Multiscale Analysis of Swelling and Mechanical Behavior of Granular media

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Eindhoven, 22 February 2022

Graduation Project
7K45M0
Words of thanks

First, I want to thank dr. ir. Payam Poorsolhjouy for all the help and support during my Master thesis. During this past year, he helped me with understanding the subjects, provided guidance during the research and helped me with great suggestions and solutions to problems. I learned a lot about granular mechanics during this past year, especially about continuum mechanics and discrete element modelling. I have also learned a lot about the use of Matlab for calculations and the use of tensor calculations.

I also want to thank dr. ir. Emanuela Bosco for her guidance during the project. Her experience with graduation projects helped a lot during the first period of the project. During the second half of the project, her guidance, help and expertise with the swelling and diffusion were really helpful.

I want to thank dr. Joshua Dijksman for providing experimental data. I want to thank both dr. Joshua Dijksman and Chandan Shakya for helping me with their knowledge of the experimental data.
Summary

Within the built environment, flow and diffusion are a subject of interest. Flow and diffusion can have an effect on a number of elements within the built environment. In particular, granular materials and their pore spaces endure these effects. Due to the diffusion of water, a material or particle packing can start to expand. This can be due to the fact that particles can adsorb water and start to swell. This moisture expansion can result in damage in a material. The swelling of particles and the influence of the swelling of particles on the mechanical behavior of granular material is studied. The answer to the following research question is found: How does the swelling of individual particles influence the overall response of a granular microstructure and what is the interaction between the mechanical and the swelling response?

In order to find the influence of the swelling of the particles on a granular particle packing, first, a suitable and efficient mechanical model should be found. Then, the swelling principles can be found for this method. When a correct mechanical model is found and the swelling principles have been explored, these swelling principles can be applied to the mechanical model.

Granular materials are usually modelled with the use of the granular micromechanics approach (continuum mechanics) or the particle mechanics approach (discrete element method). In the past, more research was done into the discrete element method. However, the granular micromechanics approach (GMA) is much less computationally expensive. For this reason, this research is focused on GMA. GMA needs to be experimentally or numerically calibrated, this is done for an experimental mono-disperse hydrogel particle packing. A correct mechanical model for this hydrogel particle packing is found.

Diffusion principles can now be explored for this mechanical model. In the case of swelling, the total strain in a particle packing consists of the hygroscopic strain and the elastic strain. The hygroscopic strain is based on the hygroscopic expansion coefficient and the change of moisture content. The hygroscopic expansion coefficient of a particle packing is dependent on the hygroscopic expansion coefficient of the particles and the properties of the particle packing. The relationship between micro
and macro can be found for the hygroscopic expansion coefficient with the use of homogenization and the principle of virtual work (PVW) or the equilibrium of stresses.

This micro-macro relationship can be tested on different particle packings. Mono-disperse and bi-disperse experimental particle packings can be evaluated, just as a simulated particle packing. For a packing with isotropic particles with only one type of microscopic expansion coefficient, both the micro-macro relation for the PVW and for equilibrium result in the macroscopic expansion coefficient of the packing being equal to the microscopic expansion coefficient of the particles. When a particle packing with two (or more) different expansion coefficients for the particles is used, the results that are found are physically reasonable for both the PVW and the equilibrium of stresses, however, both starting points give different results. The results which come from the homogenization with the equilibrium of stresses seems more likely.

Then this micro-macro relationship can be implemented on the mechanical model which was found for the mono-disperse hydrogel particle packing. The influence of the swelling on the stress-strain relationship is found. The stresses in a particle packing increase when swelling is applied. The rate of this increase depends on the hygroscopic strain, which depends on the hygroscopic swelling coefficient and on the change in moisture content.
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1 Introduction

Within the built environment, flow and diffusion are a subject of interest. Flow and diffusion can have an effect on a number of elements within the built environment. In particular, granular materials and their pore spaces endure these effects. Granular materials are widely used within the built environment. Structures within the built environment are in constant exposure to environmental effects. Examples of these environmental effects are freeze-thaw cycles of rain and snow water, thermal loading’s, ageing, radiation, corrosion and more [Poorsolhjouy, 2021]. A typical result of these environmental effects is the cracking of the structure. This is usually caused by the volume change of porous materials, which can be caused by changes in moisture content or temperature changes [Sovják et al., 2015].

Besides structures, there are also a number of aspects that make flow and diffusion important for soil mechanics. The influence of groundwater on soils is really large. The groundwater influences the stress transfer in soil mechanics [Verruijt, 2001]. Water within soils also endures freeze-thaw cycles, which can influence the compression strength of soils [Xie et al., 2015]. Within soils, fluctuating groundwater levels make the influence of water on granular material an interesting subject.

Diffusion of water within granular media is not only a subject of interest within the built environment. Within the pharmaceutical industry, powders and granular materials are of interest as well [Prescott and Barnum, 2000]. Pharmaceutical manufacturing is highly dependent on the behavior of granular materials, for example, the flow of powder and the compaction of the materials are of interest.

The diffusion of water can have numerous effects on a granular packing. Particles can be affected by the flow of water through the pores. These forces can be caused by the capillary force and retarding forces. Furthermore, a saturated packing has pore pressure due to the presence of water which can influence the stresses within the packing [Verruijt, 2001]. Due to the diffusion of water, a material or particle packing can start to expand. This can be due to the fact that particles can adsorb water and start to swell. This moisture expansion can result in damage in a material [Ruedrich et al., 2011]. Furthermore, a material that starts to swell while confined endures more stress due to an increase in strain.
1.1 Problem definition

In this thesis, the consequences of the diffusion of water into granular materials are evaluated. More specifically, particle swelling is studied. In order to find the influence of the diffusion of water into granular materials (and the swelling of particles), first, an understanding of the microstructure is needed. The packing should be evaluated and the mechanical properties should be determined. With this, the mechanical behavior of granular material can be modelled. With a correct model for the granular media, the influence of diffusion of water can be evaluated.

This results in the following research question: How does the swelling of individual particles influence the overall response of a granular microstructure and what is the interaction between the mechanical and the swelling response?

Together with the following sub-questions, the answer to this research question can be found:

- What is a suitable and efficient mechanical model for a particle packing?
- What is the influence of swelling on a granular packing?
- How can the influence of swelling be implemented into a mechanical model?

1.2 Theoretical importance

Granular materials are of great importance within the built environment, but also within other industries. Swelling due to moisture can cause a lot of damage in materials, especially in granular materials with their pore spaces. For granular materials, the microstructure influences the macroscopic mechanical behavior a lot. For this reason, the microscopic research into granular material is of interest. In the past, a lot of research was done on the microscopic behavior of granular materials. Most of the research was done on the use of Discrete Element Modelling (DEM) on granular materials. However, DEM is computationally highly expensive. Another approach, the Granular Micromechanics Approach (GMA), which is based on continuum mechanics can also be used to model granular materials. This approach is much less computationally expensive. However, the approach needs to be calibrated with experimental data. The fact that GMA is less computationally expensive and less research has been done in the past makes the research into the continuum approach more interesting. In this research, a correct material model will be developed to model the mechanical behavior of hydrogel particles.

The influence of the flow of water, diffusion of water and swelling has also been modelled in the past with Discrete Element Modelling (DEM), but within the continuum mechanics approach, this is a relatively new subject. With more research
into the use of continuum mechanics for the mechanical behavior of granular media, the modelling of granular media can eventually become much less computationally expensive. For this reason, this research is focused on the granular micromechanics approach.

1.3 Organization

In chapter 2, the theoretical investigation of the research will be discussed. The different methods and theories which are used in the research are explained and the literature is discussed. Chapter 3 discusses the activities that have led to the material mechanical model. Experimental data will be used and more data will be simulated in DEM. This data will be used for the calibration of the mechanical model in GMA. The found results are discussed and the calibration and validation of the model is discussed. Chapter 4 will look into the influence of water on a granular packing, more specifically the swelling of particles. Principles found in literature will be used and further explored to find a relationship between the microscopic swelling of a particle and the macroscopic swelling of packing. Chapter 5 will show the results of the swelling of particles on different particle packings. The relationship between the microscopic swelling of a particle and the macroscopic swelling of a packing, which was found in chapter 4, will be evaluated for different particle packings. The influence of the swelling on the mechanical behavior of a particle packing will be evaluated here as well. Chapter 6 will give a conclusion to the research and chapter 7 will be a recommendation for further research.
2 | Theoretical Investigations

2.1 Granular material

A granular packing is a system composed out of a large number of discrete particles. Granular materials are used in numerous different industries. There are a lot of different types of granular materials, for example, soils, powders and food. More specifically, sand, gravel, flour, medical powders, rice grains, coffee beans and more. Most of the research into the behavior of granular materials started after the pioneer work of Coulomb in 1773. After this, the research into granular materials kept growing, where also the research into soil mechanics originated. The research into granular materials and soil mechanics grew a lot during the past 20 years [Andreotti et al., 2013].

2.1.1 Grain geometry

Granular materials have a large range of grain sizes, where clays can have the size of 2 micrometre and coffee beans can have the size of 1 centimetre. Particles can also have different geometrical properties, ranging from perfectly smooth spherical shapes to irregular shapes with different aspect ratio’s. One of the important properties of granular materials is their particle size distribution (psd), which describes the frequency distribution of the sizes of the individual particles. This information is conveniently seen in grain size distribution diagrams, figure 2.1 shows an example of a grain size distribution diagram. The uniformity of the particles can be derived from the graph as well, with the use of the uniformity coefficient $C_u$:

$$C_u = \frac{D_{60}}{D_{10}}$$

(2.1)

where $D_{60}$ and $D_{10}$ can be found in the grain size distribution diagram. $D_{60}$ indicates the diameter where 60% of all particles are smaller than that diameter, this particle size can be found in the graph in figure 2.1, where the graph is 60% according to the vertical axis. $D_{10}$ indicates the diameter where 10% of all particles are smaller than that diameter, this value can also be found in the grain size distribution diagram. The slope of the diagram shows if the material is well-graded (flat slope) or poorly graded (steep slope) [Verruijt, 2001, Hicher, 1998].
2.1.2 Particle arrangement

The particle arrangement or settlement of a packing is also an important aspect. The same particle packings can have a different arrangement of particles. Figure 2.2a shows a very loose packing, where the particles are in a cubic array. The particles only have contacts in the orthogonal directions. Figure 2.2b shows a very dense packing, where the distribution of the particles is hexagonal. The cubic and hexagonal particle distribution are two examples of particle packings with spherical particles, where there are many more possible particle distributions.

