity Analysis of Model Parameters**

As shown in the above subsections, the model has 12 material parameters each has it own effect on the model predictions. The first three parameters (the non-linear elastic modulus model parameters) were found to affect the initial slope of the stress-strain curve and the slope of the volumetric strain curve as shown in Figure 4-20 through Figure 4-22. The effect of Poisson’s ratio was found to be insignificant on the stress-strain curve and relatively speaking; it has small
effect on the volumetric strains. The effect of other material parameters on the stress-strain and volumetric strain-axial strain curves are shown in Figure 4-23 through Figure 4-30 and they are self explanatory.
Figure 4-17 Comparison between Experimental Results and Numerical Predictions for Course Sand under Plane Strain Conditions.

(a) Deviatoric Stress versus Axial Strain

(b) Volumetric Strain versus Axial Strain
Figure 4-18: Comparison between Experimental Results and Numerical Predictions for Small Glass Beads (Axisymmetric Triaxial Tests).

(a) Deviatoric Stress versus Axial Strain

(b) Volumetric Strain versus Axial Strain
Figure 4-19: Comparison between Experimental Results and Numerical Predictions for Large Glass Beads (Axisymmetric Triaxial Tests).

(a) Deviatoric Stress versus Axial Strain

(b) Volumetric Strain versus Axial Strain
Figure 4-20 The Effect of $M_L$ on the Model Predictions
Figure 4-21 The Effect of $\lambda$ on the Model Predictions

(a) Stress-Strain Curve

(b) Volumetric Strain-Axial Strain Curve
Figure 4-22 The Effect of $\nu$ on the Model Predictions
Figure 4-23 The Effect of $m$ on the Model Predictions
Figure 4-24 The Effect of $\eta_1$ on the Model Predictions
Figure 4-25 The Effect of $\mu$ on the Model Predictions
Figure 4-26 The Effect of \( h \) on the Model Predictions
Figure 4-27 The Effect of $\alpha$ on the Model Predictions
Figure 4-28 The Effect of Con the Model Predictions

(a) Stress-Strain Curve

(b) Volumetric Strain-Axial Strain Curve
Figure 4-29 The Effect of $p$ on the Model Predictions
Figure 4-30 The Effect of $b$ on the Model Predictions
CHAPTER FIVE

MATHEMATICAL FORMULATIONS AND FINITE ELEMENT DISCRETIZATION

5.1 Introduction

Granular materials undergo high rotational and translational deformations inside a finite zone at failure. The rotations are the most dominant at the failure or at the bifurcation point (Oda et. al. 1997, 1998, 2002; Vardoulakis and Sulem, 1995). This finite zone is called the shear band in which the shear and volumetric plastic strains, plastic work, and void ratio reads maximum values within the whole continuum; moreover, the material or Cosserat rotation will record the highest values as well. Since the deformations are composed of high rotational and translational rates; it is of high importance to bring both of them into the formulations that describe the mechanics of the continua. The Cosserat continuum is one of the best techniques that can deal with such deformations in granular materials. In this technique, the rotations can be computed using the displacement fields if one chooses to use the constrained Cosserat continuum. Otherwise, the material or the Cosserat rotation should be treated independently from the displacement field and therefore a new degree of freedom is introduced. An internal length scale should be also involved in the solution through the couple stresses and thus one might overcome the mathematical instabilities in an analytical solution and mesh dependency in the finite element solution.

When granular materials are subjected to high stresses, particles will undergo high irreversible deformations “rotational and translational” accordingly. Many researchers support the notion that particles rotation is dominant at failure, however, it is to be proven experimentally. In the author’s opinion, if the particle assembly is compacted well then the
particles will prefer to rotate rather than to translate during loading. Thereafter, the idea that the rotations are dominant at failure is highly supported in this work. However, all the expected kinematics “rotation or/and translation” should be incorporated in the problem to solve for the instability and strain localization problems. The rotation of the grains occurs when the particles are subjected to high couple stress enough to overcome any resistance. This resistance will be essentially the surface-to-surface friction at the contact and what will be called here the polar friction which is caused by the angularity of the particles. The surface friction will depend primarily on the surface roughness and the normal stresses. On the other hand, the polar friction depends mainly on the shape of the particles (Oda et. al., 1998), porosity and the confining stresses. The polar friction, in other words, can be described as the resistance of the particles to any rearrangement or realignment processes.

It has been known for long time that granular materials exhibit plastic behavior mostly due to the permanent repositioning of the individual particles, no dislocation but high irregular and spatial rearrangements, which are irreversible most of the time. The elasto-plastic constitutive laws have been found fair enough to simulate the behavior of granular materials; therefore, it will be adopted in this study. As mentioned by Vardoulakis and Sulem (1995), and Rubin (2000), the Cosserat brothers (1909) have developed the couple stress theory by Viogt (1887), they separated the displacement gradients from the rotations and then it is possibly the best to deal with individual particles. The rotation can be considered as the individual particle rotation. The linearized or the constrained Cosserat developed by many researchers to have only one independent displacement field then the particle rotation can be easily computed from the displacement field. The formulations foundation that will be adopted in this study is the Cosserat continuum in which the granular particles will be treated as Cosserat points, which can be
considered as nonlinear continuum (Rubin, 2000). In a Cosserat point, the balance laws are nonlinear and the material is arbitrary, thus it can be applied to granulates. Then the overall material continua can be studied numerically based on the formulations that have the Cosserat point continuum as the theoretical foundation. In this aspect, the nonlinear finite elements formulations can be built and solved for the whole continuum. The Cosserat point can be defined as a zero dimensional point surrounded by small but finite region of material (Rubin, 2000).

5.2 The Updated Lagrangian Frame

Granular materials and in general the geomaterials will always undergo high or large deformations and thus choosing the reference configuration in the finite element solution is of high importance. The updated Lagrangian frame (UL) will be the basis for all the formulations in this work. In the UL configuration all the state variables increments in the current time step will be referred to the previous ones, in other words, the reference point is updated at each time step. Figure 5-1 shows an illustration for the concept of the updated Lagrangian configuration that will be adopted in this work. The updated position vector will read:

\[ n+1 \mathbf{X}_i = \mathbf{x}_i = \zeta_i (\mathbf{X}_i, t) \] (5.1)

Where \( \mathbf{x} \) is the position of the material point, \( \mathbf{X} \), at time “t” and \( n\mathbf{X}_i \) is the position of the material point \( \mathbf{X} \) at time (t-\( \Delta t \)), the dimensionless time increment will be used here. Now one can define the displacement vector as:

\[ u_i (x_i, t) = \zeta_i (X_{i-\Delta t}, t) - \zeta_i (X_{i-2\Delta t}, t - \Delta t) = x_i - X_i \] (5.2)

From now on \( x_i \) will be used for the current configuration and \( X_i \) will be used for the previous one “Update Total Lagrangian”. The velocity vector is defined as:
\[ v_i(X,t) = \frac{\partial\zeta_i(X,t)}{\partial t} = \frac{\partial u_i(X,t)}{\partial t} = \dot{u}_i \quad (5.3) \]

Figure 5-1 Initial and Current Body Configurations with the Deformation Mapping Steps using the Updated Lagrangian Configuration

Here the derivative is the total or the material time derivative. The above derivative will collapse into the ordinary time derivative when the motion is function of time and the position vector \( \mathbf{X} \) held constant. Similarly the acceleration vector can be defined as:

\[ a_i(X,t) = \frac{\partial v_i(X,t)}{\partial t} = \frac{\partial^2 u_i(X,t)}{\partial t^2} = \ddot{u}_i = \dot{\dot{u}}_i \quad (5.4) \]

The material time derivative can be defined for any function \( f \) as:

\[ \frac{Df}{Dt} = \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f \quad (5.5a) \]

Note here that the function \( f \) is a continuous \((in x and t)\) scalar or even a high order tensor. It is worth noting here that if the function \( f \) is defined in the Lagrangian frame then its gradient will vanish and Equation 5.5a becomes:

\[ \frac{Df}{Dt} = \frac{\partial f}{\partial t} \quad (5.5b) \]
One can now define the deformation gradient $F$ as:

$$ F_{ij} = \frac{\partial \zeta_i}{\partial X_j} = \frac{\partial x_i}{\partial X_j} \tag{5.6} $$

The deformation gradient is helpful to map between the deformed (current) configuration and the previous or the un-deformed configuration. The Jacobian is defined as the determinate of the nonsingular tensor $F$.

$$ J = \text{det}(F) \quad 0 < J < \infty \tag{5.7a} $$

This condition for the Jacobian is a must to satisfy the continuity. The Jacobian can also be related by knowing the current volume and the previous or initial volume and thus the $J$ can be rewritten as:

$$ J = \frac{V}{V_0} = \frac{\rho}{\rho_o} = \frac{\rho_o}{\rho} \tag{5.7b} $$

If one now wants to consider the time-material derivative for the Jacobian, then the following might be considered:

$$ \frac{DJ}{Dt} = J\text{div}(\mathbf{v}) \tag{5.8} $$

It is worth noting here that the position function has to be continuous and one-to-one and the Jacobian “det($F$)” must be positive quantity so the that the laws of continuum mechanics and compatibility will be satisfied.

5.3 **Kinematics and Kinetics in the Cosserat Continua**

5.3.1 **Kinematics**

If one assumes that granular particles are spherical then the schematic shown in
Figure 5-2 illustrates the interaction between two adjacent particles with the kinematics acting on them.

Figure 5-2 Cosserat Kinematics for two grains in 2D space (Vardoulakis and Sulem, 1995)

Referring to Figure 5-2 $v$ is the strain rate vector and $\omega^c$ is the Cosserat or the material point rotation which is independent on the translational degree of freedom.

According to Bathe (1990), the Green or the Lagrangian strain tensor can be decomposed into linear and non-linear components as:

\[ E_{ij} = e^n_{ij} + \eta_{ij} \quad (5.9a) \]
\[ e^n_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) \quad (5.9b) \]
\[ \eta_{ij} = \frac{1}{2} (u_{k,i}u_{k,j}) \quad (5.9c) \]

The definition of the quantity $u_{i,j}$ is the displacement field derivative with respect to the current position and;

\[ \dot{e}_{ij} = D_{ij} = \frac{1}{2} (v_{i,j} + v_{j,i}) \quad (19d) \]

Cosserat continuum is composed of individual particles and each particle will deform in translation and rotation based on the interaction between a specific particle and the neighboring.
The spin or the rotation of the particle can be described by $\omega^c$, which means the Cosserat or material point rotation; this rotation can be defined as a vector similar to the displacement vector, $u$. Then one might define vector as $\omega^c_i = \omega^c$. The objective or Cosserat strain rate tensor now can be redefined as:

$$^n\gamma_{ij} = ^n\dot{E}_{ij} + ^n\ddot{\chi}_{ij}$$  \hspace{1cm} (5.20a)

$$^n\dot{\chi}_{ij} = ^n\dot{\Omega}_{ij} - ^n\ddot{\Omega}_{ij}$$  \hspace{1cm} (5.20b)

Where, $\Omega$ and $\Omega^c$ are defined below and $\{\cdot\}$ is defined here as the spatial objective strain rate tensor. The strain rate tensor defined in Equation (5.20) produces non-symmetry in the stress tensor (Tomantschger, 2002). The curvature vector of deformation or the gradient of particle rotation can be defined as:

$$^n\kappa_i = ^n\omega_{j,i}$$  \hspace{1cm} (5.21a)

where Equation (5.21a) will collapse into the following form for plane-strain case:

$$^n\kappa_i = \omega_{j,i} \hspace{1cm} i=1,2$$  \hspace{1cm} (5.21b)

Equation (5.20) shows that there is one type of strain rate and two types of spin tensor, those are the classical strain – rate tensor, $\dot{E}_{ij}$, and the classical spin tensor:

$$^n\dot{\Omega}_{ij} = \frac{1}{2}(v_{i,j} - v_{j,i})$$  \hspace{1cm} (5.22)

and the Cosserat spin tensor that can be written as:

$$\Omega^c_{ij} = -e_{ijk} \omega^c_k$$  \hspace{1cm} (5.23a)

Where we have $e_{ijk}$ is the Ricci permutation tensor and again for a plane-strain problem (5.23a) will collapse into:

$$^n\Omega^c_{ij} = -e_{ij3} \omega^c_3$$  \hspace{1cm} (5.23b)
Equation (5.20) shows obviously that if the macro-rotation coincides with the grain rotation then the strain rate tensor will collapse into the classical one. The separation of the Cosserat or material point rotation from the continuum or the macro-rotation is clarified below in Figure 5-3.

The above formulations were written in the updated Lagrangian frame. Now one might consider the relative deformation as a result of the macro – micro differences and then the relative deformation tensor rate can be written as:

\[ ^n D_{ij}^R = \gamma_{ij}^m - \hat{\omega}^c_{ij} \]  \hspace{1cm} (5.24)

![Figure 5-3: The Separation between the micro- and macro- rotation and their effect on the kinematics in 2D space.](image)

Then the relative deformation-rate can be decomposed into symmetric and anti-symmetric parts as follow:

\[ D_{ij}^{RS} = D_{ij} \]  \hspace{1cm} (5.25)

\[ D_{ij}^{RA} = \hat{\Omega}_{ij} - \hat{\Omega}_{ij}^c \]  \hspace{1cm} (5.26)
The anti-symmetry here arises from the deviation between the micro and macro rotations “local spinning due to displacement and particle rotation”. Note that this step could be already concluded before doing the detailed derivation; direct conclusion from Equations (5.19d) and (5.25).