Granular materials have pore spaces between the grains. The sizes and the amount of pore space can be determined by the porosity $n$ of a material:

$$n = \frac{V_p}{V_t} \quad (2.2)$$

where the pore volume is defined by $V_p$ and the total volume is defined by $V_t$. The amount of pores can also be expressed as the void ratio $e$:

$$e = \frac{V_p}{V_s} \quad (2.3)$$
where $V_s$ is the solid volume. The porosity and the void ratio can be related to each other by the following equation:

$$e = \frac{n}{1 - n}$$

(2.4)

### 2.1.3 Mechanical behavior

The mechanical behavior of granular material is depended on the properties of a particle packing (as discussed in the previous sections) and on the particle mechanical properties. The interaction between grains is what is most important in the calculation of the mechanics of granular materials. Granular systems are usually modelled with the use of continuum mechanics or with discrete particle mechanics [Gonzalez and Cuitiño, 2012]. For the continuum mechanics modelling, the material point can be assumed as a continuum body. With the use of homogenization techniques, the particles are generalized over the whole representative volume element (RVE). For the discrete models, the particles are assumed to be individual parts of a particle packing [Poorsolhjouy and Gonzalez, 2018].

### 2.2 Granular micromechanics approach (GMA)

Continuum mechanics is based on the assumption of the material being a continuum rather than discrete particles. The method allows the derivation of stress at a material point. In most analyses, the material is assumed homogeneous and isotropic. These three assumptions are independent of each other. A few pioneers of the continuum mechanics approach are Cauchy, Navier and Green who developed the method in the early nineteenth century [Malvern, 1969, Pilvin, 2019]. Continuum mechanics is essentially based on four fundamental principles: (I) The conservation of mass, (II) The law of balance of linear momentum, (III) the law of balance of angular momentum, and (IV) the law of balance of energy [Chandrasekharaiha and Debnath, 1994, Liu, 2002].

In standard continuum mechanics, the microstructure is not considered, however, the microstructure and the micro-mechanical properties have a large impact on the macroscopic material behavior of granular material. In the granular micromechanics approach (GMA), the interaction between grains in a collection of grains is modelled. With the grain interactions in all directions, the macroscopic stress and strain tensors can be created. The granular micromechanics approach needs experimental validation to be used. GMA is based on continuum mechanics.

The granular micromechanics approach can be used with a static constraint or a kinematic constraint. Figure 2.3 shows a schematic overview of both methods. The kinematic constraint will be discussed in section 2.2.1, the static constraint will be discussed in section 2.2.2. Both methods can be used for granular packings which are
either stress-controlled or strain-controlled. For small Poisson’s ratio’s \((-1 \leq \nu \leq \frac{1}{4})\) usually the kinematic approach is used, for larger Poisson’s ratio’s \((-\frac{1}{3} \leq \nu \leq \frac{1}{2})\) the static approach is usually used [Poorsolhjouy, 2016].

![Figure 2.3: Granular micromechanics approach [Poorsolhjouy, 2016]](image)

### 2.2.1 Kinematic approach

As mentioned before, the granular micromechanics approach is based on the interaction between grains in all directions. For this reason, the first step in the kinematic approach is to identify the kinematics of grains in the material point. The displacement between two neighbour grains can be found with the macroscopic strain on a representative volume element. This is also the assumption on which the kinematic approach is based. Two neighbour grains inside the material point can be considered, grains n and p, with position vectors \(x^n_i\) and \(x^p_i\), respectively. The displacement of grain p can be written using Taylor series expansion, of the displacement of grain n. The anti-symmetric part of the grain displacement field \(u^\alpha_{ij}\) between two grains does not contribute to energy and thus also does not contribute to stress, so the grain displacement field can be replaced by the strain \(\varepsilon_{ij}\). This results in the relative displacement of two grains in the following formula:

\[
\begin{align*}
    u^p_i &= u^n_i + u^i_{n,j}(x^p_j - x^n_j) \\
    \Rightarrow \delta^\alpha_i &= u^p_i - u^n_i = u^i_{n,j}(x^p_j - x^n_j) \\
    \Rightarrow \delta^\alpha_i &= \varepsilon_{n,j}^i(x^p_j - x^n_j) = \varepsilon_{n,j}^i l^n_j \\
    \delta^\alpha_i &= \varepsilon_{n,j}^i l^n_j = l^n \varepsilon_{n,j}^i n^\alpha_j
\end{align*}
\]  

(2.5)  

(2.6)

where \(\delta^\alpha_i\) is the relative displacement between the two particles of the \(\alpha^{th}\) contact of the grain and \(l^n_j\) is the vector connecting the two centroids of the particles of contact.
Figure 2.4: Two grains in contact with the unit vectors, the global Cartesian and spherical coordinate systems, where $\theta$ is the polar angle and $\phi$ is the azimuth angle $\alpha$. The vector $l_j^\alpha$ can be replaced by the unit vector $n_j^\alpha$ and the distance between the two particle centroids. In this formula, the inter-granular displacement vector between a grain-pair is derived as the projection of the strain tensor in the direction of the grain-pair interaction line and then scaled with the length of the interaction line. This assumption is generally known as the kinematic constraint. In this thesis, subscripts follow the convention of index notation, the summation of repeated indices is used unless otherwise is stated.

In order to define a force-displacement relation, three local unit vectors are defined for a grain-pair contact. Figure 2.4 shows the unit vectors. The first unit vector is in the direction between two particle centroids, this is called the normal unit vector $n_i$. The other two vectors $s_i$ and $t_i$ are two orthogonal unit vectors in the plane whose normal vector is $n_i$. To generalize the local coordinate system, the three unit vectors are used as follows:

\begin{align*}
n_i &= \langle \cos \theta, \sin \theta \cos \phi, \sin \theta \sin \phi \rangle \\
s_i &= \langle -\sin \theta, \cos \theta \cos \phi, \cos \theta \sin \phi \rangle \\
t_i &= \langle 0, -\sin \phi, \cos \phi \rangle
\end{align*}

where $\theta$ is the polar angle, which is the angle between the 1-axis and the vector connecting the two particle centroids and $\phi$ is the azimuth angle, which is the angle between the 2-axis and the projection of the vector connecting the two particle centroids on the 2-3 plane (see figure 2.4).

With these unit vectors, the relative displacement vector can be decomposed into three components in this local coordinate system as the dot product between the
displacement vector and the unit vectors in the three directions:

\[
\delta_n = \delta_i n_i \\
\delta_s = \delta_i s_i \\
\delta_t = \delta_i t_i
\] (2.8)

With these displacement vectors, the inter-granular force vector can be found for the local contacts in the local coordinate system, by calibrating the microscopic constitutive relationship between force and displacement.

\[
\begin{bmatrix}
  f_n \\
  f_s \\
  f_t
\end{bmatrix} =
\begin{bmatrix}
  k_n & 0 & 0 \\
  0 & k_s & 0 \\
  0 & 0 & k_t
\end{bmatrix}
\begin{bmatrix}
  \delta_n \\
  \delta_s \\
  \delta_t
\end{bmatrix}
\] (2.9)

where \( k_n, k_s \) and \( k_t \) represent the grain-pair stiffness in the directions of the unit vectors of the grain-pair contact. For further use of the force-displacement relationship, it is useful to translate them into the RVE coordinate system. For that the rotational tensor should be as follows:

\[
T = \begin{bmatrix}
  n_1 & s_1 & t_1 \\
  n_2 & s_2 & t_2 \\
  n_3 & s_3 & t_3
\end{bmatrix}
\] (2.10)

This results in the following inter-granular force-displacement relationship in the RVE coordinate system:

\[
f_i = K_{ij} \delta_j \\
K_{ij} = T_{ip} k_{pq} T_{jq}
\] (2.11)

where \( K_{ij} \) is the grain-pair stiffness in the global RVE coordinate system and \( k_{ij} \) is the grain pair stiffness defined in the local unit vectors.

The internal energy density \( W \) can be defined by the principle of virtual work (PVW) as the volume average of the energies of all grain-pair interactions:

\[
W = \frac{1}{V} \sum_{\alpha=1}^{N} W^\alpha (\delta^\alpha_j) 
\] (2.12)

where \( W^\alpha \) stands for the energy in the \( \alpha^{th} \) contact, with \( N \) being the total number of contacts. The internal energy density can be defined by the stress and the strain. The Cauchy stress is defined as the work conjugate of the symmetric part of the displacement gradient tensor:

\[
\sigma_{ij} = \frac{\partial W}{\partial \varepsilon_{ij}} = \frac{1}{V} \sum_{\alpha=1}^{N} \frac{\partial W^\alpha}{\partial \delta^\alpha_i} \frac{\partial \delta^\alpha_j}{\partial \varepsilon_{ij}}
\] (2.13)
The inter-granular force vector $f_i$ can be defined as follows:

$$f_i^\alpha = \frac{\partial W^{\alpha}}{\partial \delta^\alpha_i}$$  \hspace{1cm} (2.14)

Substitution equations 2.14 into the Cauchy stress function (equation 2.13) yields:

$$\sigma_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} f_k^{\alpha} l_i^{\alpha} \frac{\partial \varepsilon^{\alpha}_{kl}}{\partial \varepsilon_{ij}}$$  \hspace{1cm} (2.15)

The grain scale strain and the overall RVE strain are set equal. The Cauchy stress function can be simplified further:

$$\sigma_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} f_k^{\alpha} l_i^{\alpha} \frac{\partial \varepsilon^{\alpha}_{kl}}{\partial \varepsilon_{ij}} = \frac{1}{V} \sum_{\alpha=1}^{N} f_k^{\alpha} l_i^{\alpha} \delta_{ik} \delta_{jl} = \frac{1}{V} \sum_{\alpha=1}^{N} f_i^{\alpha} l_j^{\alpha}$$  \hspace{1cm} (2.16)

Now utilizing the force-displacement relationship for the grain-pairs (equation 2.11) and the kinematic assumption (equation 2.6) the following equation is found:

$$\sigma_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} f_i^{\alpha} l_j^{\alpha} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ik}^{\alpha} l_j^{\alpha} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ik}^{\alpha} l_j^{\alpha} \varepsilon_{kl}$$  \hspace{1cm} (2.17)

Since the strain tensor $\varepsilon_{kl}$ is constant for the RVE it can be taken out of the summation. This leads to the following equations:

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl}$$  \hspace{1cm} (2.18)

$$C_{ijkl} = \frac{1}{V} \sum_{\alpha=1}^{N} ((l_i^{\alpha})^2 n_j^{\alpha} n_j^{\alpha} K_{ik}^{\alpha})$$  \hspace{1cm} (2.19)

where the global stiffness tensor ($C_{ijkl}$) can be found. Equations 2.19 allows the derivation of the macroscopic stiffness tensor as a function of the particle stiffness and the particle sizes. However, as it is seen in the equation, the analysis requires a summation over all contacts. Within the granular micromechanics approach, we are interested in an approximate solution for the whole RVE system, based on the grain-pair interactions. For this purpose two parameters are used, the number density of grain-pair interactions ($\rho_c$) and the inter-granular contact directional density distribution function ($\xi$) [Chang and Misra, 1990]. To get the approximate solution, these parameters are used and the summation is changed to an integration over all directions [Poorsolhjouy, 2016]. This is done by rewriting equation 2.19 into the normal and tangential components for the grain-pair stiffness tensor.
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\[ C_{ijkl} = \frac{1}{V} \sum_{\alpha=1}^{N} \left( (l^\alpha)^2 K_n^\alpha n_i^\alpha n_k^\alpha n_l^\alpha + (l^\alpha)^2 K_s^\alpha s_i^\alpha s_k^\alpha n_l^\alpha n_j^\alpha + (l^\alpha)^2 K_t^\alpha t_i^\alpha t_k^\alpha n_l^\alpha n_j^\alpha \right) \] \hspace{1cm} (2.20)

where in this equation, the terms in the summation are products of the directions as in figure 2.4. The summation can be changed from a summation over the total number of contacts into a summation over all direction (\(\phi\) and \(\theta\)) followed by a summation over all contacts (\(\rho\)) in each given direction:

\[ C_{ijkl} = \frac{1}{V} \sum_{\theta} \sum_{\phi} \left[ \left( \sum_{\rho}^{N^\rho} (l^\rho)^2 K_n^\rho \right) n_i n_k n_l n_j + \left( \sum_{\rho}^{N^\rho} (l^\rho)^2 K_s^\rho \right) s_i s_k n_l n_j + \left( \sum_{\rho}^{N^\rho} (l^\rho)^2 K_t^\rho \right) t_i t_k n_l n_j \right] \] \hspace{1cm} (2.21)

where \(N^\rho(\theta, \phi)\) is the number of grain-pair contacts for a given solid angle. The total number of contacts (\(N\)) in the packing is defined as:

\[ N = \sum_{\theta} \sum_{\phi} N^\rho(\theta, \phi) \] \hspace{1cm} (2.22)

Considering, as an example, the first term in equation 2.21, it is clear that the directional density distribution of \(l^2 k_n\) can be defined as:

\[ \xi(\theta, \phi) = \frac{\sum_{\rho} (l^\rho)^2 K_n^\rho}{\sum_{\alpha} (l^\alpha)^2 K_n^\alpha} \] \hspace{1cm} (2.23)

which also guarantees that \(\sum_{\theta} \sum_{\phi} \xi = 1\), an essential property of a density distribution function. The average value of the term \(l^2 k_n\) is defined as:

\[ \overline{l^2 k_n} = \frac{\sum_{\alpha=1}^{N} (l^\alpha)^2 K_n^\alpha}{N} \] \hspace{1cm} (2.24)

where the total number of contacts (\(N\)) in the material point can be defined as follows:

\[ N = V \rho_c \] \hspace{1cm} (2.25)

where \(\rho_c\) is the number density of grain-pair interactions. Substituting equations 2.23 and 2.24 yields:

\[ \sum_{\rho} (l^\rho)^2 K_n^\rho = \xi(\theta, \phi) N \overline{l^2 k_n} \] \hspace{1cm} (2.26)

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where $\xi$ represent the directional distribution of contact size and stiffness coefficients and enables the analysis of materials with different levels of anisotropy. For isotropic materials, as the directional distribution of contact properties should be uniform, naturally $\xi$ reduces to a mere normalization coefficient equal to $\frac{1}{4}\pi$, which ensures that $\int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \xi(\theta, \phi) \sin \theta d\theta d\phi = 1$.

These steps can be done for the tangential terms in equation 2.21 as well and the average with the density distribution function can be filled in and equation 2.21 can be rewritten into an integration.

$$C_{ijkl} = l^2 \rho_c \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (K_{ik}n_j n_l) \xi \sin \theta d\phi d\theta$$  \hspace{1cm} (2.27)$$

$$\sigma_{ij} = l \rho_c \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} f_i(\theta, \phi)n_j(\theta, \phi)\xi(\theta, \phi) \sin \theta d\phi d\theta$$  \hspace{1cm} (2.28)$$

For the specific case of linear elastic materials, the integral in equation 2.27 can be solved analytically [Poorsolhjouy, 2016]. For isotropic materials, the Young’s Modulus ($E$) and the Poisson’s ratio ($\nu$) can be derived:

$$E = l^2 \rho_c k_n \frac{2k_n + 3k_s}{4k_n + k_s}$$  \hspace{1cm} (2.29)$$

$$\nu = \frac{k_n - k_s}{4k_n + k_s}$$  \hspace{1cm} (2.30)$$

From equation 2.30 it can be seen that for positive stiffness ($0 \leq k$) the Poisson’s ratio is $-1 \leq \nu \leq \frac{1}{4}$.

### 2.2.2 Static approach

Besides the kinematic approach as explained in section 2.2.1, GMA can also be formulated in the so called static approach. While the kinematic approach is based on the relation between the inter-particle relative displacement and the strain, the static approach is based on the assumption that there is a relation between the stress and the inter-particle force. This considers the kinematic constraint in a weak sense [Liao et al., 1997, Poorsolhjouy and Gonzalez, 2018, Poorsolhjouy, 2016]:

$$\varepsilon_{pq} = \arg \min_{\varepsilon_{pq} \in \nu^2} \sum_{\alpha=1}^{N} \left\| \delta_i^{\alpha} - \varepsilon_{ij} r_i^{\alpha} \right\| = \arg \min_{\varepsilon_{pq} \in \nu^2} \sum_{\alpha=1}^{N} r_i^{\alpha} r_i^{\alpha} = \arg \min_{\varepsilon_{pq} \in \nu^2} \sum_{\alpha=1}^{N} R$$  \hspace{1cm} (2.31)$$

In the static approach, strain is defined as a macroscopic parameter, which minimizes the total error ($R$) of the kinematic assumption (see equation 2.6). In this method,
the square of the residual difference \((r^\alpha_i)\) between the inter-particle displacement and the macroscopic strain tensor is minimized. To minimize this difference, the derivative of the error function with respect to the strain tensor is set equal to zero as follows [Misra and Poorsolhjouy, 2015, Liao et al., 2000]:

\[
\frac{\partial R}{\partial \varepsilon_{mn}} = \sum_{\alpha=1}^{N} 2r^\alpha_i \frac{\partial}{\partial \varepsilon_{mn}} (\delta^\alpha_i - \varepsilon_{ij} l^\alpha_j) = \sum_{\alpha=1}^{N} 2(\delta^\alpha_m - \varepsilon_{mp} l^\alpha_p) l^\alpha_n = 0 \tag{2.32}
\]

\[
\sum_{\alpha=1}^{N} \delta^\alpha_m l^\alpha_n = \varepsilon_{mp} \sum_{\alpha=1}^{N} l^\alpha_p l^\alpha_n \tag{2.33}
\]

This results in the following function for the macroscopic strain tensor:

\[
\varepsilon_{mp} = \frac{N^{-1}}{V} \sum_{\alpha=1}^{N} \delta^\alpha_m l^\alpha_n \tag{2.34}
\]

where the strain tensor is now a function of a second rank fabric tensor \(N_{ij}\) and the volume average of the relative displacement of contacts \(\alpha\) and the vector connecting the two particle centroids of contacts \(\alpha\). The total number of contacts is \(N\) and the second fabric tensor \(N_{ij}\) is as follows:

\[
N_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} l^\alpha_i l^\alpha_j \tag{2.35}
\]

The principle of virtual work can now be introduced as follows:

\[
\sigma_{ij} \varepsilon_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} f^\alpha_i \delta^\alpha_i \tag{2.36}
\]

Substituting the macroscopic strain (equation 2.34), which was found with the static assumption, into the principle of virtual work (equation 2.36), the static constraint is found as a function of the stress:

\[
f^\alpha_i = \sigma_{ij} N^{-1} q^\alpha_j = l_i \sigma_{ij} N^{-1} n^\alpha_q \tag{2.37}
\]

With the static constraint, the force can be decomposed into normal and tangential components with the use of the unit vectors. This is done in the same way as in the kinematic method for equation 2.8.

\[
f_n = f_i n_i \tag{2.38}
\]

\[
f_s = f_i s_i
\]

\[
f_t = f_i t_i
\]
The microscopic displacement function can now also be expressed as follows:

\[
\begin{align*}
\delta_n &= \begin{pmatrix} s_n & 0 & 0 \end{pmatrix} \begin{pmatrix} f_n \end{pmatrix} \\
\delta_s &= \begin{pmatrix} 0 & s_s & 0 \end{pmatrix} \begin{pmatrix} f_s \end{pmatrix} \\
\delta_t &= \begin{pmatrix} 0 & 0 & s_t \end{pmatrix} \begin{pmatrix} f_t \end{pmatrix}
\end{align*}
\]

(2.39)