### 5.3.2 Kinetics

One begins defining the Cauchy stress tensor in the \( n^{th} \) configuration and as, \( ^n\sigma_{ij} \) and then the second Piola-Kirchoff stress tensor is expressed as:

\[
^nS_{ij} = ^n\sigma_{ij} + \Delta^nS_{ij}
\]  

(5.27)

In the particles continuum and according to the Schneebelli medium over a distance \( l \), the macroscopic stress tensor, \( \sigma_{ij} \), is related to the intergranular stress tensor \( \Sigma_{ij} \). The stress tensor \( \sigma_{ij} \) is the average of \( \Sigma_{ij} \) over the distance \( 2l \) (Vardoulakis and Sulem, 1995) as:

\[
^n\sigma_{11} = \int_{-l}^{l} ^n\Sigma_{11} dx_2 \quad \text{(5.28a)}
\]

\[
^n\sigma_{22} = \int_{-l}^{l} ^n\Sigma_{22} dx_1 \quad \text{(5.28b)}
\]

\[
^n\sigma_{12} = \int_{-l}^{l} ^n\Sigma_{12} dx_1 \quad \text{(5.28c)}
\]

\[
^n\sigma_{21} = \int_{-l}^{l} ^n\Sigma_{21} dx_2 \quad \text{(5.28d)}
\]

Figure 5-4 shows the inter-particle stresses acting on an macro-element. It is worth noting that the Cauchy stress tensor here is non-symmetric and:

\[
^n\Sigma_{ij} = \frac{1 - n}{\pi l} \sum_{k=1}^{N} ^nP_{ij}^kn_{jk}^k \quad \text{(5.29)}
\]
Where \( n \) is the medium porosity, \( l \) is the dimension of the macro-element that contains \( N \) grains, \( nP_i^k \) is the \( k^{th} \) inter-granular forces at the \( k^{th} \) contact with the unit normal \( n^k_j \) in the \( n^{th} \) configuration. One might define the couple stress for 2D Cosserat continuum as:

\[
\int_{\Sigma} \Sigma = l^l n d\xi x_3 113323 \mu
\]  
\[\text{(5.30)}\]

\[
\int_{\Sigma} \Sigma = l^l n d\xi x_1 113323 \mu
\]  
\[\text{(5.31)}\]

The rate-of-deformation tensor can be decomposed into symmetric and anti-symmetric parts as:

\[
\dot{\gamma}_{(ij)} = \dot{E}_{ij}
\]  
\[\text{(5.32a)}\]

\[
\dot{\gamma}_{[ij]} = \dot{\Omega}_{ij} - \dot{\Omega}^c_{ij} = \dot{\chi}_{ij}
\]  
\[\text{(5.32b)}\]

The inertial forces and couples respectively will read:

\[
f_i = -\rho \dot{\chi}_i
\]  
\[\text{(5.33a)}\]

\[
\sigma_i = -I \dot{\omega}_i^c
\]  
\[\text{(5.33b)}\]

Where, the first moment of inertial for the micro-medium, \( I \), reads:

Figure 5-4: Schematic Distribution of the inter-granular stresses on a macro-element.
The micro-medium density is:

\[ \rho = (1 - n) \rho_g \]  

(5.33d)

Where \( \rho_g \) is the density or the specific gravity of the grains.

In the 2D Cosserat continuum one has essentially two couple stresses; they are:

\[ m_1 = \mu_{21} \text{ and } m_3 = \mu_{23} \]  

(5.34)

The couple stress will cause the main anti-symmetry in the stress tensor and thereafter the material stiffness matrix becomes anti-symmetric, the loss of symmetry is shown in Figure 5-5.

Figure 5-5: Loss of Stress Symmetry in Cosserat Continua

5.4 Equations of Virtual Work

Following Bathe (1990), the virtual work in an updated Lagrangian reference reads:

\[ \int_{\Omega} (n_1 S_y \delta(n_1 E_y)) dV = n_1 R \]  

(5.35)

Where, \( R \) is the external virtual work. Incorporating the Cosserat couple stresses and rotations, the virtual work equation becomes:

\[ \int_{\Omega} (n_1 S_y \delta(n_1 E_y) + n_1 m_i \delta(n_1 K_i)) dV = n_1 R \]  

(5.36)
\[ R = \int_{\Omega} \left( \rho_{ij} \dot{\epsilon}_{ij} + m \Omega_{ij} \right) \mu^{n+1} S + \int_{\Omega} \left( \rho_{ij} \dot{\epsilon}_{ij} + I \dot{\omega}^c \right) \mu^{n+1} \nu \]  

(5.37)

Where,

\[ \gamma_{ij} = e_{ij} + \eta_{ij} + \Omega_{ij} - \Omega_{ij} = E_{ij} + \chi_{ij} \]  

(5.38a)

\[ m = m_{ni} \]  

(5.38b)

\[ T_i = \sigma_{ij} n_j \]  

(5.38c)

Now the Cauchy stress tensor can be related to the second Piola–Kirchoff stress tensor through the Jacobian and the deformation gradient Abu-Farsakh et al. (1998) as:

\[ \sigma_{ij}^{n+1} = J^{-1} X_{i,l} X_{j,l}^{n+1} S_{lj} \]  

(5.39a)

\[ X_{i,l} = \frac{\partial x_i}{\partial x^l} = \frac{\partial^n X_i}{\partial^n x^l} \]  

(5.39b)

### 5.5 Constitutive Relations

#### 5.5.1 Lade’s Single Hardening Model

As shown earlier in Chapter Four Lade and co-workers developed a constitutive model with a single hardening function and non-linear elasticity relations. The Lade’s constitutive model will be discussed very briefly. The following non-linear elasticity modulus was proposed and used in this work.

\[ E = M_l P_a \left[ \left( \frac{I_1}{P_a} \right) + R_l \left( \frac{J_2}{P_a^2} \right)^{\frac{1}{2}} \right] \]  

(5.40a)

All the parameters in Equation (5.40) have been defined in Chapter Four and the second deviatoric stress invariant is enhanced to account for the couple stress effect as follow:

\[ J_2' = h_3 \left( (\sigma_{11} - \sigma_{22})^2 + (\sigma_{33} - \sigma_{22})^2 + (\sigma_{11} - \sigma_{33})^2 \right) + \sigma_{12}^2 + \frac{h_4}{I^2} (m_1^2 + m_2^2) \]  

(5.40b)
Where, $h_3$ and $h_4$ are the balancing factors between the couple stress ($m_i$) and the stress ($\sigma_{ij}$) and $l$ is an internal length scale. The following plastic potential function was proposed:

$$g_p = \left[ \Psi_1 \frac{I_i^3}{I_{III}} - \frac{I_i^2}{I_{II}} + \Psi_2 \left( \frac{I_i}{P_a} \right)^h \right]^p$$ \hspace{1cm} (5.41)

The plastic strain increment can be obtained from the plastic potential function; non-associated flow rule is adopted here:

$$\dot{\varepsilon}_{ij}^p = \dot{\lambda}_p \frac{\partial g_p}{\partial \sigma_{ij}}$$ \hspace{1cm} (5.42a)

Where $\dot{\lambda}_p$ is a positive plastic proportionality constant and can be expressed as:

$$\dot{\lambda}_p = \frac{\dot{W}_p}{\mu g_p}$$ \hspace{1cm} (5.42b)

Lade and Kim (1988) has developed a yield function based on the work – hardening and softening law for frictional materials. The following function was proposed:

$$f_p = f_p^*(\sigma) - f_p^\alpha(W_p) = 0$$ \hspace{1cm} (5.43)

This is the yield criterion they have proposed, $W_p$ is the plastic work and;

$$f_p^* = \left[ \Psi_1 \frac{I_i^3}{I_{III}} - \frac{I_i^2}{I_{II}} \left( \frac{I_i}{P_a} \right)^h \right] e^q$$ \hspace{1cm} (5.44a)

$$f_p^\alpha = \left( \frac{1}{D} \right)^{1/p_a} \left( \frac{W_p}{P_a} \right)^{1/p_a}$$ \hspace{1cm} (5.44b)

This acts as the plastic work hardening during the hardening regime, where the softening is an exponential function expressed as:

$$f_p^\alpha = A e^{-B \left( \frac{W_p}{P_a} \right)}$$ \hspace{1cm} (5.44c)

Now the plastic work is estimated during the isotropic (hydrostatic) loading as:
\[ W_p = C P_e \left( \frac{I_1}{p a} \right)^p \]  

(5.45a)

At any further stresses it can be estimated as:

\[ W_p = D P_e \left( f_p^n \right)^n \]  

(5.45b)

### 5.5.2 Phenomological Enhancement for Lade’s Model

In this study, the stress invariants will be modified to account for the couple stresses; in this sense weighting factors will be postulated and latter on the model will be calibrated to estimate those model parameters, such parameters will depend on the shape of the grains and on the assumed contact distribution function:

\[ I_1 = \sigma_{ii} \]  

(5.46a)

\[ I_{II} = h_1 \left[ \sigma_{12} \sigma_{21} - \sigma_{11} \sigma_{22} - \sigma_{11} \sigma_{33} - \sigma_{22} \sigma_{33} \right] - h_2 \frac{m_1 m_2}{l_s^2} \]  

(5.46b)

\[ I_{III} = \left[ \sigma_{11} \sigma_{22} \sigma_{33} - \sigma_{33} \sigma_{12} \sigma_{21} \right] \]  

(5.46c)

Where, \( h_r (r = 1, 2) \) are weighing coefficients for statics. Vardoulakis and Sulem (1995) have used similar approach in modifying stress second invariant; the following values were used in their work:

\[ h_r = \{1/2, 1\} \]  

(5.46d)

And \( l_s \) is an internal length scale that represents the length of the contact surface between two adjacent particles and it should be chosen carefully. In this case, the internal length scale is the length of the contact surface between two particles as shown in Figure 5-6.
5.5.3 Elasto-Plastic Constitutive Equations

The total strain and rotation tensors can be decomposed into elastic and plastic strains as:

\[
\dot{E}_{ij} = \dot{E}_{ij}^e + \dot{E}_{ij}^p \\
E_{ij} = E_{ij}^e + E_{ij}^p
\]  
(5.47)

\[
\dot{\kappa}_i = \dot{\kappa}_i^e + \dot{\kappa}_i^p \\
\kappa_i = \kappa_i^e + \kappa_i^p
\]  
(5.48)

\[
\dot{\gamma}_{ij} = \dot{\gamma}_{ij}^e + \dot{\gamma}_{ij}^p \\
\gamma_{ij} = \gamma_{ij}^e + \gamma_{ij}^p
\]  
(5.49)

The stress tensor can be written such that the couple stresses are incorporated as:

\[
[\sigma] = \begin{bmatrix}
\sigma_{11} & \sigma_{12} & \sigma_{13} & 0 & 0 & 0 \\
\sigma_{21} & \sigma_{22} & \sigma_{23} & 0 & 0 & 0 \\
\sigma_{31} & \sigma_{32} & \sigma_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{m_1}{l_s} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{m_2}{l_s} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{m_3}{l_s}
\end{bmatrix}
\]  
(5.50)

In 2D Cosserat the above stress matrix can be expressed in the following vector (Equation (5.51)) for simplicity in finite element implementation. For a plane strain condition,
the continuum has a constraint on the displacement in the intermediate principal direction \((u_2 = 0)\) and the Cosserat rotations are locked except the out of plane rotation then: \(\gamma_{22} = \gamma_{12} = \gamma_{21} = \gamma_{23} = \gamma_{32} = 0, \ \sigma_{12} = \sigma_{21} = \sigma_{23} = \sigma_{32} = 0, \ \text{and} \ \omega^c_1 = \omega^c_2 = 0.\)

\[
\{\sigma\} = \begin{bmatrix} \sigma_{11} & \sigma_{22} & \sigma_{33} & \sigma_{13} & m_1/l_s & m_3/l_s \end{bmatrix}
\] (5.51a)

One can express the stress and couple stress components as follow:

\[
\{\Sigma\} = \begin{bmatrix} \sigma \\ \mu \end{bmatrix}
\] (5.51b)

Note that the stress in the minor principal direction might be held constant to represent the effective confining stress level. The displacement in the intermediate direction, \(u_2\) is constrained. The strain matrix for 2D Cosserat continuum can be expresses in a vector form as:

\[
\{\gamma\} = \begin{bmatrix} \gamma_{11} & \gamma_{22} & \gamma_{33} & \gamma_{13} & l_a \kappa_1 & l_a \kappa_3 \end{bmatrix}
\] (5.52a)

where; \(l_a\) is the length of the arm of rotation. To this end the author is trying to separate two different length scales, one is the contact surface and the other is the arm of rotation. The strain and curvature of rotations can also be decoupled as:

\[
\{\gamma\} = \begin{bmatrix} \varepsilon \\ \kappa \end{bmatrix}
\] (5.52b)

According to Schaefer (1962) the stress-strain equations for 2D-isotropic linear elastic Cosserat continuum are:

\[
\sigma_{11} = (G + K)E_{11} + (K - G)E_{33}
\] (5.53a)

\[
\sigma_{33} = (K - G)E_{11} + (K + G)E_{33}
\] (5.53b)

\[
\sigma_{13} = 2GE_{13} + 2G^c (\Omega_{13} - \Omega_{13}^c)
\] (5.54c)

\[
\sigma_{31} = 2GE_{31} + 2G^c (\Omega_{31} - \Omega_{31}^c)
\] (5.54d)

\[
m_1 = M \kappa_1 \quad m_3 = M \kappa_3
\] (5.54e)
These elasticity equations can be extended to the 3D as:

\[
\begin{align*}
\sigma_{11} &= (G + K)E_{11} + (K - G)E_{22} + (K - G)E_{33} \quad (5.55a) \\
\sigma_{22} &= (K - G)E_{11} + (K + G)E_{22} + (K - G)E_{33} \quad (5.55b) \\
\sigma_{33} &= (K - G)E_{11} + (K - G)E_{22} + (K + G)E_{33} \quad (5.55c) \\
\sigma_{12} &= 2GE_{12} + 2G^c(\Omega_{12} - \Omega_{12}^c) \quad (5.55d) \\
\sigma_{21} &= 2GE_{21} + 2G^c(\Omega_{21} - \Omega_{21}^c) \quad (5.55e) \\
\sigma_{13} &= 2GE_{13} + 2G^c(\Omega_{13} - \Omega_{13}^c) \quad (5.55f) \\
\sigma_{31} &= 2GE_{31} + 2G^c(\Omega_{31} - \Omega_{31}^c) \quad (5.55g) \\
\sigma_{32} &= 2GE_{32} + 2G^c(\Omega_{32} - \Omega_{32}^c) \quad (5.55h) \\
\sigma_{23} &= 2GE_{23} + 2G^c(\Omega_{23} - \Omega_{23}^c) \quad (5.55i) \\
m_1 &= M\kappa_1 \quad m_2 = M\kappa_2 \quad m_3 = M\kappa_3 \quad (5.55j)
\end{align*}
\]

where \( K \) is the material bulk modulus, \( G \) is the shear modulus, \( G^c \) is the shear modulus that relates the anti-symmetric part of the relative deformation to the anti-symmetric part of the resulted shear stress component and \( M \) is the bending modulus that takes the unit of a force.

The following relations hold in order to obtain the above moduli (Vardoulakis and Sulem, 1995):

\[
l = \sqrt{\frac{M}{G}} \quad (5.56a)
\]

where; \( l \) is the material bending length and it might be taken as an internal length, for example the grain size can be considered to represent this length then one will be able to compute the bending modulus.
\[ \frac{K}{G} = 1/(1 - 2\nu) \]  
(5.56b)

Where \( \nu \) is the Poisson’s ratio that.

\[ \alpha = 1/\sqrt{1 + G/G^c}; \quad 0 \leq \alpha \leq 1 \]  
(5.56c)

The shear modulus (the classical one) is related to the Cosserat shear modulus, \( G^c \) through a constant called coupling number (Vardoulakis and Sulem, 1995). The lower and the upper bounds of this number actually are meaningful in the sense that when \( \alpha = 1 \), this means \( G^c \) is infinitely large. In other words, \( \omega = \omega^c \) which leads to the constrained Cosserat and symmetric stress tensor. Equations 5.55c and 5.55d are linked with Equation (5.56c) to yield:

\[ \sigma_{13} = 2G\left[E_{13} + \frac{\alpha^2}{(1 - \alpha^2)}(\Omega_{e13} - \Omega_{13})\right] \tag{5.57a} \]

\[ \sigma_{31} = 2G\left[E_{31} + \frac{\alpha^2}{(1 - \alpha^2)}(\Omega_{e31} - \Omega_{31})\right] \tag{5.57b} \]

Based on Equations 5.57 the stress tensor will show non-symmetry and deviate from the classical one. The objective Cosserat strains can be rewritten as:

\[ \gamma_{11} = E_{11} = e_{11} + \eta_{11} \]  
(5.58)

\[ \gamma_{22} = E_{22} = e_{22} + \eta_{22} \]  
(5.59)

\[ \gamma_{33} = E_{33} = e_{33} + \eta_{33} \]  
(5.60)

\[ \gamma_{13} = \left[E_{13} + \frac{\alpha^2}{(1 - \alpha^2)}(\Omega_{e13} - \Omega_{13})\right] \]  
(5.61a)

\[ \gamma_{31} = \left[E_{31} + \frac{\alpha^2}{(1 - \alpha^2)}(\Omega_{e31} - \Omega_{31})\right] \]  
(5.61b)

Displacements constrains will be applied on the \( x_2 \)-direction to satisfy the plane strain conditions.
To obtain the elasto-plastic stiffness matrix the non-associated flow rule of plasticity will be adopted in this thesis and the following relationships are proposed here as:

\[
\dot{\varepsilon}^p_{ij} = \dot{\lambda}_p \frac{\partial g}{\partial \sigma_{ij}} \quad (5.63a)
\]

\[
\dot{\kappa}^p_i = \dot{\lambda}_p \frac{\partial g}{\partial \kappa_i} \quad (5.63b)
\]

Where \( \dot{\lambda}_p \) is positive plastic proportionality. In general, one will have the following relation for the stress and strain tensors holds:

\[
\dot{\gamma}^p_{ij} = \dot{\lambda}_p \frac{\partial g}{\partial \sigma_{ij}} \quad (5.63c)
\]

It is more convenient to deal with time rates then the following constitutive laws can be used:

\[
\{\dot{\sigma}\} = [D]\{\dot{\gamma}\} \quad (5.64)
\]

Where, \([D]\) is the elasto-plastic stiffness matrix. To derive a formula for \([D]\) one might begin with:

\[
\{\dot{\sigma}\} = [D^e]\{\dot{\gamma}^e\} = [D^e]\{\dot{\gamma} - \dot{\lambda}_p \frac{\partial g}{\partial \sigma}\} \quad (5.65a)
\]

Substitute (5.63c) into (5.65) and then:

\[
\{\dot{\sigma}\} = [D^e]\{\dot{\gamma}^e\} = [D^e]\{\dot{\gamma} - \dot{\lambda}_p \frac{\partial g}{\partial \sigma}\} \quad (5.65b)
\]
Recalling Equations 5.43 and 5.44 will yield:

\[ f_p = f'_p(\sigma) - f'_p(W_p) = 0 \Rightarrow \dot{f} = 0 \Rightarrow \]

\[ \frac{\partial f'_p}{\partial \sigma} : \dot{\sigma} - \frac{\partial f'_p}{\partial W_p} \dot{W}_p = 0 \quad \text{(5.66)} \]

Now from Equation 5.42b one has:

\[ d\lambda_p = \frac{dW_p}{\mu\gamma} \rightarrow \dot{W}_p = \mu\gamma p \dot{\lambda}_p \quad \text{(5.67)} \]

If one substitute Equation 5.67 into Equation 5.66 with use of Equation 5.65a will get:

\[ \dot{\lambda}_p = \frac{\{\frac{\partial f'_p}{\partial \sigma}\}^T[D']\{\dot{\gamma}\}}{\frac{\partial f'_p}{\partial \sigma} \{D'\} + \frac{\partial f'_p}{\partial W_p} \mu\gamma p} \quad \text{(5.68)} \]

Substitute Equation 5.68 into the constitutive Equation 5.65b results:

\[ \{\sigma\} = \left[D' - \left\{\frac{\partial f'_p}{\partial \sigma}\right\}^T[D']\left\{\frac{\partial g_p}{\partial \sigma}\right\} + \frac{\partial f'_p}{\partial W_p} \mu\gamma p \right\}\{\dot{\gamma}\} \quad \text{(5.69)} \]

The following general elasto-plastic matrix is obtained accordingly:

\[ [D] = \left[D' - \left\{\frac{\partial f'_p}{\partial \sigma}\right\}^T[D']\left\{\frac{\partial g_p}{\partial \sigma}\right\} + \frac{\partial f'_p}{\partial W_p} \mu\gamma p \right\} \quad \text{(5.70a)} \]
Where \(<1>\) is a switch function that accounts for the plastic deformations when it kicks on and can be expressed as:

\[
< 1 > = \begin{cases} 
1 & \text{if } f_p \geq 0 \\
0 & \text{otherwise}
\end{cases}
\]  

(5.70b)

The elasto-plastic matrix shown above is a coupled stiffness matrix in both stresses and couple stresses aspects. For 2D problem the above material stiffness matrix is (7x7) and can be subdivided into four sub-matrices (5x5, 5x2, 2x5 and 2x2), this matrix reads:

\[
\mathbf{D} = \begin{bmatrix} 
\mathbf{D}^{sx}_{5x5} & \mathbf{D}^{sx}_{5x2} \\
\mathbf{D}^{kx}_{2x5} & \mathbf{D}^{kx}_{2x2}
\end{bmatrix}
\]  

(5.71)

The decoupled stress-strain matrix, \(\mathbf{D}^{\varepsilon}_{5x5}\) takes the form of:

\[
\mathbf{D}^{\varepsilon}_{5x5} = \mathbf{D}^{\varepsilon}_{5x5} - \frac{1}{H_p} \left( \mathbf{D}^{\varepsilon}_{5x5} : \mathbf{G} \right) \otimes \left( \mathbf{F}^T : \mathbf{D}^\varepsilon_{5x5} \right)
\]  

(5.72)

In which \(H_p\) is the scalar hardening modulus and can be defined as:

\[
H_p = \mathbf{F}^T : \mathbf{D}^{\varepsilon}_{5x5} : \mathbf{G} + \frac{\partial f_p^e}{\partial w_p} \mu g_p
\]  

(5.73a)

\(\mathbf{F}\) and \(\mathbf{G}\) are the partial derivative vectors of the yield function and plastic potential function with respect to the associated tresses, respectively, and they read:

\[
\mathbf{F} = \begin{bmatrix} 
\frac{\partial f_p^e}{\partial \mathbf{\sigma}} \\
\frac{\partial g_p}{\partial \mathbf{\sigma}}
\end{bmatrix}
\]  

(5.73b)

\[
\mathbf{G} = \begin{bmatrix} 
\frac{\partial g_p}{\partial \mathbf{\sigma}}
\end{bmatrix}
\]  

(5.73c)

The coupled material stiffness matrices \(\mathbf{D}^{sx}_{5x2}\) and \(\mathbf{D}^{sx}_{2x5}\) read:
\[
    D_{5x2}^{ex} = D_{5x2}^e - \frac{1}{H_p} \left( D_{5x5}^e : G^e \right) \otimes \left( F^{exT} : D_{2x2}^e \right) 
\]  
\[
    D_{2x5}^{ex} = D_{2x5}^e - \frac{1}{H_p} \left( D_{2x2}^e : G^e \right) \otimes \left( F^{exT} : D_{5x5}^e \right) 
\]  
(5.74a)

(5.74b)

Finally, the decoupled couple stress-rotation matrix \( D_{2x2}^{ex} \) reads:

\[
    D_{2x2}^{ex} = D_{2x2}^e - \frac{1}{H_p} \left( D_{2x2}^e : G^e \right) \otimes \left( F^{exT} : D_{2x2}^e \right) 
\]  
(5.75)

It is worth noting here that following conditions hold for the elastic stiffness matrix in which we have:

\[
    D_{5x2}^e = D_{2x5}^e = 0 
\]  
(5.76)

This is obviously shown in Equation 5.62.

### 5.6 Formulating the Virtual Work Equations in the UL Frame

The relationship between the second Piola-Kirchhoff stress and the Cauchy stress tensor can be rewritten according to Voyiadjis and Abu-Farsakh (1997) as:

\[
    ^{n+1}_n S_{ij} = JX_{i,j}X_{j,i} \sigma_{ij} 
\]  
(5.77)

The time derivative of Equation 5.77 according to Voyiadjis (1988) can be expressed as:

\[
    ^{n+1}_n \dot{S}_{ij} = J\dot{v}_{i,k}X_{i,j}X_{j,i} \sigma_{ij} + JX_{i,i}X_{j,j} \dot{\sigma}_{ij} - JX_{i,k}v_{k,i}X_{j,i} \sigma_{ij} - JX_{i,i}X_{j,k}v_{k,j} \sigma_{ij} 
\]  
(5.78)

The indices will tell the configuration of interest (Eulerian or Lagrangian); lower case denotes the spatial or the Eulerian space whereas the upper case denotes Lagrangian or material space. A combination between the lower and upper cases mean the current position referred to the previous state and vice versa. Equation 5.78 can be rewritten as:

\[
    ^{n+1}_n \dot{S}_{ij} = JX_{i,i}X_{j,j} \left[ v_{k,i} \sigma_{ij} + \dot{\sigma}_{ij} - v_{i,k} \sigma_{kj} - v_{j,k} \sigma_{ik} \right] 
\]  
(5.79)
Note that all the stresses are effective, since the problems being treated here are all under dry condition (i.e. no pore fluid pressure will be dealt with in the current formulations). If the stress tensor is symmetric, Equation (5.79) collapses into:

\[
\mathbf{n}_{ij} \frac{\partial K_{ij}}{\partial J_{ij}} \mathbf{I} + \mathbf{I} - \mathbf{I} = 0
\]  

(5.80)

The strain rate tensor in the Lagrangian space or what is called the material strain rate can be defined as:

\[
\frac{\mathbf{n}_{ij}}{\partial J_{ij}} = \mathbf{X}_{i,j} \mathbf{X}_{j,i} \frac{\mathbf{n}_{ij}}{\partial J_{ij}}
\]  

(5.81)

One now can substitute for velocity gradient in Equation 5.81 and then:

\[
v_{k,k} = \dot{e}_{kk}
\]  

(5.82)

This will yield:

\[
\mathbf{n}_{ij} \frac{\partial \dot{K}_{ij}}{\partial \dot{J}_{ij}} \mathbf{I} + \mathbf{I} - \mathbf{I} = 0
\]  

(5.83)

Where the modified elasto-pastic matrices are given as:

\[
\mathbf{D}_{ijkl} = \left( \mathbf{D}_{ijkl} + \delta_{kl} \sigma_{ij} - \delta_{ik} \delta_{ml} \sigma_{lj} - \delta_{jk} \delta_{ml} \sigma_{il} \right) \mathbf{X}_{k,K} \mathbf{X}_{l,L} \mathbf{X}_{j,J} \mathbf{X}_{i,I} 
\]  

(5.84a)

\[
\mathbf{D}_{ijkl}^{**} = \mathbf{D}_{ijkl} \mathbf{X}_{k,K} \mathbf{X}_{l,L} \mathbf{X}_{j,J} \mathbf{X}_{i,I}
\]  

(5.84b)

\[
\mathbf{D}_{ijkl}^{***} = \left( \mathbf{D}_{ijkl} - \delta_{ik} \mathbf{D}_{ml} \sigma_{lj} - \delta_{jk} \mathbf{D}_{ml} \sigma_{il} \right) \mathbf{X}_{k,K} \mathbf{X}_{l,L} \mathbf{X}_{j,J} \mathbf{X}_{i,I}
\]  

(5.84c)

If one now integrates Equation 5.83 with respect to time will get the stress increment that transfers the material from the Piola-Kirchhoff stress to the Cauchy stress space as:

\[
\Delta \mathbf{S}_{ij} = \mathbf{D}_{ijkl}^{*} \Delta \mathbf{e}_{KL} + \mathbf{D}_{ijkl}^{**} \Delta \eta_{KL} + \mathbf{D}_{ijkl}^{***} \Delta \Omega_{KL} - \mathbf{D}_{ijkl}^{****} \Delta \Omega_{KL}
\]  