The local compliance tensor components are related to the local stiffness tensor components as \( s_n^\alpha = 1/k_n^\alpha, \) \( s_s^\alpha = 1/k_s^\alpha \) and \( s_t^\alpha = 1/k_t^\alpha. \)

Just as in the kinematic method, the rotation tensor needs to be used to rewrite the displacement-force relationship into the RVE coordinate system for the local contact.

\[
\delta_i = S_{ij} f_j \\
S_{ij} = T_{ip} s_{pq} T_{jq}
\]

(2.40)

where \( S_{ij} \) is the grain-pair compliance in the global coordinate system and \( s_{ij} \) is the grain pair compliance defined in the local unit vectors. With the principle of virtual work (equation 2.36), the static constraint (equation 2.37), the macroscopic strain tensor (equation 2.34) and the displacement force relationship in the RVE coordinate system, the global compliance tensor can be derived:

\[
S_{ijkl} = \frac{N_{jr}^{-1} N_{ls}^{-1}}{V} \sum_{\alpha=1}^{N} (l^\alpha)^2 n_r^\alpha n_s^\alpha S_{ik}^\alpha
\]

(2.41)

Just as in the kinematic approach, the approximate solution is more interesting in GMA. For that reason, the compliance tensor and the strain tensor are rewritten into an integral form. The same can be done as in the kinematic method, where the values are averaged and the same number density of grain-pair interactions \( (\rho_c) \) and the same directional density distribution function \( (\xi) \) as was found in the kinematic method can be found. This results in the following compliance tensor and the strain tensor in integral form:

\[
S_{ijkl} = l^2 \rho_c N_{jr}^{-1} N_{ls}^{-1} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (S_{ik} n_r n_s) \xi \sin \theta d\phi d\theta
\]

(2.42)

\[
\varepsilon_{ij} = S_{ijkl} \sigma_{kl}
\]

(2.43)

For the specific case of linear elastic materials, the integral in equation 2.42 can be solved analytically. For isotropic materials, the Young’s Modulus \( (E) \) and the Poisson’s ratio \( (\nu) \) can be derived:

\[
E = \frac{5l^2 \rho_c K_n K_s}{3 \left( 2K_n + 3K_s \right)}
\]

(2.44)
\[ \nu = \frac{K_n - K_s}{2K_n + 3K_s} \]  

(2.45)

From equation 2.45 it can be seen that for positive stiffness \(0 \leq k\) the Poisson’s ratio is \(-\frac{1}{3} \leq \nu \leq \frac{1}{2}\).

### 2.3 Particle mechanics

The Particle mechanics approach can also be generally referred to as a branch of the Discrete Element Method (DEM). DEM is based on the computation of motion and effect of a large number of small particles, where every particle is considered individually. DEM was first introduced by Cundall and Strack [Cundall and Strack, 1979]. In the paper of Cundall and Strack, the Discrete Element Model is introduced as a numerical model capable of describing the mechanical behavior of assemblies of discs and spheres. Cundall originally developed this method to evaluate rock mechanics. This method was constantly improved by multiple researchers. In 1985 Cundall and Hart [Cundall and Hart, 1985] developed codes to perform DEM in three dimensions. The motion of every particle in DEM follows from Newton’s second law.

\[ \mathbf{F} = \mathbf{Ma} \]  

(2.46)

With Newton’s second law of motion, the particle motion is modelled and the interaction between particles can be found. DEM calculates the contact interaction between each individual particle with normal contact laws and tangential contact laws. For the normal contacts, usually, Hertz law is used [Gelnar and Zegzulka, 2019]. Hertz law, together with other models, will be explained further in section 2.3.2. Parameters such as particle size and material properties are input values for the models.

#### 2.3.1 Geometries

The first step in DEM is to determine the geometry of the particles and the intersections between particles. In the most simple form of DEM, spherical particles are used in 3D and disc particles in 2D. These particles are an oversimplification of reality. However, with changing the particle to a more complex geometry, the computational expense increases [Barreto and Leak, 2021].

#### 2.3.2 Contact model

The determination of the contact model is the most important part of the DEM analysis. The contact between two grains is evaluated as a normal contact relation and a tangential contact relation. Normal and tangential models are described
with the use of the Kelvin-Voigt model for viscoelasticity. This model consists of a 
Newtonian damper for a viscous materials and a Hookean elastic spring for an elastic 
material. Combined they can describe a viscoelastic material (see figure 2.5). With 
the use of the contact models, the force-displacement relations can be found. A few 
example’s of contact models will be described next.

![Figure 2.5: Normal and tangential contact model with a spring and a dashpot](image)

**Elastic contact model**

The most used normal contact model is based on Hertz theory. The contact force 
($F$) between two elastic spherical particles can be calculated with the use of normal 
displacement ($\gamma_n$) [Grohn et al., 2019].

$$F_{n}^{Hertz}(\gamma) = \frac{4}{3} E^* \sqrt{R^* \gamma_n^3}$$  \hspace{1cm} (2.47)

The normal displacement ($\gamma_n$) causes a contact radius between two particles of:

$$a = \sqrt{R^* \gamma_n}$$  \hspace{1cm} (2.48)

With the effective Young’s modulus ($E^*$) and the radius ($R^*$) defined as:

$$\frac{1}{E^*} = \frac{1 - \nu_1^2}{E_1} + \frac{1 - \nu_2^2}{E_2}$$  \hspace{1cm} (2.49)

$$\frac{1}{R^*} = \frac{1}{R_1} + \frac{1}{R_2}$$  \hspace{1cm} (2.50)

with the radius and Young’s modulus of the particles in contact.
Elastic-Plastic contact model

Besides elastic contact models, there are also elastic-plastic contact models. Thornton proposed a model which initially considers contacts in the same way as the Hertz model would, but Thornton extended the model after the yield limit is reached. Walton and Braun also developed a model for linear plastic-elastic behavior. In the model of Walton and Braun, the unloading slope is higher than the loading slope, which causes the elastic-plastic behavior. Besides the models of Thornton, and Walton and Braun, there are more elastic-plastic contact models [Rojek et al., 2019].

Visco-elastic contact model

Tsuiji developed a viscoelastic model by extending Hertz model with a damping term to account for the viscous effects [Grohn et al., 2019]. Kuwabara and Kono also extended Hertz’s theory for visco-elastic particles [Horabik and Molenda, 2016].

Nonlocal contact model

Generally, for small deformations and low relative densities, the contact behavior between two elastic particles is described by Hertz theory. Gonzalez and Cuitino (2012) developed a nonlocal formulation for the contacts that take the interplay of deformations due to multiple contacts into account. Figure 2.6 shows the difference between Hertz contact law and the nonlocal formulation.

![Figure 2.6: Two spheres in contact under a general configuration of multiple concentrated forces. Left: schematic of the loading configuration with all forces rotated about the z-axis and represented on the zr-plane. Middle: contact loading-conditions for Hertz theory. Right: contact loading-conditions for the nonlocal contact formulation proposed in this work [Gonzalez and Cuitino, 2012].](image)

By using the principle of superposition, the contributions of nonlocal deformations ($W_{P_k}$) induced by all other forces ($P_k$) on a particle are taken into account. The
following nonlocal displacement is then found:

\[ \gamma_{NL} = \sum_{k=1,2} \sum_{i=1}^{N_{P_k}} W_{P_k} \]  

(2.51)

By taking into account the nonlocal contacts as in figure 2.6, the Hertz formula (equation 2.47) is adapted to the following equation:

\[ F_{NL}(\gamma) = \frac{4}{3} E^{*} \sqrt{R^{*}} (\gamma_{n} + \gamma_{NL})^{3/2} \]  

(2.52)

where the contribution of the nonlocal forces is taken into account by \( \gamma_{NL} \) [Gonzalez and Cuitiño, 2012].

**Tangential contact model**

Mindlin (1949) and Mindlin-Deresiewicz (1953) developed the basis of the most important tangential contact models. The tangential contact force is a function dependent on the tangential displacement (\( \gamma_{t} \)) and the normal displacement (\( \gamma_{n} \)):

\[ F_{t}^{Mindlin}(\gamma_{t}) = -K_{t}\gamma_{t} \]  

(2.53)

\[ K_{t}^{Mindlin} = 8G^{*}\sqrt{R^{*}}\gamma_{n}^{3/2} \]  

(2.54)

with \( G^{*} \) being the effective shear modulus.

\[ \frac{1}{G^{*}} = \frac{2 - \nu_{1}}{G_{1}} + \frac{2 - \nu_{2}}{G_{2}} \]  

(2.55)

The tangential contact model of Mindlin and Deresiewicz (Equation 2.53) is usually used in combination with the hertz normal contact model [Horabik and Molenda, 2016, Di Renzo and Paolo Di Maio, 2005]. Multiple variations on this model have been developed ever since the publication in 1949 and 1953.

**2.4 Experimental data**

Bares, Brodu, Zheng and Dijksman released their experimental data on hydrogel particle packings in 2019. Figure 2.7 shows a typical experimental setup. For these experiments, the tank is filled with hydrogel particles. The particles are almost incompressible, which results in a Poisson’s ratio of \( \nu \approx 0.5 \) for the particles. The estimated friction coefficient of the hydrogel particles is \( \mu \approx 0.03 \). The Young’s modulus of the hydrogel particles is \( E \approx 23 \) kPa [Brodu et al., 2015]. The hydrogel particles have been saturated with a fluorescent dye and are surrounded by a solution of water and polyvinylpyrrolidone (PVP). In this setup, a camera is held by a stage.
The camera is equipped with a red filter and a laser which creates a red light sheet. This camera scans the beads which are loaded by three plates that can move in three orthogonal directions.

Figure 2.7: Schematic view of the experimental set-up [Barés et al., 2019]

The beads are mechanically loaded by the three different moving plates. Figure 2.8 shows the four different types of experiments that were done. The four different types of experiments are explained in the following sections.