(5.85)

Equations 5.83 through 5.85 were written in a general form to deal with any stress and strain tensor. For the case being treated here, the following expressions hold:

\[
\Delta \mathbf{S}_{ij} = \mathbf{D}_{ijkl}^{*} \Delta \mathbf{e}_{KL} + \mathbf{D}_{ijkl}^{**} \Delta \eta_{KL} + \mathbf{D}_{ijkl}^{***} \Delta \Omega_{KL} - \mathbf{D}_{ijkl}^{****} \Delta \Omega_{KL}
\]  

(5.86)

Where, \((i, j, k, l, I, J, K, L = 1, 3)\)
Now the same argument will be used so that the couple stresses will be updated in the updated Lagrangian space as:

\[ m_{i}^{n+1} = m_{i}^{n} + \Delta m_{i}^{n} \tag{5.87} \]

One can write the couple stress rate in an expression similar to Equation 5.83:

\[ \dot{m}_{i}^{n} = JX_{k} X_{j} \left[ v_{i,k} \sigma_{j} + \sigma_{ij} - v_{i,k} \sigma_{j} - v_{j,k} \sigma_{i} \right] \]

\[ v_{i,k} = \dot{\epsilon}_{ik} + \dot{\Omega}_{ik} \quad v_{j,k} = \dot{\epsilon}_{jk} + \dot{\Omega}_{jk} \]

\[ M_{2,j2k}^{*} = JX_{j} X_{k,k} \left[ M_{2,j2k}^{*} - \delta_{jk} m_{2j} \right] \tag{5.88} \]

The time derivative for Equation (5.88) reads:

\[ \Delta m_{21}^{*} = \int_{t}^{t+\Delta t} M_{212k}^{*} \dot{k}_{2k} dt = M_{212k}^{*} \Delta \kappa_{2K} \tag{5.89} \]

Similarly,

\[ \Delta m_{23}^{*} = \int_{t}^{t+\Delta t} M_{232k}^{*} \dot{k}_{2k} dt = M_{232k}^{*} \Delta \kappa_{2K} \tag{5.90} \]

\[ \dot{m}_{2j}^{n+1} = M_{2,j2k}^{*} \dot{\omega}_{2,k}^{c} = m_{2j}^{n+1} \tag{5.91} \]

\[ M_{2,j2k}^{*} = JX_{j} X_{k,k} \left[ M_{2,j2k}^{*} - \delta_{jk} m_{2j} \right] \tag{5.92} \]

Recalling the virtual work equation (5.35) one will have:

\[ \int \left[ \left( ^{n} \sigma_{ij} \right) \delta \left( ^{n} \dot{\epsilon}_{ij} + ^{n} \dot{\Omega}_{ij} - ^{n} \dot{\Omega}_{ij}^{c} \right) + \left( ^{n} m_{i} \right) \delta \left( ^{n} \dot{k}_{i} + \left( \Delta ^{n} \dot{S}_{g} \right) \right) \right] dV = ^{n+1} R \tag{5.93} \]

Now recall the Equations 5.86 and 5.89, substitute into (5.93) yields:
\[
\int_V \left[ \sigma_{ij} \left( \dot{n} \epsilon_{ij} + n \dot{\Omega}_{ij} - n \Omega_{ij} \right) \right] dV \\
+ \int_V \left( D_{ijkl} \Delta \epsilon_{kl} + D_{ijkl} \Delta \eta_{kl} + D_{ijkl} \Delta \Omega_{kl} - D_{ijkl} \Delta \Omega_{kl} \right) \delta^n dV = n+1 \]

5.7 Discretization of the Virtual Work Equations

Cosserat continuum will have a new degree of freedom which is the rotation of the grains. In the Plane Strain condition one will have this degree of freedom in the \( x_1-x_2 \) plane. In other words, the two displacements will be \( u_1 \) and \( u_3 \) and the only rotation will be \( \omega_3 \). Now the new strain-curvature tensor will be:

\[
\gamma = \nabla \mathbf{u} = \{ \gamma_{11}, \gamma_{33}, \gamma_{13}, l_1 \kappa_1, l_3 \kappa_3 \} \quad (5.95)
\]

In finite element implementation each node in the plane strain Cosserat continuum will have the following degrees of freedom:

\[
\mathbf{u} = \{ u_1, u_3, \omega_2 \}^T \quad (5.96)
\]

Therefore, the displacement is constrained in the \( x_2 \) direction but there will be stress that will evolve in this direction, \( \nabla \) is a differential operator matrix defined by Equation 5.97. It takes care of the linear, non-linear strains in addition to the rotations and their curvatures. Figure 5-7 shows a schematic diagram for the prismatic sample that will be used to simulate the plane strain conditions:

\[
\nabla = \begin{bmatrix}
\frac{\partial}{\partial x_1} + \frac{1}{2} \left( \frac{\partial}{\partial x_1} \right)^2 & 1 \left( \frac{\partial}{\partial x_1} \right)^2 & 0 \\
\frac{1}{2} \left( \frac{\partial}{\partial x_2} \right)^2 & \frac{\partial}{\partial x_2} + \frac{1}{2} \left( \frac{\partial}{\partial x_2} \right)^2 & 0 \\
\frac{1}{2} \left( \frac{\partial}{\partial x_3} \right)^2 & \frac{\partial}{\partial x_3} + \frac{1}{2} \left( \frac{\partial}{\partial x_3} \right)^2 & \frac{\alpha^2}{1-\alpha^2} \\
\frac{1}{2} \left( \frac{\partial}{\partial x_1} \right)^2 + \frac{\alpha^2}{1-\alpha^2} \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_1} + \frac{1}{2} \left( \frac{\partial}{\partial x_1} \right)^2 + \frac{\alpha^2}{1-\alpha^2} \frac{\partial}{\partial x_1} & -\frac{\alpha^2}{1-\alpha^2} \\
0 & 0 & \frac{\partial}{\partial x_1} \\
0 & 0 & \frac{\partial}{\partial x_1}
\end{bmatrix} \quad (5.97)
\]
Now the stress-couple vector can be written in the following form:

$$\Sigma = \{\sigma_x, \sigma_z, \sigma_{xz}, \frac{m_1}{l_x}, \frac{m_3}{l_x}\}^T$$  \hspace{1cm} (5.98)

Figure 5-7: Schematic Diagram Showing Specimen under a Plane Strain Condition.

The length scales, \(l_a\) and \(l_s\), in Equations (5.95) and (5.98) are not necessarily the same parameter. In Equation 5.95 the length scale represents the distance from the center of the particle to the point of contact under consideration while in Equation 5.98, it is the length of contact surface under consideration. Now one can use a global shape function (\(N\)) to compute the strains, positions, etc. within the nodal points. It depends on the type of the element adopted. It is possible to write the objective strain vector as:

$$\gamma = Bu$$  \hspace{1cm} (5.99a)

$$B = \nabla N$$  \hspace{1cm} (5.99b)

The finite element equations in the updated Lagrangian configuration are done within the framework of the virtual work principles. The current domain is subdivided into elements and
the total number of the nodes is \( n_N \). The current position in finite element, given a specific space dimension, \( n_{SD} \), can be approximated by:

\[
x_i(X, t) = N_I(x)x_{iI}(t) \quad I = 1, \ldots, n_N \quad i = 1, \ldots, n_{SD}
\]  \hspace{1cm} (5.100)

Again, \( N_I(x) \) is the shape function being used in the formulations, then the nodal displacement field can be defined as:

\[
u_i(t) = x_{iI}(t) - X_{iI}
\]  \hspace{1cm} (5.101)

Accordingly, the displacement, velocity and acceleration fields can be defined respectively as follow:

\[
u_i(X, t) = v_{iI}(t)N_I(x)
\]  \hspace{1cm} (5.102)

\[
v_i(X, t) = v_{iI}(t)N_I(x)
\]  \hspace{1cm} (5.103)

\[
a_i(X, t) = a_{iI}(t)N_I(x)
\]  \hspace{1cm} (5.104)

The summation will be over the repeated index. Following the same arguments above one can define the spin, curvature and the angular acceleration fields of the grains (Cosserat fields) as:

\[
\omega_i(X, t) = \omega_{iI}(t)N_I(x)
\]  \hspace{1cm} (5.105)

\[
\kappa_i(X, t) = \kappa_{iI}(t)N_I(x)
\]  \hspace{1cm} (5.106)

\[
\dot{\omega}_i(X, t) = \dot{\omega}_{iI}(t)N_I(x)
\]  \hspace{1cm} (5.107)

If one considers the parent coordinates by \( \xi \) then the displacement, velocity and acceleration fields will be:

\[
u_i(\xi, t) = v_{iI}(t)N_I(\xi)
\]  \hspace{1cm} (5.108)

\[
v_i(\xi, t) = v_{iI}(t)N_I(\xi)
\]  \hspace{1cm} (5.109)

\[
a_i(\xi, t) = a_{iI}(t)N_I(\xi)
\]  \hspace{1cm} (5.110)
Using the chain rule one can express the derivatives with respect to the parent coordinates in terms of the derivative with respect to the current space coordinates, if \( f \) is any continuous function that represent any quantity in the system then:

\[
 f_{,\xi} = f_{,x} x_{,\xi} 
\]  

(5.111)

In 2D space the following parent coordinates will be used:

\[
 \xi = [\xi \quad \eta]^T
\]  

(5.112)

In this study a quadrilateral isoparametric 4-noded element is used, isoparametric means identical shape functions for both geometrical and displacements quantities (Cook et al. 1989). The 4-node element is chosen here for minimize the stiffness and any expected locking in the element (Belytschko 2000). The element size will be related to the rigid grain size for better physical simulation. Figure 5-8 shows the element with its parent coordinates. The nodal numbering is taken counter-clockwise to be consistent with the finite element programs since most of them follow the same convention. Based on this type of element a bi-linear shape function will be used, this function is expressed in parent coordinates as shown in Equation (5.113).

![Figure 5-8: 4-node isoparametric 2D element with parent coordinates](image)
\[ N_i(\xi) = \frac{1}{4} \left( 1 + \xi \xi_i \right) \left( 1 + \eta \eta_i \right) \]  

(5.113a)

\[
\begin{bmatrix}
N_1 & 0 & 0 & N_2 & 0 & 0 & N_3 & 0 & 0 & N_4 & 0 & 0 \\
0 & N_1 & 0 & 0 & N_2 & 0 & 0 & N_3 & 0 & 0 & N_4 & 0 \\
0 & 0 & N_1 & 0 & 0 & N_2 & 0 & 0 & N_3 & 0 & 0 & N_4 \\
\end{bmatrix}
\]  

(5.113b)

Referring to Figure 5-8 one can write the following:

\[
\xi = \begin{bmatrix} \xi_i \\ \eta_i \end{bmatrix} = \begin{bmatrix} -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 \end{bmatrix} 
\]  

(5.114)

If one recalls the differential operator and the shape function then the virtual work equation might be rewritten as:

\[
\int_{V} \left[ B_0 \delta \mathbf{U} + B_{col} m \delta \omega^e \right] dV \\
+ \int_{V} \left[ \mathbf{D}' \mathbf{B}' L \Delta \mathbf{U} + \mathbf{D}' \mathbf{B}' NL \Delta \mathbf{U} + \mathbf{D}' \mathbf{B}' SP \Delta \mathbf{U} - \mathbf{D}' \mathbf{B}' B_{col} \Delta \mathbf{U} \right] \mathbf{B}_0 \delta \mathbf{U} + = n^T R 
\]  

(5.115a)

\[
\int_{V} \left[ B_0 \delta \mathbf{U} + B_{col} m \delta \omega^e \right] dV \\
+ \int_{V} \left[ \mathbf{B}' \mathbf{D}' \mathbf{B}' L + \mathbf{B}' \mathbf{D}' \mathbf{B}' NL + \mathbf{B}' \mathbf{D}' \mathbf{B}' SP - \mathbf{B}' \mathbf{D}' \mathbf{B}' B_{col} \right] \Delta \mathbf{U} \delta \mathbf{U} + = n^T R 
\]  

(5.115b)

One can decouple the stress and the couple stress terms as:

\[
\int_{V} \left[ B_{col} m \delta \omega^e \right] dV + \int_{V} \left[ \mathbf{B}'_{col} \mathbf{M}' \mathbf{B}'_{col} \right] \Delta \omega^e \delta \omega^e dV = n^T R^{\omega^e} 
\]  

(5.116a)

\[
\int_{V} \left[ B_0 \delta \mathbf{U} \right] dV + \int_{V} \left[ \mathbf{B}' \mathbf{D}' \mathbf{B}' L + \mathbf{B}' \mathbf{D}' \mathbf{B}' NL + \mathbf{B}' \mathbf{D}' \mathbf{B}' SP - \mathbf{B}' \mathbf{D}' \mathbf{B}' B_{col} \right] \Delta \mathbf{U} \delta \mathbf{U} dV = n^T R^{\sigma^e} 
\]  

(5.116b)

In general the equilibrium equations can be stated as in the disceretized following forms to simplify the finite element implementation for the boundary value problem:
\[ \delta u^T K \Delta u = \delta u^T \Phi \] (5.117a)

and

\[ K \Delta u = \Phi \] (5.117b)

where;

\[ K = K_L + K_{NL} + K_{SP} - K_{CO1} + K_{CO2} \] (5.118)

\[ K_L = \int B^T D L B_L d^n V \] (5.119a)

\[ K_{NL} = \int B^T D ^{NL} B_{NL} d^n V \] (5.119b)

\[ K_{SP} = \int B^T D ^{SP} B_{SP} d^n V \] (5.119c)

\[ K_{CO1} = \int B^T D ^{CO1} B_{CO1} d^n V \] (5.119d)

\[ K_{CO2} = \int B^T _{CO2} M^{pq} B_{CO2} d^n V \] (5.119e)

The residual force vectors read:

\[ R^m = \int_{n+1}s \left( N^T M \right) d^{n+1} S + \int_{n+1}y \rho N^T c d^{n+1} V - \int_{n+1}y B^T_{CO2} m d^{n+1} V \] (5.120a)

\[ R^p = \int_{n+1}s N^T \rho d^{n+1} S + \int_{n+1}y \rho N^T b d^{n+1} V - \int_{n+1}y B^T a d^{n+1} V \] (5.120b)