Figure 2.8: Experimental loading [Barés et al., 2019]
2.4.1 Uniaxial Compression

A packing of 514 mono-disperse hydrogel particles are vertically compressed, while confined in the other directions (figure 2.8a). The hydrogel particles have a mean diameter of 2.1 cm. The base plate of this packing is 16.5 × 16.5 cm and the uncompressed height is 15 cm [Brochu et al., 2015]. The compression test exists of 10 and 20 cycles of loading. Each loading cycle consists of 60 steps, which include loading and unloading. In each step, the plate moves 1 mm with a total strain of 13.4%. Besides the compression test on mono-disperse hydrogel particles, also a compression test was performed on a packing of bi-disperse hydrogel particles. A bi-disperse packing of 1573 particles with a mean diameter of 1.16 cm and 348 particles with a mean diameter of 2.1 cm is compressed in 60 steps of 0.5 mm with a maximum strain of 10.2%. The particles with a mean diameter of 2.1 cm are the same particles as for the mono-disperse compression experiments.

2.4.2 Intrusion

In a packing of 823 mono-disperse hydrogel particles (with a mean diameter of 2.1 cm), one hydrogel sphere with a diameter of 6.3 cm is pushed back and forth into the packing (fig. 2.8b). The large sphere is pushed up and down in the packing for 20 cycles. Each loading cycle consists of 60 steps, which include loading and unloading. In each step, the sphere moves 1 mm, with a total displacement of 3 cm.

2.4.3 2D shear

In the biaxial shear experiment (fig. 2.8c) a packing of 757 mono-disperse particles is compressed in one horizontal direction, while expanded in the orthogonal direction for 20 cycles. The loading walls move 0.5 mm in each step, with a total of 20 steps in each cycle for loading and unloading. The orthogonal plate moves in such a way that the total volume stays constant. The mean diameter of the particles is 2.1 cm.

2.4.4 3D shear

In the triaxial shear experiment (fig. 2.8d) a packing of 882 mono-disperse particles is compressed in one horizontal direction, while expanded in the two orthogonal directions for 25 cycles. The loading walls move 0.5 mm in each step, with a total of 34 steps in each cycle for loading and unloading. The orthogonal plates move in such a way that the total volume stays constant. The mean diameter of the particles is 2.1 cm.


2.5 Moisture expansion

The swelling of particles can occur in multiple different circumstances. A well-known cause of swelling and shrinkage is temperature change. Besides thermal expansion, a material can also expand due to moisture. A particle packing that is fully saturated can start to swell, but a material can also swell during diffusion or flow of water. Furthermore, a material can swell also due to a change in relative humidity of the air. Swelling and shrinkage due to a change in temperature is a well-known principle and much research has been done into thermal expansion. This is much less for moisture expansion, while the moisture expansion of a material can be in the same order or even larger than the deformation caused by temperature change [Teverovsky, 2002]. The condition in which moisture expansion occurs can be categorised into two categories. Swelling due to the contact with immersed water is called hydric-swelling, while the swelling caused by a change in relative humidity is called hygric-swelling. Moisture expansion includes both hydric- and hygric-swelling [Sovják et al., 2015, Ruedrich et al., 2011].

The rate of swelling of a material due to moisture can be defined by the hygroscopic expansion coefficient. The hygroscopic expansion coefficient ($\beta$) in one direction can be expressed as follows:

$$\beta = \frac{\Delta L}{L} / \Delta M$$

(2.56)

where $\Delta L$ and $L$ are the change in length and the original length and $\Delta M$ is the change in moisture content [Poenninger and Defoort, 2003, Toman and Cerný, 1996, Lin et al., 2020]. These values should be experimentally determined for a certain material. Both $\frac{\Delta L}{L}$ and $\Delta M$ have the unit of %, which makes the hygroscopic expansion coefficient unitless. The hygroscopic strain can be expressed as [Bosco et al., 2015, Perez et al., 2012]:

$$\varepsilon^{\Delta M}_{ij} = \beta_{ij} \Delta M$$

(2.57)

If the material is isotropic, the hygroscopic expansion coefficient should be identical in all directions. Furthermore, the off-diagonal components should be zero. This results in the following relationship for the hygroscopic expansion for isotropic materials:

$$\beta_{ij} = \beta_{\delta ij}$$

(2.58)

The mechanical behavior of a material that starts to swell can be described by the total strain ($\varepsilon^{tot}_{ij}$), the elastic strain ($\varepsilon^{el}_{ij}$) and the hygroscopic strain ($\varepsilon^{\Delta M}_{ij}$).

$$\varepsilon^{tot}_{ij} = \varepsilon^{el}_{ij} + \varepsilon^{\Delta M}_{ij}$$

(2.59)
The stress in a particle packing is induced by the elastic strain ($\varepsilon^{el}$) and can be calculated as follows [Bosco et al., 2015, Perez et al., 2012, Lin et al., 2020]:

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl}$$  \hspace{1cm} (2.60)

$$\sigma_{ij} = C_{ijkl} (\varepsilon^{tot}_{kl} - \varepsilon^{\Delta M}_{kl})$$
3 | Mechanical model

In order to model the swelling of particles in a granular material and to evaluate the effects on the granular material behavior, first an accurate model for the material behavior of a granular structure needed to be evaluated. As was mentioned in Chapter 2, granular systems are usually modelled with the use of continuum mechanics (section 2.2) or with particle mechanics (section 2.3).

The continuum mechanics approach can only be used after several experimental calibrations, which is not the case for the Particle Mechanics approach. However, the Particle Mechanics approach is computationally much more expensive than the approach which is based on continuum mechanics [Gonzalez and Cuitiño, 2012]. As mentioned before, this research focuses on the granular micromechanics approach.

Experimental results were needed to find the correct normal force-displacement and tangential force-displacement relationship in the Granular Micromechanics Approach. At least two different experimental tests with the same packing were needed to derive the two functions. A third experiment could then be used to verify if the model works correctly. The experiments needed to be different in their loading type. Unfortunately, the experiments which were done by Barés et al. (2019) all had different packings for different loading types. For this reason, DEM was used to generate more results for the same packing as the compression test of the experiments. The packing of the experimental data of Barés et al. (2019) could be used in DEM. Different load paths could then be implemented on the packing to get multiple stress-strain relationships for the calibration and validation in GMA.

3.1 Granular Micromechanics Approach

First, an appropriate and suitable mechanical model needs to be developed. For this, the Granular Micromechanics Approach is used. The mechanical model in GMA should be strain-controlled. Chapter 2.2 gave the derivation of the method. The calculation of the stress due to the imposed strain will be explained further in this section. The calculations can then be done in Matlab with the kinematic or static constraint, depending on the Poisson’s ratio of the packing.
3.1.1 Kinematic approach

The relative displacement caused by the imposed strain at a certain increment can be calculated with:

\[ \delta^\alpha_i = \varepsilon_{ij} l^\alpha_j = l^\alpha \varepsilon_{ij} n^\alpha_j \] (3.1)

where \( l \) is the distance between two particle centroids and \( n \) is the unit vector connecting the centres of the two particles in contact. In order to find the normal and tangential relative displacements between the particles, the relative displacements should be translated to the microscopic inter-granular contact coordinates \( n, s \) and \( t \).

\[ \delta_n = \delta_i n_i \] (3.2)
\[ \delta_s = \delta_i s_i \]
\[ \delta_t = \delta_i t_i \]

Instead of using both tangential direction \( s \) and \( t \), one tangential relative displacement can be used \( \delta_w = \sqrt{\delta_s^2 + \delta_t^2} \). With the relative displacements between particles in the normal and the tangential direction, the force between particles in normal and tangential direction can be found with the use of correct force-displacement relationships. These force-displacement relationships depend on the type of granular material which is evaluated and need to be calibrated with that material.

\[ \begin{bmatrix} f_n \\ f_w \end{bmatrix} = \begin{bmatrix} k_n & 0 \\ 0 & k_w \end{bmatrix} \begin{bmatrix} \delta_n \\ \delta_w \end{bmatrix} \] (3.3)

With the force-displacement relationships, the stiffness in both normal and tangential directions can be found, as the derivative of the force-displacement relationship. With the use of the rotational tensor, the interparticle stiffness can be rewritten to the RVE direction.

\[ f_i = K_{ij} \delta_j \] (3.4)
\[ K_{ij} = T_{ip} k_{pq} T_{jq} \]

The inter-particle stiffness in RVE direction can then be used to calculate the global stiffness tensor \( C_{ijkl} \).

\[ C_{ijkl} = \frac{1}{V} \sum_{\alpha=1}^{N} \left( (l^\alpha)^2 n^\alpha_i n^\alpha_j K_{ik} \right) \] (3.5)

This stiffness tensor can be changed into an integration for the approximate calculation:

\[ C_{ijkl} = l^2 \rho_c \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (K_{ik} n_j n_l) \xi \sin \theta d\phi d\theta \] (3.6)
With the stiffness tensor for a certain strain increment, the stress increment can be calculated:

\[ d\sigma_{ij} = C_{ijkl}d\varepsilon_{kl} \tag{3.7} \]

With the stress of the previous increment and the incremental increase of the stress, the new stress can be found. The Matlab script which is used for this calculation can be found in appendix A.

### 3.1.2 Static approach

The force between two particles in the RVE coordinate system can be calculated with the use of the stress of the previous increment:

\[ f_i = \sigma_{ij}N^{-1}_{jq}l_q = l\sigma_{ij}N^{-1}_{jq}n_q \tag{3.8} \]

where \( l \) is the distance between two particle centroids, \( n \) is the unit vector connecting the centres of two particles and \( N_{jq} \) is the fabric tensor. In order to find the normal and tangential forces between the particles, the forces should be translated to the microscopic intergranular contact coordinates \( n, s \) and \( t \).

\[ f_n = f_in_i \tag{3.9} \]
\[ f_s = f_is_i \]
\[ f_t = f_it_i \]

Instead of using both tangential direction \( s \) and \( t \), one tangential force can be used \( f_w = \sqrt{f_s^2 + f_t^2} \). With the force between particles in the normal and the tangential direction, the relative displacements between particles in normal and tangential direction can be found with the use of correct displacement-force relationships. These force-displacement relationships depend on the type of granular material which is evaluated and need to be calibrated with that material.

\[ \begin{bmatrix} \delta_n \\ \delta_w \end{bmatrix} = \begin{bmatrix} s_n & 0 \\ 0 & s_w \end{bmatrix} \begin{bmatrix} f_n \\ f_w \end{bmatrix} \tag{3.10} \]

With the displacement-force relationships, the compliance in both normal and tangential direction can be found, as the derivative of the displacement-force relationship. With the use of the rotational tensor, the interparticle compliance can be rewritten to the RVE direction.

\[ \delta_i = S_{ij}f_j \tag{3.11} \]
\[ S_{ij} = T_{ip}s_{pq}T_{jq} \]
The inter-particle compliance tensor in the RVE direction can then be used to calculate the global compliance tensor $S_{ijkl}$.

$$S_{ijkl} = \frac{N_{jr}^{-1} N_{ls}^{-1}}{V} \sum_{\alpha=1}^{N} ((l^n)\alpha n_r \alpha n_s \alpha S_{ik})$$  \hspace{1cm} (3.12)

This compliance tensor can be changed into an integration for the approximate calculation:

$$S_{ijkl} = l^2 \rho_c N_{jr}^{-1} N_{ls}^{-1} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (S_{ik} n_r n_s) \xi \sin \theta d\phi d\theta$$  \hspace{1cm} (3.13)

With the compliance tensor known for a strain increment, the stress increment can be calculated as follows:

$$d\sigma_{ij} = S_{ijkl}^{-1} d\varepsilon_{kl}$$  \hspace{1cm} (3.14)

With the stress of the previous increment and the incremental increase of the stress, the new stress can be found. This stress is then used for the calculation of the next increment. The Matlab script which is used for this calculation can be found in appendix B.

### 3.2 Experimental data

As explained before, the GMA mechanical model needs to be calibrated with experimental data. For this reason, the model is specifically calibrated with a certain material. The model is specifically made for hydrogel particles, which were experimentally tested [Barés et al., 2019]. More specifically, the mono-disperse packing of 514 hydrogel particles (section 2.4.1) was evaluated. The particle distribution of the experiment is shown in figure 3.1. The first loading cycle of the experiment with 10 cycles is used, one cycle consists of 30 loading steps and 30 unloading steps. The particles have a mean diameter of 2.1 cm. The particles have a Poisson’s ratio of 0.5 and an E-modulus of 23 kPa.

![Figure 3.1: Experimental Packing [Barés et al., 2019]](image)
3.2.1 Results

A stress-strain figure can be plotted with the experimental data of Barés et al. (2019). In figure 3.2 the first loading cycle of the compression experiment with 10 cycles is plotted. One loading has 30 loading steps, however, stress does not start to increase at the first loading step, due to the settlement of the particles. The figure starts with the loading step where stress starts to increase. The stress due to gravity is neglected in this figure.

![Stress-strain curve](image)

Figure 3.2: Stress-strain curve for the first loading cycle, of the experimental data of uniaxial compression with 10 loading cycles

3.2.2 Poisson’s ratio

For the Granular Micromechanics Approach, the correct constraint has to be determined. This is done by determining the Poisson’s ratio of the packing. For small Poisson’s ratio’s ($-1 \leq \nu \leq \frac{1}{3}$) the kinematic method should be used, for larger Poisson’s ratio’s ($-\frac{1}{3} \leq \nu \leq \frac{1}{2}$) the static method should be used [Poorsolhjouy, 2016]. The Poisson’s ratio of the hydrogel packing can be calculated with the use of Hooke’s law.

\[
\begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{23} \\
\sigma_{13} \\
\sigma_{12}
\end{bmatrix} = \frac{E}{(1 + \nu)(1 - 2\nu)} \begin{bmatrix}
1 - \nu & \nu & \nu & 0 & 0 & 0 \\
\nu & 1 - \nu & \nu & 0 & 0 & 0 \\
\nu & \nu & 1 - \nu & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1 - 2\nu}{2} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1 - 2\nu}{2} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1 - 2\nu}{2}
\end{bmatrix} \begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33} \\
\varepsilon_{23} \\
\varepsilon_{13} \\
\varepsilon_{12}
\end{bmatrix},
\] (3.15)
In the case of the Uniaxial compression experiment, only $\varepsilon_{11} \neq 0$, the other directions have no strain.

$$\sigma_{11} = \frac{E(1 - \nu)}{(1 + \nu)(1 - 2\nu)}\varepsilon_{11}$$ (3.16)

$$\sigma_{22} = \frac{E\nu}{(1 + \nu)(1 - 2\nu)}\varepsilon_{11}$$ (3.17)

This results in the following equation for the Poisson’s ratio:

$$\frac{\sigma_{11}(1 + \nu)(1 - 2\nu)}{E(1 - \nu)} = \frac{\sigma_{22}(1 + \nu)(1 - 2\nu)}{E\nu}$$ (3.18)

$$\nu = \frac{\sigma_{22}}{\sigma_{22} + \sigma_{11}}$$ (3.19)

The Poisson’s ratio of the hydrogel packing of 514 mono-disperse particles is about 0.41.

### 3.2.3 E-modulus

The E modulus of a particle packing can also be calculated with the use of Hooke’s law (equation 3.15). Also with assuming that only $\varepsilon_{11} \neq 0$ and the rest of the strains are zero. The following equation can be found when for a certain strain increment:

$$d\sigma_{11} = \frac{E(1 - \nu)}{(1 + \nu)(1 - 2\nu)}d\varepsilon_{11}$$ (3.20)

$$E = \frac{d\sigma_{11}(1 + \nu)(1 - 2\nu)}{d\varepsilon_{11}} \frac{1}{1 - \nu}$$ (3.21)

The material, however, does not show a linear relationship between stress and strain. For this reason, the E-modulus can not be found for the whole material relationship, it can only be found for certain stages of the compression experiment, which results in the tangent modulus. The tangent modulus between each loading increment in the uniaxial compression experiment (figure 3.2) can be calculated.

### 3.3 Particle mechanics

The data from the compression test with a packing of 514 hydrogel particles (figure 3.1) was used in DEM. The experimental data [Barès et al., 2019] has the coordinates of the particles and the radius of these particles. These were scanned with the laser and camera methods in each step. Besides the particle data, also the wall locations and directions are known for each step. However, only the initial locations ($\varepsilon = 0$) are needed. With these locations, the boundary conditions and the particle properties,
the experiment can be generated in DEM. The Hertz contact model and the nonlocal contact model are used. For both, they are assumed frictionless.

First, the uniaxial compression experiment which was done by Barès et al. (2019) was simulated to verify the DEM results. The normal force-displacement relationship for GMA can be easily found by using a hydrostatic loading on the packing, since only normal forces occur in the packing under hydrostatic loading. The hydrostatic loading is modelled with the use of the particle and wall data of the Uniaxial Compression experiment [Barès et al., 2019]. With the use of hydrostatic loading, the normal force-displacement relationship can be derived. With the use of the Uniaxial Compression test, the tangential force-displacement relationship can then be found. To verify the force-displacement functions, a third loading type can be modelled in DEM. For this, a Biaxial compression test is simulated.

### 3.3.1 Uniaxial compression

In order to compare the particle mechanics method with the experimental data, the compression experiment is modelled with the particle mechanics method. Figure 3.3 shows the results of the uniaxial compression experiment and the particle mechanics (DEM) simulation together. Figure 3.3a shows the stresses in the direction of the loading and figure 3.3b shows the stresses in the directions perpendicular to the loading direction.

The particle mechanics simulation is done for the Hertz contact formulation and for the non-local contact formulation. It can be seen in figure 3.3 that the non-local contact formulation gives a more accurate result when compared to the experimental result. Both contact models still give a difference with the experimental results. This difference can be due to the fact that the particles are assumed to be frictionless. Since the non-local results were more accurate, only the non-local contact formulation is used for the next simulations. The difference between the particle mechanics simulation and the experimental results is neglected, since the goal of this research is not to get a perfect DEM simulation, but to find a representative mechanical model in GMA.

**Poisson’s ratio and E-modulus**

For the discrete element method, the Poisson’s ratio and E-modulus can also be calculated for the particle packing. This differs a bit from the experimental found results, since there was a difference in the stress-strain relationship. For the calculation of the E-modulus and the Poisson’s ratio, again equations 3.21 and 3.19 can be used, respectively. The Poisson’s ratio of the packing which is found for the particle mechanics simulation is 0.40. Again the tangent modulus can be found between each loading increment.
Figure 3.3: Stress-strain curve for the particle mechanics and the experimental results for uniaxial compression

(a) Stress and strain both in the direction of the loading

(b) Strain in the directions of the loading, stress perpendicular to the loading
3.3.2 Hydrostatic compression

As explained before, a hydrostatic compression simulation is modelled in particle mechanics. This is done again with the same particle packing of the 514 monodisperse hydrogel particles. The nonlocal contact model is used and the material is assumed frictionless. The particle packing is compressed until the same relative density is reached as in the uniaxial compression simulation in DEM ($\rho = 0.7$).

The particle mechanics simulation of the hydrostatic loading can be found in figure 3.4. The strain in all three directions is equal, the stress in the three directions is almost the same. Figure 3.4 shows three graphs which are about the same. The small difference in stress in the three directions can be explained by the different particle distributions in the different directions.

![Hydrostatic compression](image)

**Figure 3.4**: Stress-strain curve for the particle mechanics hydrostatic compression

3.3.3 Biaxial compression

As mentioned before, a third loading type can then be used for the validation of the mechanical model. For this, biaxial compression is used. Biaxial compression can be done in multiple different ways. For this research it was done twice, to see the influence of a different loading in the two directions. So first, a biaxial compression loading is simulated where $\varepsilon_x = \varepsilon_y$. Then a biaxial compression loading is simulated where $2 \varepsilon_x = \varepsilon_y$. For these, again the experimental particle packing of 514 monodisperse hydrogel particles is used in DEM and the packing is again compressed until a relative density of $\rho = 0.7$. The nonlocal contact model is used and the material is assumed frictionless.
Biaxial compression $\varepsilon_x = \varepsilon_y$

A biaxial compression loading, where $\varepsilon_x = \varepsilon_y$, is modelled in DEM. Figure 3.5a shows the stress in plane x to the strain of plane x and the stress in plane y to the strain of plane y. Figure 3.5b shows the stress in plane z to the strain of plane x and plane y. In figure 3.5b, only one graph is visible, this is due to the fact that they are exactly the same, which is what is expected of this graph, since $\varepsilon_x = \varepsilon_y$.