Where I is the angular momentum of inertia, c and b are body force vectors, T and m are the surface traction and moment respectively.

\[ \delta \gamma = B \delta \dot{u} \] (5.121a)

\[ \delta \kappa = B_{CO2} \delta \dot{u} \] (5.121b)

\[ \Delta \gamma = B \Delta u \] (5.121c)

\[ B_L = \nabla^{(1)} N \] (5.122a)
\( B_{NL} = \nabla^{(2)} N \) \hspace{1cm} (5.122b)

\( B_{SP} = \nabla^{(3)} N \) \hspace{1cm} (5.122c)

\( B_{CO1} = \nabla^{(4)} N \) \hspace{1cm} (5.122d)

\( B_{CO2} = \nabla^{(5)} N \) \hspace{1cm} (5.122e)

Where the above operators can be extracted from the main differential operator Equation (5.97) and then one will have:

\[
\nabla^{(i)} = \begin{bmatrix}
\frac{\partial}{\partial x_i} & 0 & \frac{1}{2} \left( \frac{\partial}{\partial x_3} \right) & \frac{1}{2} \left( \frac{\partial}{\partial x_5} \right) & 0 & 0 \\
0 & \frac{\partial}{\partial x_3} & \frac{1}{2} \left( \frac{\partial}{\partial x_1} \right) & \frac{1}{2} \left( \frac{\partial}{\partial x_5} \right) & 0 & 0 \\
0 & 0 & \frac{1}{2} \left( \frac{\partial}{\partial x_1} \right) & \frac{1}{2} \left( \frac{\partial}{\partial x_3} \right) & 0 & 0
\end{bmatrix}^T
\] \hspace{1cm} (5.123a)

\[
\nabla^{(2)} = \begin{bmatrix}
\frac{1}{2} \left( \frac{\partial}{\partial x_1} \right)^2 & \frac{1}{2} \left( \frac{\partial}{\partial x_3} \right)^2 & \frac{1}{2} \left( \frac{\partial}{\partial x_1} \frac{\partial}{\partial x_5} \right) & \frac{1}{2} \left( \frac{\partial}{\partial x_1} \frac{\partial}{\partial x_5} \right) & 0 & 0 \\
\frac{1}{2} \left( \frac{\partial}{\partial x_1} \right)^2 & \frac{1}{2} \left( \frac{\partial}{\partial x_3} \right)^2 & \frac{1}{2} \left( \frac{\partial}{\partial x_1} \frac{\partial}{\partial x_5} \right) & \frac{1}{2} \left( \frac{\partial}{\partial x_1} \frac{\partial}{\partial x_5} \right) & 0 & 0 \\
0 & 0 & \frac{1}{2} \left( \frac{\partial}{\partial x_1} \frac{\partial}{\partial x_5} \right) & \frac{1}{2} \left( \frac{\partial}{\partial x_1} \frac{\partial}{\partial x_5} \right) & 0 & 0
\end{bmatrix}^T
\] \hspace{1cm} (5.123b)

\[
\nabla^{(3)} = \begin{bmatrix}
0 & 0 & \frac{1}{2} \left( \frac{\alpha^2}{1-\alpha^2} \frac{\partial}{\partial x_5} \right) & \frac{1}{2} \left( -\frac{\alpha^2}{1-\alpha^2} \frac{\partial}{\partial x_3} \right) & 0 & 0 \\
0 & 0 & \frac{1}{2} \left( \frac{\alpha^2}{1-\alpha^2} \frac{\partial}{\partial x_1} \right) & \frac{1}{2} \left( \frac{\alpha^2}{1-\alpha^2} \frac{\partial}{\partial x_1} \right) & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}^T
\] \hspace{1cm} (5.123c)
\[ \nabla^{(a)} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\alpha^2}{1-\alpha^2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\alpha^2}{1-\alpha^2} & 0 & 0 \end{bmatrix} \]  
\tag{5.123d}

\[ \nabla^{(b)} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{L_0}{\partial x_1} & \frac{L_0}{\partial x_3} \end{bmatrix} \]  
\tag{5.123e}

Then the second term in Equation (5.117b) is expressed as:

\[ \Phi = \int_{V} \left( B^T \sigma + B_{c02}^T m \right) dV = \int_{V} \left( B^T \sigma + B_{c02}^T m \right) dV \]  
\tag{5.126}

5.8 **Length Scales**

Cosserat theory is more physically based and realistic in the sense that it separates the micro-rotation of a material point from the overall rotation of the continuum. In granular materials the particle rotation can be represented by a Cosserat point and thus some internal length scale that characterizes the particle micro-properties can be incorporated. To this end, the only length scale that has been introduced and used effectively is the mean particle size which is needed to link the curvature of rotation to the couple stress. In this section, new micro-length scales will be introduced and incorporated in the formulations. As will be shown later in Chapter Seven, the surface roughness and shape indices are essentially of high influence on the behavior of frictional materials. The Micropolar theory or Cosserat rotation allows using the particle size to represent the length of the contact surface and the arm of rotation. Equation 5.21 suggests that a length scale should be used to adjust for the units; most researchers use the mean particle size to represent this parameter. However, this argument is not necessarily true unless the particles are spherical. Figure 5-6 shows that the arm of particle rotation is not a unique values; it depends on the shape and the surface roughness. It is not possible to account for the change in this
parameter along the particle perimeter in finite element formulation; however, an alternative approximation might be used to account for such variation in the length scale. Figure 5-9 shows an arbitrary particle subdivided into eight regions to account for the shape and surface roughness into the length scale.

The arm of particle rotation, \( r \), seems to oscillate depending on the surface roughness, \( R_{\text{rough}} \), and the shape indices that were discussed in Chapter Three. If the surface roughness to be assumed uniform with an average value; Figure 5-10 can be used to represent such oscillation (sinusoidal oscillation is assumed here).

Assuming a uniform surface roughness with some average value measured at the micro-scale will allow us to incorporate this parameter in the formulations at the finite element level. The following modification for the angular momentum of inertia is proposed.

\[
I_i = \rho \oint_0^R \int_0^{R_{\text{rough}}} \left( r + R_{\text{rough}} \sin(\theta) \right)^3 dr d\theta 
\]

\[
I = \sum_{i=1}^{8} I_i
\]  

\( \sum_{i=1}^{8} \)

Figure 5-9: Arbitrary Particle Showing the Non-uniformity in Shape and the Surface Roughness
The surface roughness effect will be embedded into Equation (5.126) and as a micro-property of the grain, will have a contribution to the overall behavior of the material.

The shape of the particles will affect the behavior of the material as well; it is argued here that the more particle angularity the more the polar friction and as a result the dilation will be higher. The surface of contact between adjacent particles is highly affected by the shape of those particles; Figure 5-11 shows different particle shapes and the nature of their contact surface.
Granular particles have the tendency to lay on their long direction (Figure 5-12) for more stability; based on this assumption the column-like structure will be built and column buckling phenomenon will most probably occur as a result of loading. It is worth noting here that couple stress depends on the size of the contact surface, we will call it here the bending length, as shown in (Figure 5-11) which is affected by the shape of the particles. The shape indices, $I_R$ and $I_{sph}$, will be used to account for the shape non-uniformity.

Looking at the particles at the micro-scale, one can measure infinite number of radii from the center of gravity to the surface of the particles and then these radii can be adjusted to account for the surface roughness. The adjusted radii, $R^{adj}$, can be used together with the shape indices to be used as the arm of rotation and the length of the contact surface. In this work the real particle images taken by the SEM will be subdivided into eight regions as shown in Figure 5-9.

Figure 5-12 The Bucking of Column-Like Structure in Granular Materials as a Result of Couple Stresses and Particles Rotation.
CHAPTER SIX

FINITE ELEMENT IMPLEMENTATION

6.1 Introduction

The finite element implementation for the discretized equations shown earlier in Chapter Five was done using the finite element program (ABAQUS). This program does not provide an element with material rotation; therefore a User Element Subroutine (UEL) is needed to solve the system of the finite element equations within the Micropolar framework. A 4-noded isoparametric element with four integration points was used. However, selective reduced integration technique was used to avoid any possible volumetric locking during the softening regime. In this sense, full integration was used for all the state variables and only reduced integration technique was used for the volumetric strains. The finite element program ABAQUS uses Newton Raphson iteration technique to fulfill the static equilibrium equations and the load–displacement increments are updated using an implicit integration scheme within the standard version of ABAQUS. The problem in hand is a mixed control problem (load-displacement control) and all the internal state variables (such as stresses, plastic work, void ratio, etc.) are updated within the UEL using the explicit forward Euler integration scheme. Thereafter the ABAQUS postprocessor is used to show the analysis results.

6.2 Governing Equations

As shown in Chapter Five the finite element governing equations were represented in their weak form and this system of equations can be decoupled into stress and couple stress based components as:

\[
\begin{align*}
\int_{\Omega} \left[ [B^*][u] \right] dV + \int_{\Gamma} \left( B^T D^* B_L + B^T D^* D^* B_{NL} + B^T D^* D^* D^* s_{sp} - B^T D^* D^* B_{Bsd} \right) \delta u dV &= \delta U^T \mathbb{R}^T \quad (6.1a)
\end{align*}
\]
The strong form for the global system of equilibrium equations was proposed as:

\[ K \Delta u = \Phi \]  \hspace{1cm} (6.2)

\[ K = K_L + K_{NL} + K_{SP} - K_{CO1} + K_{CO2} \]  \hspace{1cm} (6.3)

Where; \( K_L, K_{NL}, K_{SP}, K_{CO1}, \) and \( K_{CO2} \) have been defined earlier in Chapter Five.

The Jacobin, \( J \), is required to map between the current and previous configuration if one chooses to use the updated Lagrangian frame. To compute this quantity at any time increment, the deformation gradient, \( F \), is needed therefore.

\[ F_{ij}^o = \frac{\partial X_i}{\partial \xi_j} \]  \hspace{1cm} (6.4)

Where in the current configuration the deformation gradient reads:

\[ F_{ij}^n = \frac{\partial X_i}{\partial \xi_j} = F_{ij}^o + \frac{\partial u_i}{\partial \xi_j} \]  \hspace{1cm} (6.5)

For the 4-noded quadratic element one will have (Belytschko et. al, 2000):

\[ \frac{\partial X_i}{\partial \xi_j} = \sum_{k=1}^{4} X^k_i \frac{\partial N^k}{\partial \xi_j} \]  \hspace{1cm} (6.6a)

\[ \frac{\partial u_i}{\partial \xi_j} = \sum_{k=1}^{4} u^k_i \frac{\partial N^k}{\partial \xi_j} \]  \hspace{1cm} (6.6b)

For the global system with total number of elements (NE) and total number of nodes (NN) one will have:
\[
\sum_{k} \sum_{i=1}^{n} \left( M^{T} B_{k} + \int_{e_{i,y}} IN^{T} c d^{n+1}V \right) = \int_{e_{i,y}} B_{k}^{T} m d^{n+1}V \tag{6.7a}
\]
\[
\sum_{k} \sum_{i=1}^{n} \left( N^{T} T^{n+1} T^{n+1} + \int_{e_{i,y}} \rho N^{T} b d^{n+1}V \right) = \int_{e_{i,y}} B_{k}^{T} \sigma d^{n+1}V \tag{6.7b}
\]

In this sense the residual load vector must vanish to satisfy the equilibrium equations and hence:
\[
\sum_{k} \left( \delta o^{T} R^{m} + (\delta u)^{T} R^{e} \right) = 0 \tag{6.8}
\]

Where \( k (k = 1...4) \) denotes the node number for a given element in system, \( K (K = 1, 2...NE) \) is the element number and \( N \) is the node number in the global system \( (N = 1, 2...NN) \).

6.3 Numerical Integration for Equilibrium Equations

The numerical integration for the surface and volumetric integrands is achieved using the Gaussian integration technique (Belytschko et al., 2000). For the 4-noded isoparametric element (2D space) used in this study with four integration points, the following integration technique was used for any function \( g(x,y) \) within the element.

\[
\int_{e_{i,y}} g(x,y) dV = \sum_{i=1}^{n_{i}} g^{'}(\xi_{i},\eta_{i}) J^{i} J^{i} d\xi d\eta = \sum_{i=1}^{n_{i}} g^{'}(\xi_{i},\eta_{i}) J^{i}(\xi_{i},\eta_{i}) W_{ii} \tag{6.9}
\]

Where, \( g^{'}(\xi,\eta) \) is any function within an element as function of the parent coordinates, \( J^{i} \) is the Jacobin value at the current time step, \( ii \) denote the Gaussian integration point, \( ni \) is the total number of Gaussian points used in the element, and \( W_{ii} \) is the Gaussian weighting factor for the \( ii^{th} \) Gaussian point. If one chooses to use full integration then 2x2 integration scheme is needed for a 4-noded element. However, full integration causes volumetric or shear locking most of the time which will add unrealistic stiffness to the element leading to a very poor or divergent solution. This type of locking is very common in plasticity and one way to overcome is the so called reduced or selective reduced integration. Such technique will still require a minimum
number of integration points that we may not go below to assure that finite element solution is converging to the correct solution. For 4-noded element the minimum number of integration points is one, which can be used and the solution will be accurate enough. The reduced integration technique will require less memory and computationally inexpensive.