![Biaxial compression x-y](image1)

(a) Stress and strain both in the direction of the loading

![Biaxial compression x=y](image2)

(b) Strain in the directions of the loading, stress perpendicular to the loading

Figure 3.5: Stress-strain curve for the particle mechanics Biaxial compression for $\varepsilon_x = \varepsilon_y$
**Biaxial compression** $2\varepsilon_x = \varepsilon_y$

The same thing can be done with different loadings in the two loading directions. The strain in the y-direction is twice the strain in the x-direction. Figure 3.6a shows the stress in plane x to the strain of plane x and the stress in plane y to the strain of plane y. Figure 3.6b shows the stress in plane z to the strain of plane x and plane y.

![Biaxial compression x and y](image)

(a) Stress and strain both in the direction of the loading

![Biaxial compression x and y](image)

(b) Strain in the directions of the loading, stress perpendicular to the loading

Figure 3.6: Stress-strain curve for the particle mechanics Biaxial compression for $2\varepsilon_x = \varepsilon_y$
3.4 Calibration in the Granular micromechanics approach

With a Poisson’s ratio of 0.41, the static constraint of the Granular Micromechanics Approach should be used, to have positive grain-pair stiffnesses. For the static constraint in the Granular Micromechanics Approach, a correct microscopic constitutive relationship or displacement-force relationship should be found. This relationship can then be rewritten into a force-displacement relationship.

3.4.1 Normal force-displacement relationship

As explained before, a hydrostatic loading only results in normal forces between particles. For this reason, only the normal force-displacement relationship has an effect on this loading type. The normal force-displacement relationship can thus be adapted until the most perfect fit between the GMA and DEM graphs is found. The DEM results which were shown in figure 3.4 are used for this fitting. The average of the three curves is used.

The stress-strain relationships shows an exponential relationship, where with a linear increasing strain, the stress increases exponentially, as could be seen in figure 3.4. For this reason, the force-displacement relationship is assumed exponential as well. This means that in the static method, the displacement-force relationship should be a root function, with an unknown coefficient ($C_n$) and a power ($p_n$):

$$\delta_n = \frac{1}{C_n} (f_n)^{1/p_n} \quad (3.22)$$

The standard error of estimation ($S_{est}$) and the $R^2$-value can be used to find the best fit for the normal force-displacement relationship for the hydrostatic compression simulation in DEM:

$$S_{est} = \sqrt{\frac{\sum (y - y_{est})^2}{N - 2}} \quad (3.23)$$

$$R^2 = \frac{\sum (y - y_{mean})^2 - \sum (y - y_{est})^2}{\sum (y - y_{mean})^2} \quad (3.24)$$

where $y_{est}$ is the modelled value (GMA) which is calibrated with the data $y$ (DEM), where the amount of data points is $N$ and $y_{mean}$ is the average of the data sets. With the use of equation 3.22 and equations 3.23 and 3.24, the standard error of estimation and the $R^2$-value can be evaluated for multiple combinations of $C_n$ and $p_n$. The results for this can be found in figures 3.7 and 3.8. It can be seen that the $R^2$ has the best results for a diagonal region over the graphs. The red dot in this diagonal region gives the best found combination for $C_n$ and $p_n$. For some powers in
this diagonal region, the best found coefficient is shown in table 3.1. The $R^2$-value for the combination of those powers and coefficients can be found in this table as well.

Figure 3.7: Standard error of estimation for combinations of $C_n$ and $p_n$

Figure 3.8: $R^2$-values for combinations of $C_n$ and $p_n$
Table 3.1: Best $R^2$-values for each power for the normal force-displacement relationship

<table>
<thead>
<tr>
<th>$p_n$</th>
<th>$C_n$</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>100</td>
<td>0.648267</td>
</tr>
<tr>
<td>1.05</td>
<td>100</td>
<td>0.862605</td>
</tr>
<tr>
<td>1.1</td>
<td>100</td>
<td>0.945881</td>
</tr>
<tr>
<td>1.15</td>
<td>109</td>
<td>0.958377</td>
</tr>
<tr>
<td>1.2</td>
<td>120</td>
<td>0.966865</td>
</tr>
<tr>
<td>1.25</td>
<td>132</td>
<td>0.974145</td>
</tr>
<tr>
<td>1.3</td>
<td>144</td>
<td>0.980296</td>
</tr>
<tr>
<td>1.35</td>
<td>156</td>
<td>0.985406</td>
</tr>
<tr>
<td>1.4</td>
<td>168</td>
<td>0.989545</td>
</tr>
<tr>
<td>1.45</td>
<td>180</td>
<td>0.992769</td>
</tr>
<tr>
<td>1.5</td>
<td>191</td>
<td>0.995219</td>
</tr>
<tr>
<td>1.55</td>
<td>203</td>
<td>0.996851</td>
</tr>
<tr>
<td>1.6</td>
<td>214</td>
<td>0.997776</td>
</tr>
<tr>
<td>1.65</td>
<td>225</td>
<td>0.998002</td>
</tr>
<tr>
<td>1.7</td>
<td>236</td>
<td>0.997611</td>
</tr>
<tr>
<td>1.75</td>
<td>247</td>
<td>0.99665</td>
</tr>
<tr>
<td>1.8</td>
<td>258</td>
<td>0.99514</td>
</tr>
<tr>
<td>1.85</td>
<td>268</td>
<td>0.993098</td>
</tr>
<tr>
<td>1.9</td>
<td>279</td>
<td>0.990605</td>
</tr>
<tr>
<td>1.95</td>
<td>289</td>
<td>0.987672</td>
</tr>
<tr>
<td>2</td>
<td>299</td>
<td>0.984312</td>
</tr>
</tbody>
</table>

The best fit is found for a power of 1.65 with a coefficient of 225. This has a $R^2$-value of 0.998, which is a quite accurate estimation. This gives the following force-displacement relationship:

$$\delta_n = \frac{1}{225} (f_n)^{1.65}$$  \hspace{1cm} (3.25) \\
$$f_n = 7605(\delta_n)^{1.65}$$

Figure 3.9 shows the stress-strain graphs of the GMA simulation for this normal force-displacement relationship and the DEM simulation of the hydrostatic compression. The standard error of estimation between the GMA and the DEM simulation is 4.62 and the $R^2$-value is 0.998. This is a really good $R^2$-value, since a $R^2$-value of 1 means that it is a perfect fit. It shows that the fitting between DEM and GMA is good.
Figure 3.9: Stress-strain curve for the calibration between particle mechanics simulation and GMA calculation of hydrostatic compression
3.4.2 Tangential force-displacement relationship

With the normal force-displacement relationship known, another type of loading is needed to find the tangential force-displacement relationship. This can be done with the uniaxial compression simulation in DEM (see figure 3.3). Now only the tangential force-displacement relationship should be adapted to find the most perfect fit between the GMA simulation of stress and strain and the DEM simulation. For the tangential force-displacement relationship, also an exponential relationship is assumed. In this relationship, also a linear relationship is evaluated, when the power is equal to one.

\[ \delta_w = \frac{1}{C_w (f_w)^{1/p_w}} \]  \hspace{1cm} (3.26)

The standard error of estimation (equation 3.23) and the \( R^2 \)-value (equation 3.24) can be used for the tangential force-displacement relationship as well. With the use of equation 3.26, the standard error of estimation and the \( R^2 \)-value can be evaluated for multiple combinations of \( C_w \) and \( p_w \). This evaluation is done in the three directions (x, y and z) combined. The result for this can be found in figures 3.10 and 3.11. It can be seen that the \( R^2 \) and the standard error of estimation have the best result for a diagonal region over the graphs. The red dot in this diagonal region gives the best found combination for \( C_w \) and \( p_w \).

The best fit is found for the following tangential force-displacement relationship:

\[ \delta_w = \frac{1}{35 (f_w)^{1/\alpha}} \]  \hspace{1cm} (3.27)
\[ f_w = 207 (\delta_w)^{1.5} \]

Figure 3.12a shows the stress-strain graphs in the direction of the loading of the GMA simulation and the DEM simulation of the uniaxial compression. The standard error of estimation and the \( R^2 \)-value between the GMA and the DEM simulation can be calculated for the stress-strain results in the direction of the loading and result in 9.60 and is 0.979 respectively. Figure 3.12b shows the stress-strain graphs in the directions perpendicular to the loading. The average of the two DEM graphs is used. The standard error of estimation and the \( R^2 \)-value between the GMA and the DEM simulation can be calculated for the stress-strain results in the direction perpendicular to the loading and result in 11.44 and 0.943 respectively.

It can be seen in both the figures and the \( R^2 \)-value that the fitting in the direction of the loading is better than the fitting in the direction perpendicular to the loading. However, both estimations are quite well, since they fit both for more than 94%.
Figure 3.10: Standard error of estimation for combinations of $C_w$ and $p_w$

Figure 3.11: $R^2$-values for combinations of $C_w$ and $p_w$
(a) Stress and strain both in the direction of the loading

(b) Strain in the direction of the loading, Stress perpendicular to the loading

Figure 3.12: Stress-strain curve for the calibration between particle mechanics simulation and GMA calculation of uniaxial compression
3.4.3 Validation of the model

Now that the microscopic constitutive relations are known, the mechanical model in GMA, with these normal and tangential force-displacement relationships can be tested. To ensure the validity of the calibrated relationships, the force-displacement relationships are validated with a third loading type. This can be done with the biaxial compression tests which were shown in figure 3.5 and figure 3.6. First, the loading in both directions of the biaxial compression is the same, thus $\varepsilon_x = \varepsilon_y$. The same loading is applied in GMA and the DEM and GMA results can be compared. Then the biaxial compression test is done for different loadings in the loading directions, namely $2\varepsilon_x = \varepsilon_y$. This is then again compared for DEM and GMA.