6.4 Solution Technique for the Governing Equations

The constitutive relations used in this study are high non-linear type of relations and require that the one should be careful during the implementation. The loading mechanism in this study is applied as mixed control type of loading; initially the specimen is confined with all-around pressure (first step) and the second step is the deviatoric loading through strain-controlled loading. A total displacement is subincremented over certain period of time, $T$. However, the problem in hands is a time independent problem since all the relations used here are homogeneous in time. The finite element program (ABAQUS) uses the well-known Newton-Raphson method to solve the equilibrium equations in which the solution for high non-linear equations will converge most of time. The time increment used in ABAQUS can be a variable within minimum and maximum values. ABAQUS will always choose the largest increment that will lead the solution to converge; in other words it always tries to save in the computational cost and reach a good solution. Since the finite element solution is just a numerical approximation then Equation 6.8 can never be met and instead some tolerance is to be used as:

$$\left( R^m (\omega^c + \Delta \omega^c) + R^w (\mathbf{u} + \Delta \mathbf{u}) \right) = 0 \quad (6.10)$$

With coupled system at the $i^{th}$ N-R iteration one will have:

$$K^i \Delta \mathbf{u}^{i+1} = \mathbf{R}^i \quad (6.10a)$$

$$\mathbf{u}^{i+1} = \mathbf{u}^i + \Delta \mathbf{u}^{i+1} \quad (6.10b)$$

Then the convergence criterion will require that:
\[ \left\| \Delta \mathbf{u}^{i+1} \right\| \leq \text{tolerence}_u \]  
\[ \left\| \Delta \mathbf{R}^{i+1} \right\| \leq \text{tolerence}_r \]

The convergence criteria are to be satisfied inside ABAQUS and the user can just control the required tolerance.

6.5 **Model Features and Capabilities**

The model implemented into UEL for ABAQUS has the capabilities to deal with any geomaterial, confining pressure, and boundary/loading conditions. The numerical model was implemented in this Chapter using material properties for loose fine silica sand, which were documented by Lade and Kim (1988) to show its features and capabilities. The present numerical model was able to predict to some extent a shear band features (thickness and inclination) with very little dependency on the mesh size.

As shown in Figure 6-1 the shear band bonuses or reflects on a certain angle once it hits the boundary, this can be justified physically by the existence of high friction at the boundary. One feature of the constitutive relations is that they are not directly dependent on the initial void ratio but the material parameters are influenced by the initial void ratio. Therefore, the void ratio effect is accounted for implicitly within the model; however, the void ratio, plastic work and/or the effective plastic strain are good variables that can be used to monitor the features of the shear band (Figure 6-2).
Figure 6-1 Shear Band Independence on the Mesh Size.

10x20 mesh

15x30 mesh

20x40 mesh
In this work the void ratio was used to measure the thickness of the shear band as will be discussed later in this Chapter. The profiles A-A, B-B and C-C in Figure 6-2 were used to predict the shear band thickness; the void ratio values were plotted against the distance along each of those profiles and the results (Figure 6-3) were used to measure the shear band thickness. The shear band location and mode was found to be highly influenced by the boundary conditions and the geometry of the specimen, which consistent with experimental observations.

The Cosserat rotation or the couple stresses were found to sharply switch their sign at the middle of the localization zone (Figure 6-4) which is consistent with the literature. If one chooses to change the length to the width ratio and make it larger than 2.0 then the failure will not, to some extent, be affected by the boundary and a single shear band might be obtained (Figure 6-5).
Figure 6-3 Void Ratio Values along Profiles A-A, B-B and C-C Used to Predict the Shear Band Thickness (t).

Figure 6-4 Couple Stress Values along the Profiles A-A, B-B and C-C.
Figure 6-5 Effective Plastic Strain Contours and Shear Bands in A Specimen with Length to Width ratio of 2.2.

Figure 6-6 Shear Band Progress during Different Loading Stages under 300.0 kPa Confining Pressure.
It was noticed in this study that strain localization commence during the hardening regime. Figure 6-6 and Figure 6-7 show the shear band progress during loading. The present model predicts that the material will behave homogeneously until a late stage of the hardening regime where the continuum will split into three or more regions. The first region is classified as the localization zone where the material will show tremendous volumetric and shear strains. This localization region will essentially separate two other regions that will experience elastic rebound and behave homogeneously as a rigid block as shown earlier in this Chapter. The stress-strain behavior and the volumetric change will show homogeneity until localization begins and thereafter the localization zone will continue deforming and the rigid regions will show zero volumetric changes and less softening. The stress-strain curves were extracted from the finite element results using the assigned three elements shown in Figure 6-8 for the same material discussed above. The results were obtained for two confining pressures (100 and 150 kPa) at the
same initial void ratio (same material properties). Figure 6-9 shows that the same material fails at higher strain lever under higher confining pressure.

Figure 6-8 Elements Chosen for Monitoring the Deviatoric Stress and the Void Ratio Changes during Loading.

Figure 6-9 Deviatoric Stress Distribution within the Rigid and the Localization Zones at Two Different Confining Pressures.
As discussed earlier the material will behave as a rigid body outside the localization zone, the numerical findings in this dissertation supports this theory. The void ratio was found to be almost constant outside the localization zone during the softening regime (Figure 6-10). Showing the local stresses versus the local vertical strain; the one might conclude that material outside the localization zone will exhibit elastic rebound while high vertical strains will be experienced within the shear band (Figure 6-11 and Figure 6-12). Now if one chooses to change the boundary conditions then the behavior of the material will change, an example was performed by constraining the movement at the bottom of the specimen in all directions then crossing shear bands were obtained at a strain level of 6% (Figure 6-13). At later strain level the cross shear band started collapsing into one single shear band. The fact that the global stiffness matrix is a non-symmetric matrix might explain this phenomenon.

Figure 6-10 Void Ratio Distribution within the Rigid and the Localization Zones at Two Different Confining Pressures.
Figure 6-11 Local Deviatoric Stresses versus the Local Axial Strains

Figure 6-12 Local Void Ratio versus the Local Axial Strains
Figure 6-13 Shear Band Evolution in a Fixed Base Specimen

Axial Strain = 6 %

Axial Strain = 13.5 %
CHAPTER SEVEN

RESULTS AND DISCUSSION

7.1 Introduction

As shown in the previous Chapters the numerical model was developed in the Cosserat continuum to investigate the shear band thickness and inclination for granular materials. The model was used to study such phenomena for the F-Sand, C-Sand, small and large glass beads, whose material parameters were estimated in Chapters Three and Four. Experimental data for some of those materials are available in the literature (Alshibli, 1995) which was used for verification purposes. In this Chapter, the shear band occurrence and the factors affecting its thickness and inclination angle are discussed. Material heterogeneity and the mapping of such heterogeneity of the material into the finite element mesh and its influence on the strain localization is investigated accordingly. The heterogeneity in the material properties is basically represented by the spatial distribution of the particle size, surface roughness and shape indices. However, the heterogeneity of the material, which influences its behavior, is not accounted for in this study due to the limitations in the constitutive model.

7.2 Results for F-75 Sand

7.2.1 Medium-Dense F-Sand

Alshibli (1995) has published experimental results for shear bands in F-75 Ottawa sand. The study involved several experiments under different initial void ratio and confining pressures. Material parameters for this material were evaluated and presented in Chapter Four. For the medium-dense F-sand with initial void ratio of 0.629 ($D_r = 55\%$) and confining pressure of 15.0 kPa; laboratory observations showed that the shear band thickness was about 2.97mm after the
specimen was loaded until it reached a nominal axial strain of about 10.2% and the inclination angle was 52.5°. The model predictions under the same conditions were a thickness of 3.1 mm and an inclination angle of 51.6°. Figure 7-1 shows a specimen at the beginning of test and at an axial strain of about 10.2%.

![Primary shear band](image)

(a) Axial Strain = 0%  
(b) Axial Strain = 10.2%

Figure 7-1 Medium-Dense F-Sand Plane Strain Specimen Tested in the Laboratory under 15.0 kPa Confining Pressure with Initial Void Ratio of 0.629, (Alshibli, 1995).

As shown in Figure 7-1, the specimen failed through conjugate shear bands. The movement of the bottom of the specimen was restrained in all directions during the test and that might be a strong reason for multiple shear bands to develop in the specimen. This phenomenon does not appear in the numerical model prediction due to the fact that roller boundaries were assigned at the bottom of the specimen which allows the specimen to slide in the lateral direction allowing only one shear band to develop most of the time. Figure 7-2 shows the model predictions for the same material under the same initial relative density and confining pressure.
The plane strain tests in the laboratory were video-taped and the shear bands were captured using the same video camera as shown in Figure 7-1. However, the whole specimen was not completely captured due to focusing issues and only certain part of the specimen was imaged. Therefore, a window with the same video image size was projected on Figure 7-2 for comparison purposes. Figure 7-3 shows comparison between the measured and predicted shear band for the medium-dense F-sand under 15.0 kPa confining pressure.

![Figure 7-2 Prediction for the Medium-Dense F-Sand Plane Strain Specimen under 15.0 kPa Confining Pressure with Initial Void Ratio of 0.629 Loaded to 10.2% Axial Strain.](image)

As illustrated in Figure 7-3, the present model yields good prediction of strain localization in the Medium-Dense F-sand. The shear band in the simulation was triggered by a numerical imperfection introduced in the very upper right edge of the specimen; this imperfection was introduced by reducing the material parameter, $M_L$, by 5% in one element as shown in Figure 7-4 a.
Figure 7-3 Comparison between Predicted and Measured Shear Band Thickness and Inclination Angle for the Medium-Dense F-sand under Confining Pressure of 15.0 kPa at 10.2% Axial Strain.

(a) Axial Strain = 0%     (b) Axial Strain = 10.2%

Figure 7-4 Initiation of Strain Localization Using Material Imperfection (Effective Plastic Strain).
The material imperfection represent a numerical weakness that will trigger the strain localization, however the shear band should not necessarily pass through the numerical imperfection. As shown in Chapter Six the shear band thickness is identified by a finite zone with high volumetric strains, effective plastic strain, Cosserat rotations and concentration of void ratio. Profiles for void ratio, effective plastic strain and Cosserat rotation crossing the centerline of the shear band will be a representative measurement of the thickness of the shear band (Figure 7-5 and Figure 7-6). Figure 7-6 shows that the Cosserat rotation reads the highest value at the shear band center while the rotation curvature and the couple stresses at failure will vanish outside the shear band and they switch their direction at the center of the shear band. This phenomenon has a physical meaning in the sense that the centerline of the shear band can be considered as a slip surface where the particles will be sheared with tremendous shearing loads and therefore their rotational gradient and couple stresses will flip from clockwise to counter clockwise, (Figure 7-7).

The angle that the shear band centerline makes with respect to the minor principal axis represents the shear band inclination, (Figure 7-8). The same material with the same initial void ratio was simulated by the model under 100 kPa confinement; the shear band thickness was slightly less than the one obtained at the low confining pressure (15 kPa) with larger inclination angle. However, the experimental observations by Alshibli (1995) showed no obvious trend in this regard.

The laboratory measurements for the shear band thickness and the inclination angle under a confining pressure of 100 kPa were 2.91 mm and 55°, respectively; whereas the numerical predictions were 2.85 mm and 53.7°, respectively. Figure 7-9 shows comparison between measurement and model prediction.
Figure 7-5 Effective Plastic Strain Profile along the Shear Band Centerline for Medium-Dense F-sand.

Figure 7-6 Cosserat Rotation Profile along the Shear Band Centerline for Medium-Dense F-sand.
Figure 7-7 Gradient of Cosserat Rotation across the Shear Band Centerline for the Medium-Dense Sand.

\[ \theta = \tan^{-1}\left(\frac{y}{x}\right) = 51.6^\circ \]

Figure 7-8 Shear Band Inclination Predicted by the Present Numerical Model for the Medium-Dense F-75 Sand.
Again as shown in Figure 7-9 (b) two shear bands were obtained under biaxial testing for the F-sand; this phenomenon might be justified by the fact that the movement was restrained in all directions at the bottom of the specimen.

![Image of model prediction and experimental result]

(a) Model Prediction  (b) Experimental

Figure 7-9 Comparison between Measured and Predicted Shear Band Thickness and Inclination Angle for the Medium Dense F-sand under Confining Pressure of 100 kPa at 12.7% Axial Strain.

### 7.2.2 Very Dense F-Sand.

Results on the same F-sand at a very dense state with initial void ratio of 0.495 ($D_r = 97\%$) under two different confining pressures (15 and 100 kPa) were also reported by Alshibli (1995). The experimental tests under plane strain conditions were simulated numerically using the present model. Experimental measurements of the shear band thicknesses were 3.01 mm and 3.05 mm for confining pressures 15.0 kPa and 100 kPa, respectively. On the other hand, the
predicted values were 3.0 mm and 2.78 mm under 15.0 kPa and 100.0 kPa, respectively. The very dense F-sand failed at angle of 57° under the 15.0 and 100 kPa confining pressures while the model predicted inclinations of 58° and 59.2° for those two confinements, respectively. It can be seen here that the model has a trend in decreasing the shear band thickness as the confining pressures increases and at the same time the inclination angle will increase with increasing the confining pressure. In this simulation, the same methodology was followed to trigger the shear band, a weak element was assigned at the very top left of the sample. Figure 7-10 shows the a specimen tested in the laboratory under plane strain conditions with dimensions of 150.0 mm in height and 80mm in width and under confining pressure of 15 kPa.

Figure 7-10 F-Sand Plane Strain Specimen Tested in the Laboratory under 15 kPa Confining Pressure with Initial Void Ratio of 0.495 (Alshibli 1995).
The model simulation using a fine mesh of (35x70) elements showed that a single shear band will develop under the same initial void ratio and confining pressure (Figure 7-11).

![Figure 7-11 Prediction for F-Sand Plane Strain Specimen under 15.0 kPa Confining Pressure with Initial Void Ratio of 0.495.](image)

(a) Axial Strain = 0.0%  
(b) Axial Strain = 10.1%

For the very dense sand with a slightly different void ratio, specimen was tested under a confining pressure of 100.0 kPa and simulated by the present model. Figure 7-12 shows comparison between the experimental results and the numerical simulation. Same window was projected on both the video image and the predicted mesh for comparison purposes.

### 7.3 Results for C-Sand

The material parameters for the C-sand were calibrated and presented in Chapter Four. Those parameters were used in the numerical model to simulate the strain localization for this material under confining pressures of 15.0 and 100.0 kPa. The specimen size was the same as the
F-sand specimen and the initial void ratio was of about 0.767. Figure 7-13 shows a video image obtained for the C-sand specimen at the beginning of the test and at an axial strain of 10.4%.

It is well known from a geotechnical point of view that the loose sand will dilate under low confining pressure and dense sand might contract under high confining pressure. The shear band thickness can be always linked to the amount of the localized dilation (i.e. the more the dilation the thicker the shear band). This explanation might be confusing in the sense that thicker shear bands give less shear strength while higher dilation gives higher shear strength. The argument that loose sand will show thicker shear band (high localized dilation) under low confining pressure is highly supported by the author and the present numerical model. The
dilation phenomenon is not discussed globally in this study; localized dilation is discussed instead. The loose C-sand showed a thicker crossing shear bands as shown in Figure 7-13; this might be due to the relatively high localized dilatancy given that the sample is loose and the confining pressure is relatively low (15.0 kPa). The fact that the shear band thickness highly depends on the size and the shape of the particles explains the experimental findings in this regard which showed a shear band thickness of 17.33 mm. The model prediction for the loose C-sand under the same initial void ratio and the same confining pressure 15.0 kPa is shown in Figure 7-13.

Figure 7-13 C-Sand Plane Strain Specimen Tested in the Laboratory under 15.0 kPa Confining Pressure with Initial Void Ratio of 0.767 (Alshibli, 1995).
The predicted shear band thickness was of about 18.04 mm and the inclination angle was 51.4° which compares well with the experimental results 17.33 mm and 50°, respectively, for the same material under the same conditions.

The C-sand was tested almost under the same initial void ratio and higher confining pressure 100.0 kPa; the shear band thickness decreased to 17.00 mm and the inclination angle decreased to 48° as well. These experimental findings are for some reason confusing due to the lack of any trend or agreement with the physical laws. From fundamental geotechnical point of view, the loose sand will always dilate under low confining pressure (15.0 kPa) which will lead to a thicker failure zone (shear band) and to a smaller failure angle.

Figure 7-14 Prediction for C-Sand Plane Strain Specimen under 15.0 kPa Confining Pressure with Initial Void Ratio of 0.767.
The experimental results did not show such clear trends for the sands mentioned above. The model predictions for the loose C-sand under a confining pressure 100.0 kPa were 16.4 mm for the thickness and an onset of 53.2°. Figure 7-15 shows the experimental results for the loose C-sand under confining pressure of 100.0 kPa (Alshibli, 1995) and Figure 7-16 shows the numerical predictions for the same specimen under the same conditions at the same strain level (10.8%).

### 7.4 Small and Large Glass Beads

The glass beads used in this study were characterized in Chapter Three; the shape of those beads was fairly spherical which did not allow obtaining wide range of void ratio. In other words the range between the minimum and the maximum void ratios was very narrow. The nature of the glass beads also will not, in general, lead to high dilative behavior of such materials and the heterogeneity level is relatively low, therefore no clear shear bands might be obtained. The numerical model in its current shape does not account for the effects of the particle shape and surface roughness on strain localization and still predicts strain localization with poor characterizing features reflected from the material parameters.

Experimental results on strain localization for small glass beads with mean particle size of about 0.22 mm under plane strain conditions were reported by Alshibli (2004) using a specimen of 136 mm high by 42 mm width. Figure 7-17 shows X-ray Computed Tomography image for the specimen at 0.0 and 7.34% axial strain level. The shear band thickness of these glass beads was about 4.9 mm (i.e., 22.3d₅₀) with inclination angle of 61.5°. For the small glass beads at a void ratio of 0.587 and confining pressure of 75.0 kPa the model prediction is shown in Figure 7-18. For the large glass beads at a void ratio of 0.592 and under a confining pressure of 75.0 kPa; the prediction results are shown in Figure 7-19.
Figure 7-15 C-Sand Plane Strain Specimen Tested in the Laboratory under 100 kPa Confining Pressure with Initial Void Ratio of 0.767 (Alshibli, 1995).

Figure 7-16 Prediction for C-Sand Plane Strain Specimen under 100.0 kPa Confining Pressure with Initial Void Ratio of 0.767.
The model predictions for the small and large glass beads are shown in Figure 7-18 and Figure 7-19, respectively. As shown in the analysis for the small and large glass beads clear localization zone was obtained although such materials (glass beads) seem to have low degree of heterogeneity in the material properties and local void ratio.

The surface roughness, shape indices and particle size for such, relatively speaking, uniform material are, to some extent, uniformly distributed and therefore those types of distributions led to global failure in the material with no clear strain localization.
Figure 7-18 Prediction for Small Glass Beads Plane Strain Specimen under 75.0 kPa Confining Pressure with Initial Void Ratio of 0.587.

Figure 7-19 Prediction for Large Glass Beads Plane Strain Specimen under 75.0 kPa Confining Pressure with Initial Void Ratio of 0.592.
7.5 **Summary of the Experimental and Numerical Results**

The experimental and numerical results for the materials used in this study were shown and discussed above. However, in this subsection a summary for those results will be tabulated to simplify the comparison process for the interested reader (Table 7-1 and Table 7-2). Table 7-3 shows the values of the axial strain at which strain localization began for all the materials used in this study. All the simulated and tested specimens showed that the localization would always start at a very late stage of the hardening regime and observation was more obvious in the very dense material which can be explained by higher dilation tendency in such materials.

Table 7-1 Comparison between Measured and Predicted Shear Band Thickness.

<table>
<thead>
<tr>
<th>Material</th>
<th>Confining Pressure (kPa)</th>
<th>Initial Void Ratio</th>
<th>Mean Grain Size (mm)</th>
<th>Predicted Shear Band Thickness (mm)</th>
<th>Measured Shear Band Thickness (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>F-Sand</td>
<td>15.00</td>
<td>0.629</td>
<td>0.22</td>
<td>3.10 ($14.1d_{50}$)</td>
<td>2.97±0.24</td>
</tr>
<tr>
<td>F-Sand</td>
<td>100.0</td>
<td>0.629</td>
<td>0.22</td>
<td>2.85 ($13d_{50}$)</td>
<td>2.91±0.2</td>
</tr>
<tr>
<td>F-Sand</td>
<td>15.00</td>
<td>0.495</td>
<td>0.22</td>
<td>3.00 ($13.64d_{50}$)</td>
<td>3.00±0.29</td>
</tr>
<tr>
<td>F-Sand</td>
<td>100.0</td>
<td>0.495</td>
<td>0.22</td>
<td>2.78 ($12.64d_{50}$)</td>
<td>3.05±0.18</td>
</tr>
<tr>
<td>C-Sand</td>
<td>15.00</td>
<td>0.767</td>
<td>1.60</td>
<td>18.04 ($11.28d_{50}$)</td>
<td>17.33±0.4</td>
</tr>
<tr>
<td>C-Sand</td>
<td>100.0</td>
<td>0.767</td>
<td>1.60</td>
<td>16.40 ($10.25d_{50}$)</td>
<td>17.00±0.57</td>
</tr>
<tr>
<td>S- Beads</td>
<td>100.0</td>
<td>0.587</td>
<td>0.80</td>
<td>18.4 ($23d_{50}$)</td>
<td>22.2 $d_{50}$</td>
</tr>
<tr>
<td>L-Beads</td>
<td>100.0</td>
<td>0.592</td>
<td>3.3</td>
<td>50.00 ($15.15d_{50}$)</td>
<td>22.2 $d_{50}$</td>
</tr>
</tbody>
</table>

Table 7-2 Comparison between Measured and Predicted Shear Band Inclination Angle.

<table>
<thead>
<tr>
<th>Material</th>
<th>Confining Pressure (kPa)</th>
<th>Initial Void Ratio</th>
<th>Mean Grain Size (mm)</th>
<th>Predicted Shear Band Inclination (°)</th>
<th>Measured Shear Band Inclination (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>F-Sand</td>
<td>15.00</td>
<td>0.629</td>
<td>0.22</td>
<td>52.5</td>
<td>51.6</td>
</tr>
<tr>
<td>F-Sand</td>
<td>100.0</td>
<td>0.629</td>
<td>0.22</td>
<td>55.0</td>
<td>53.7</td>
</tr>
<tr>
<td>F-Sand</td>
<td>15.00</td>
<td>0.495</td>
<td>0.22</td>
<td>57.0</td>
<td>58.0</td>
</tr>
<tr>
<td>F-Sand</td>
<td>100.0</td>
<td>0.495</td>
<td>0.22</td>
<td>57.0</td>
<td>59.2</td>
</tr>
<tr>
<td>C-Sand</td>
<td>15.00</td>
<td>0.767</td>
<td>1.60</td>
<td>50.0</td>
<td>51.4</td>
</tr>
<tr>
<td>C-Sand</td>
<td>100.0</td>
<td>0.767</td>
<td>1.60</td>
<td>48.0</td>
<td>53.2</td>
</tr>
<tr>
<td>S- Beads</td>
<td>100.0</td>
<td>0.587</td>
<td>0.80</td>
<td>61.5</td>
<td>58.7</td>
</tr>
<tr>
<td>L-Beads</td>
<td>100.0</td>
<td>0.592</td>
<td>3.3</td>
<td>NA</td>
<td>51.0</td>
</tr>
</tbody>
</table>
Table 7-3 Comparison between Measured and Predicted Onset of Localization.

<table>
<thead>
<tr>
<th>Material</th>
<th>Confining Pressure (kPa)</th>
<th>Measured Axial Strain (%)</th>
<th>Predicted Axial Strain (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>M-D F-Sand</td>
<td>15.0</td>
<td>2.9</td>
<td>2.08</td>
</tr>
<tr>
<td>M-D F-Sand</td>
<td>100.0</td>
<td>3.3</td>
<td>2.7</td>
</tr>
<tr>
<td>V-Dense F-Sand</td>
<td>15.0</td>
<td>2.2</td>
<td>1.76</td>
</tr>
<tr>
<td>V-Dense F-Sand</td>
<td>100.0</td>
<td>2.5</td>
<td>1.9</td>
</tr>
<tr>
<td>C-Sand</td>
<td>15.0</td>
<td>5.4</td>
<td>4.61</td>
</tr>
<tr>
<td>C-Sand</td>
<td>100.0</td>
<td>6.1</td>
<td>4.72</td>
</tr>
<tr>
<td>S- Beads</td>
<td>75.00</td>
<td>3.94</td>
<td>5.3</td>
</tr>
<tr>
<td>L-Beads</td>
<td>100.0</td>
<td>NA</td>
<td>7.2</td>
</tr>
</tbody>
</table>

7.6 Effect of Surface Roughness on the Behavior of Granular Materials

As shown in Chapter Three, Alshibli and Alsaleh (2004) proposed a method to measure the surface roughness of granular materials. The effect of the surface roughness on the peak friction angle and the dilatancy angle was studied and discussed. A series of biaxial (plane strain) experiments were performed on the three sands using prismatic specimens that measure 83.3mm wide by 80.8mm long by 152.4mm high. Loose (relative density, $D_r =39-66\%$) and dense specimens ($D_r = 80-100\%$) were tested under 15 and 100 kPa confining-pressure conditions (see Alshibli & Sture 2000 for more details about the experiments). Figure 7-20 shows the relationship between surface roughness (represented by the mean $R_a$ value) and peak friction angle ($\phi^p$) and the dilatancy angle ($\psi$). Some of the specimens did not reach the critical state, which made it difficult to calculate the critical state friction angle; therefore, peak friction angles were used in the analysis. It is well known that the frictional resistance of granular materials is mainly attributed to interparticle sliding resistance and particles' rearrangements/ interlocking (dilatancy effects). Figure 7-20 shows that $\phi^p$ and $\psi$ increase as surface roughness increases for all cases. Furthermore, dense specimens have higher $\phi^p$ and $\psi$ values compared to loose specimens tested under the same confining pressure. $\phi^p$ and $\psi$ values are also higher for
specimens tested at low confining pressure (15 kPa) compared to those tested at high confining pressures (100 kPa) with similar densities. Finally, it seems that there is a consistency in the trend of the rate of increase of $\phi^p$ with surface roughness (i.e., the slope and shape of the curve) for specimens tested at the same confining pressure value. It is obvious that the surface roughness will significantly affect the dilatancy behavior of the granular materials which in its turn will affect the shear band thickness. To assess this effect numerically or theoretically a micromechanical model is needed. However, this effect might be accounted for, to some extent, at the finite element level using phenomenological constitutive relations as shown in the previous Chapters.

The effect of the surface roughness of the particles on strain localization in granular material was accounted for through the angular momentum of inertial where the grain size is needed as shown in Chapter Five. A parametric study for the effect of the surface roughness on the shear band thickness was performed numerically for the F-sand in which all the parameters (initial void ratio, confining pressure, and material parameters) were assumed to be constant. Figure 7-21 shows that the shear band thickness will increase slightly with increasing the surface roughness of the particles.

These findings and conclusions drawn from this study support the argument that the micro-structural properties will highly affect the behavior of the granular materials. Yet no explicit studies are available in the literature to investigate this phenomenon and therefore, it is a very challenging task that might face the researcher. The surface roughness and shape indices of granular materials, to some extent, are difficult to quantify. However, the author has successfully addressed those parameters as discussed earlier in Chapter Three.
Figure 7-20: Effect of Surface Roughness on Friction Angle, and on Dilatancy Angle
(Experimental Data (Alshibli, 1995))
Moreover, the physical link between the surface roughness and the shear band thickness is not addressed well in this study due to the lack of the micromechanical-based relations.

Figure 7-21 Numerical Simulation Showing the Effect of Surface Roughness on Shear Band Thickness at Different Initial Void Ratios under Low and High Confining Pressures for the F-Sand

It is obviously clear that the shear band thickness would increase as the surface roughness increases due to the fact that the shear band thickness is dependent on the internal length scale which is affected by the roughness. This finding is in full agreement with the physical justification in the sense that the shear band thickness is highly dependent on the dilation that would increase with the increasing the roughness of the surface of contact between the particles. In Figure 7-21 and as was shown earlier the increase of the confining pressure will cause a decrease in the shear band thickness due to the decrease of the dilation.
7.7 **Effect of Shape Indices on the Behavior of Granular Materials**

The shape and size of the particles will always affect the internal length scale used in this study; many researchers have used the same length scale \( d_{50} \) which is not necessarily accurate and most of the time will be a significant source for error in modeling the behavior of granular material. In Cosserat continuum the model requires two length scales; one is the length of contact surface and another is the arm of rotation (See Chapter Five). These two parameters were found to be highly dependent on the shape and the size of the particle. The more the particle is elongated in shape the longer is the contact surface and less the arm of rotation. Based on this argument, a proportionality factors are proposed as follows:

\[
l_s = \frac{l_{SPH}}{I_R} \quad I_{ave}
\]

(7.1)

Where, \( l_s \), \( I_{SPH} \), \( I_R \) and \( I_{ave} \) are the length of the surface of contact, sphericity index, roundness index and the mean particle size (equivalent to \( d_{50} \)), respectively.

\[
l_a = \frac{I_R}{I_{SPH}}l_{ave} + R_a
\]

(7.2)

Where, \( l_a \) and \( R_a \) are the length of the arm-of-rotation and the mean surface roughness respectively. For the same F-sand a value for \( R_a \) was assumed to be constant and the shape indices were changed and their effect on the shear band thickness was as significant as the surface roughness or the confining pressure (Figure 7-22).

Again this was a hypothetical example assuming material properties for medium dense and very dense F-sand and changing the shape indices to investigate the response of the numerical model for such changes. The numerical model response was basically through the effect of Equations 7.1 and 7.2, which in a way has a physical meaning extracted from the previous Chapters. The effect of the roundness index is pretty much non-linear with low degree
of nonlinearity as illustrated in Figure 7-22 and this is also justified by the way the mathematical formulation was done in the Equations 7.1 and 7.2.

![Figure 7-22](image.png)

Figure 7-22 Effect of the Roundness Index on Shear Band Thickness at Different Initial Void Ratios under Low and High Confining Pressures for the F-Sand.

The sphericity effect of the granular materials on the strain localization was studied for the same F-sand under the same assumptions mentioned earlier. Figure 7-23 shows the effect of sphericity on the shear band thickness.

The shape indices ($I_R$ and $I_{SPH}$) will basically affect the polar friction (resistance to any rotation, realignment or reallocation of the particles). The higher those two indices the larger the dilation which will lead to a thicker localization zone. The purpose of this parametric study was just to show the sensitivity of the numerical model to those micro-structural properties and thereafter these parameters will be used to represent the heterogeneity of the material. Again,
micromechanics within constitutive laws will be an interesting and more accurate approach to investigate the effect of such micro-properties on the behavior of granular materials.

Figure 7-23 Effect of the Sphercity Index on Shear Band Thickness at Different Initial Void Ratios under Low and High Confining Pressures for the F-Sand.

7.8 **Effect of the Initial Density and the Confining Pressure**

As illustrated earlier in Figure 7-21 through Figure 7-23 the effect of the initial void ratio (density) and the confining pressure was investigated using the F-75 Ottawa sand. The shear band thickness was found to decrease as the confining pressure increases which agrees with the fundamentals of geomechanics. The medium dense sand under the same confining pressure was found to show a thicker shear band than the very dense sand. This might be misleading if one does not consider the localization issue in the sense that the denser the sand will dilate more. As a matter of fact, the global dilation, which is measured in the laboratory, will be always higher for
the higher density; however, dilation within the shear band will be higher for looser granular material which will lead to a thicker shear band. The critical soil mechanics supports this finding in the sense that the loose specimen will exhibit higher volumetric change to transfer the state from the initial void ratio to the critical values as illustrated in Figure 7-24. Numerical results reported by Huang et. al. (2002) are consistent with the authors results.

Figure 7-24 Critical State Soil Mechanics Illustration
7.9  Mapping the Material Heterogeneity into the Finite Element Model

The granular media or in general the soil media is composed of discrete particles that makes the mechanical behavior complicated and difficult to understand or to simulate. The randomness in the shape and size of the particles make local properties very different. As a result, strain localization will always occur following the settings of the applied loads and the boundary conditions. To this end, the strain localization has been triggered by assigning a numerical defect in one (or more) element within the finite element mesh; this element will be chosen based on some experimental experience. However, if one succeeds to map some actual local properties of the domain into the finite element mesh, the results will be more representative and accurate. In this subsection some spatial distributions for the length scales was generated based on the SEM images shown in Chapter Three. Then mapping between the material properties and the finite element mesh was performed to pick local properties for each element based on the assigned spatial distribution (Figure 7-25). It is worth noting here that one should be careful regarding the element size; in other words an element size close to the particle size will violate the physical assumptions used in the model. The minimum element size used in this study was about 5 times the mean particle size to avoid any theoretical deformation for the particle itself. However, physically particle crushing will most likely occur if the soil mass is loaded under high confining pressure; this will need some damage representation within the model. In this dissertation the assumption that particles will not crush alternatively, rigid body translation and rotation are assumed.

A high resolution computed tomography will be an accurate way to capture the heterogeneity of the domain and then the mapping between the spatial distribution for the material properties and the finite element will be more representative.
It was found that different spatial distributions for the same material properties will yield different localization features. Results for the dense F-sand under 100.0 kPa are shown in this subsection to investigate the mapping approach. The spatial distributions for the particle size and the shape indices were obtained from SEM images using 10 images (each has about 6 particles), however such distributions were statistical and more accurate spatial distributions are needed. Based on those distributions each element in the FE mesh will contain few particles, which will have an average values for the particle size, surface roughness and the shape indices. Those values will be used at each integration point for a given element in the domain for computational purposes.

Figure 7-25 Hypothetical Sketch Showing the Mapping between the Finite Element Mesh and the Material Properties.

The displacement field will be heterogeneous at early stages of the loading stage yielding a heterogeneous field for all the internal state variables, accordingly; this will lead to strain
localization around the failure stress. Figure 7-26 shows the spatial distributions for the particle size and the shape index $I_R$.

The statistical random distribution for the material properties was found to effectively trigger the strain localization phenomenon using the present numerical model. Figure 7-27 shows the shear band characteristics as a result of the first statistical distributions shown in Figure 7-26. However, changing the above distribution to the distribution shown below in Figure 7-28 was found to change the shear band characterization as shown in Figure 7-29.

Figure 7-26 Spatial Distributions for the Particle Size and the Shape Index, $I_R$.  
(a) Particle Size (mm)  
(b) Shape Index, $I_R$
Figure 7-27 Prediction of the Shear Band Thickness and Inclination Angle for the Very Dense F-sand under Confining Pressure of 100.0 kPa using the Material Spatial Distribution I.

(a) Undeformed                           (b) Deformed (Axial Strain = 9.6%)

Figure 7-28 Spatial Distributions II for the Particle Size and the Shape Index, $I_R$.

(a) Particle Size (mm)             (b) Shape Index, $I_R$
Figure 7-29 Prediction of the Shear Band Thickness and Inclination Angle for the Very Dense F-sand under Confining Pressure of 100 kPa using the Material Spatial Distribution II

It is worth noting here that the spatial material distribution will always affect the numerical results; in other words the numerical model was able to detect any material heterogeneity within the continuum. Accordingly, an accurate estimation for such material heterogeneity is essential and makes the finite element solution closer to the discrete element solutions in the sense that it will deal each element as a small continuum.

7.10 Application of the Model for Real Geotechnical Problem

The behavior of the granular material beneath a shallow foundation is simulated using the numerical model. A strip footing of 2.0 m width at an embedment depth of 2.0 m laid on the F-75 sand was modeled using the numerical model. The footing was assumed to be on ground surface and the embedment depth was simulated by applying a surcharge of 36.0 kPa on the surface. The footing was assumed to be very stiff (steel material was assumed) and the soil stratum modeled as the foundation soil was assumed to be of 13.0 m width and 6.5 m thick to avoid the boundary
effects. The loading was performed through three stages; the first was applying the surface surcharge, the second was applying the vertical and horizontal effective overburden pressure adding the effect of the surface surcharge and the last stage was pushing the footing towards the foundation soil; the footing was pushed a total of 20.0 mm. It is known that shallow foundations might fail via one of three common failure modes; the first is the general shear failure which occurs in dense sand, the second is the local shear failure in medium dense sand and the third is the punching shear failure which is common in very dense sand (Figure 7-30).

Figure 7-30 Failure Modes of Shallow Footings Resting on Granular Materials.
The type of failure will essentially depend on the stiffness of the footing, the soil properties and the depth of the embedment. The results of the numerical model showed the foundation soil failed with local shear failure mode. Figure 7-31 shows the undeformed and deformed shape of the structure, respectively.

\[ \sigma_v = \gamma z + q \]
\[ \sigma_h = \sigma_v k_o \]

Figure 7-31 Model for Strip Footing Resting on Medium Dense F-75 Sand.
The vertical stress distribution beneath the strip footing induced from the applied load is shown in Figure 7-32; the shape of stress distribution obtained from the numerical solution is expected based on the available analytical solutions.

Figure 7-32 Vertical Stress Distribution beneath a Strip Footing Resting on the Medium Dense F-75 Sand using the Numerical Model (kPa)

Figure 7-33 shows the volumetric strain distribution beneath the footing; this distribution agrees to some extent with the failure pattern shown in Figure 7-30b which indicates a local shear failure mode in this type of granular material.
Figure 7-33 Volumetric Strain Distribution beneath a Strip Footing Resting on the Medium Dense F-75 Sand using the Numerical Model.
CHAPTER EIGHT

CONCLUSIONS AND RECOMMENDATIONS

8.1 Conclusions

The dissertation involved enhancing Lade’s constitutive model by implementing Cosserat rotation. The model was implemented into the finite element program ABAQUS to predict strain localization in granular materials. User material and user element subroutines (UMAT and UEL) were needed to solve for the problem.

The model was used to study such phenomena for the F-Sand, C-Sand, small glass beads and large glass bead, which were characterized in Chapters Three and Four. Available experimental data in the current literature was used for comparison and verification purposes. The following conclusions are drawn:

- Cosserat theory was found to be an efficient non-local theory that can be used to investigate the localization phenomenon in granular materials.

- The enhanced model gave good predictions of strain localization in granular materials.

- Non local theory with representative length scales is required to overcome the mathematical ill-posedness and mesh dependency to capture strain localization in materials.

- Plasticity models in their original shapes are not properly equipped to accommodate such length scales. Therefore, special treatment for such models is needed to incorporate the effect of the internal length scales through the Cosserat rotation and the couple stresses.

- The confining pressure was found to have an effect on the shear band thickness.
• The shear band thickness will decrease as the confining pressure increases; while the inclination angle increases with increasing the confining pressure.

• The model showed that the initial density has also a significant influence on the shear band thickness; Shear band thickness decrease as the initial density increases.

• Microstructural characterization for the Silica sands the glass beads was performed to investigate the effect of such properties on the behavior of granular materials. The size, surface roughness and the shape indices were evaluated using imaging techniques and some statistical distributions were proposed.

• The mean particle size, surface roughness and the shape indices were used in the model as internal length scales and were found to affect the shear band thickness significantly.

• The shear band thickness increases as the mean particle size and the particle surface roughness increase.

• Shear band thickness increases as the particle sphericity and roundness decreases.

• Strain localization was found to begin at late stages of the hardening regime for the sand and the glass beads.

• The Cosserat rotation was found to be maximum at center of the shear band at the failure point.

• The couple stresses and the rotation curvature have almost zero values outside the shear band and they switch their direction at the center line of the shear band reading maxima within the localization zone.

• The couple stress values were found to be very small compared with the stress values; however, they have a significant effect on the behavior of the material.
• The void ratio at the center of the shear band might exceed the maximum global void ratio for a certain material. Very large volumetric and shear strains were observed within the shear band.

• Material imperfection is always needed to trigger the localization zone; this imperfection can be introduced as a small weak area within the continuum. However, Shear band might not pass through the material imperfection.

• The numerical model can respond to any material heterogeneity once such heterogeneity distribution is available and mapped into the finite element model.

• The numerical model was used to predict the behavior of shallow footing and the results were in good agreement with the theory.

8.2 Recommendations for Future Research

• The present model was developed by enhancing the Lade’s model to incorporate the effect of the couple stresses; however, polar-based constitutive relations will be of more efficient.

• The micro-structural properties were incorporated at the finite element level; however such properties need to be incorporated at the constitutive level and therefore a micromechanical derivation is needed.

• The initial material properties used in the model are assumed to be constant throughout the simulation; however it is believed that as the material deforms the void ratio will change and the material properties will change accordingly. Some evolution criteria need to be established to account for such changes.

• More controlled experiment with reliable measurements at different densities and confining pressure are needed.
• High resolution images are needed to evaluate the material heterogeneity distributions and map such heterogeneities into the finite element model.

• The numerical model was developed to work under plane strain conditions, however it can be enhanced to work for 3D and axisymmetric elements.

• Correlations and comparisons need to be made to compare the Cosserat approach with the different proposed gradient models
REFERENCES


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VITA

Mustafa Ibrahim Alsaleh was born on the 5th of November, 1972, in a small town in the northern part of Jordan called Al Sareih. He finished his high school in the same town in 1991 and started going to the Jordan University of Science and Technology (JUST) to get his bachelor of science degree in civil engineering with geotechnical engineering emphasis; was ranked the fourth among 86 students in the same batch. Right after he got his bachelor degree, (Jan.1996) Mr. Alsaleh started his master’s study at the same school (JUST) working on developing a new design methodology for driven piles in sand considering the post-driving residual stresses under the supervision of the Prof. Ahmad Alawneh. He got his master of science degree in geotechnical engineering in June 1998 and started working as a geo-environmental engineer for Al-Shamil engineering, Amman-Jordan. In May 1999 he got an offer to work with Arab Center for Engineering Studies in Abu-Dhabi, United Arab Emirates, where he worked for a year. Mr. Alsaleh started his doctor of philosophy study at the University of Akron in July 2000, he attended there for a year and then decided to transfer to Louisiana State University in August 2001, where he started working in the field of strain localization of granular materials under the supervision of Dr. Alshibli and Dr.Voyiadjis. He will earn the degree of Doctor of Philosophy at the August 2004 Commencement.