**Biaxial compression $\varepsilon_x = \varepsilon_y$**

Figure 3.13a shows the stress-strain comparison of DEM and GMA of the biaxial compression loading in the loading direction where the strain in both loading directions is equal. Figure 3.13b shows the stress-strain comparison of DEM and GMA of the biaxial compression loading in the direction perpendicular to the loading. The standard error of estimation (equation 3.23) and the $R^2$-value (equation 3.24) can again be calculated. The standard error of estimation in the direction of the loading is 4.95 and the $R^2$-value is 0.997. The standard error of estimation in the direction perpendicular to the loading is 9.61 and the $R^2$-value is 0.981. Just as for the uniaxial compression simulation, the simulation in the direction of the loading is better than the simulation perpendicular to the loading. However, again both $R^2$-values are good.

**Biaxial compression $2\varepsilon_x = \varepsilon_y$**

Figure 3.14a shows the stress-strain comparison of DEM and GMA of the biaxial compression loading in the loading direction where the strain is not equal in both directions. Figure 3.14b shows the stress-strain comparison of DEM and GMA of the biaxial compression loading in the direction perpendicular to the loading. The standard error of estimation (equation 3.23) and the $R^2$-value (equation 3.24) can again be calculated. The standard error of estimation in the x-direction is 3.16 and the $R^2$-value is 0.997. The standard error of estimation in the y-direction is 3.46 and the $R^2$-value is 0.998. The standard error of estimation in the direction perpendicular to the loading (z-direction) is 3.86 and the $R^2$-value is 0.990.
Figure 3.13: Stress-strain curve for the validation between particle mechanics simulation and GMA calculation of biaxial compression $\varepsilon_x = \varepsilon_y$

(a) Stress and strain both in the direction of the loading

(b) Strain in the directions of the loading, stress perpendicular to the loading
Mechanical model

Chapter 3

(a) Stress and strain both in the directions of the loading

(b) Strain in the directions of the loading, stress perpendicular to the loading

Figure 3.14: Stress-strain curve for the validation between particle mechanics simulation and GMA calculation of biaxial compression $2\varepsilon_x = \varepsilon_y$

These figures show that both the functional forms as well as the numerical values calibrated for the model are correct. More experiments can be performed to better ensure the validity of the used relationships. The whole script for the mechanical model for the particle packing of 514 mono-disperse hydrogel particles can be found in the Appendix. Appendix B gives the calculation of the Granular Micromechanics approach with the static constraint and appendix C gives the correct force-displacement relationship.
4 | Swelling of particles

Before we start evaluating the swelling principles, first, the most important principles which were found in the literature will be repeated here. The moisture expansion or hygroscopic swelling of a material can result in changes in the stresses and strains in a material. The total strain \( \varepsilon_{ij}^{\text{tot}} \) in a material is based on the hygroscopic strain \( \varepsilon_{ij}^{\Delta M} \) and the elastic strain \( \varepsilon_{ij}^{\text{el}} \) (see figure 4.1).

\[
\varepsilon_{ij}^{\text{tot}} = \varepsilon_{ij}^{\text{el}} + \varepsilon_{ij}^{\Delta M}
\]  

(4.1)

As found in the literature, the strain which is caused by the hygroscopic swelling of a material can be expressed as follows:

\[
\varepsilon_{ij}^{\Delta M} = \beta_{ij} \Delta M
\]  

(4.2)

where \( \Delta M \) is the change in moisture content and \( \beta \) the hygroscopic expansion coefficient. If the material is isotropic, the hygroscopic expansion coefficient is as follows:

\[
\beta_{ij} = \beta \delta_{ij}
\]  

(4.3)

If the hygroscopic expansion is constraint, the total strain \( \varepsilon_{ij}^{\text{tot}} = 0 \), if the hygroscopic expansion is not constraint the elastic strain \( \varepsilon_{ij}^{\text{el}} = 0 \).

The influence of this hygroscopic expansion can be evaluated for the stress-strain relationship of a particle packing. The influence of the swelling of the material and thus the swelling of the particles can be implemented into the mechanical model for the calculation of the stress and strain relationship in the Granular Micromechanics Method.

Figure 4.1: Total strain is defined by the hygroscopic strain and the elastic strain
4.1 Kinematic constraint

The relative deformation between two particles now has two contributing factors. In section 2.2.1 the relative displacement between two particles was described by the relative displacement of the grain centroids. When there is hygroscopic swelling or another type of swelling for example due to temperature change, there can be relative deformation between two particles, while the centroids of the particles have no relative displacement. This second contributing factor is caused by the hygro-strain (or thermal strain). This results in the following relation for the relative deformation ($\gamma$):

$$\gamma_\alpha = \delta_{\alpha}^{\text{tot}} - \delta_{\alpha}^{\Delta M} = u_{ij}^{\alpha} l_j^{\alpha} - \beta_{ij}^{\alpha} \Delta M_j^{\alpha} = \varepsilon_{ij}^{\alpha,el} l_j^{\alpha} \quad (4.4)$$

where the relative deformation of the two particle centroids is described by $\delta^{\text{tot}}$ and the swelling of the particles is described by $\delta^{\Delta M}$. The relative deformation between two particle centroids can be described by the displacement between the particles centroids ($u$) and the original distance between the two particle centroids ($l$). The superscript $\alpha$ stands for the $\alpha$th contact of the grain. The graphical representation of these particle displacements can be seen in figure 4.2.

With the relative deformation, we can write the microscopic constitutive relation with the relative deformation as follows:

$$f_i = K_{ij} \gamma_j \quad (4.5)$$

With the stiffness tensor in the RVE system ($K_{ik}$), the stiffness tensor in the material point ($C_{ijkl}$) can be found and the macroscopic constitutive relationship is as follows:

$$d\sigma_{ij} = C_{ijkl} \, d(\varepsilon_{kl}^{\text{tot}} - \beta_{kl} \Delta M) \quad (4.6)$$

$$d\sigma_{ij} = C_{ijkl} \, d\varepsilon_{kl}^{\text{el}} \quad (4.7)$$

![Figure 4.2: Elastic deformation is defined by total deformation between particle centroids and hygroscopic expansion](image)

45 Multiscale Analysis of Swelling and Mechanical Behavior of Granular media
4.1.1 Homogenization based on the principle of virtual work

Homogenization is the averaging of microscopic variables towards those that are macroscopically observable. If the hygroscopic expansion coefficient of a particle is known, a relation between the microscopic expansion of a particle and the macroscopic expansion of the RVE can be made by homogenization [Lui, 2018].

The macroscopic work can be expressed as the stress and the elastic strain. The stress can be reformulated with the macroscopic constitutive relationship. The elastic strain can then be rewritten into the total strain and the hygroscopic strain. This results in the following macroscopic work:

\[
W = \sigma_{ij} \varepsilon_{ij}^\text{el} = C_{ijkl} (\varepsilon_{kl}^\text{tot} - \beta_{kl} \Delta M) (\varepsilon_{ij}^\text{tot} - \beta_{ij} \Delta M) \tag{4.8}
\]

The work can be formulated for the microscopic side as the volume average of the work for all grain pair interactions. Where the superscript \( \alpha \) stands for the \( \alpha \)th contact and \( N \) is the total number of contacts. The work in a grain pair interaction is the force and the relative deformation. The force can be reformulated with the microscopic constitutive relationship. The relative deformation can then be rewritten as the displacement of the particle centroids and the deformation due to moisture change. This results in the following microscopic work:

\[
W = \frac{1}{V} \sum_{\alpha=1}^{N} W^\alpha = \frac{1}{V} \sum_{\alpha=1}^{N} f_\alpha^\text{\alpha} \gamma_\alpha^{\alpha} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{\alpha} \varepsilon_\alpha \gamma_\alpha^{\alpha} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{\alpha} \varepsilon_\alpha \gamma_\alpha^{\alpha} (\varepsilon_{kl}^\text{tot} - \beta_{kl} \Delta M) (\varepsilon_{ij}^\text{tot} - \beta_{ij} \Delta M) \tag{4.9}
\]

The microscopic work can be set equal to the macroscopic work with the principle of virtual work:

\[
\sigma_{ij} \varepsilon_{ij}^\text{el} = \frac{1}{V} \sum_{\alpha=1}^{N} f_\alpha^\text{\alpha} \gamma_\alpha^{\alpha} \tag{4.10}
\]

Having this micro-macro relationship for equations 4.8 and 4.9 give the following relationships:

\[
C_{ijkl} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{\alpha} \varepsilon_\alpha \gamma_\alpha^{\alpha} \tag{4.11}
\]

\[
C_{ijkl} \beta_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{\alpha} \varepsilon_\alpha \gamma_\alpha^{\alpha} \beta_{ij} \tag{4.12}
\]

\[
C_{ijkl} \beta_{kl} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{\alpha} \varepsilon_\alpha \gamma_\alpha^{\alpha} \beta_{kl} \tag{4.13}
\]

\[
C_{ijkl} \beta_{kl} \beta_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{\alpha} \varepsilon_\alpha \gamma_\alpha^{\alpha} \beta_{kl} \beta_{ij} \tag{4.14}
\]
Appendix D gives the full derivation of equations 4.11 to 4.14.

With equation 4.12 or 4.13, and equation 4.14 the relationship between the microhygroscopic expansion coefficient and the macrohygroscopic expansion coefficient can be found. For convenience, we reformulate the right hand side of equation 4.12 to:

$$R_{kl} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ikl}^{\alpha} \beta_{ij}^{\alpha}$$  \hspace{1cm} (4.15)$$

To show that equation 4.12 and equation 4.13 are equal, we can reformulate equation 4.15 to:

$$R_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{pij}^{\alpha} \beta_{pq}^{\alpha}$$  \hspace{1cm} (4.16)$$

The subscript $p$ can be replaced by the subscript $k$ and the subscript $q$ can be replaced by the subscript $l$ since they are both dummy indices:

$$R_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ikl}^{\alpha} \beta_{kl}^{\alpha}$$  \hspace{1cm} (4.17)$$

Since the stiffness tensor is symmetric ($k_{ik} = k_{ki}$) this can be rewritten to:

$$R_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ikl}^{\alpha} \beta_{kl}^{\alpha}$$  \hspace{1cm} (4.18)$$

Which is the same as the right hand side of equation 4.13. With the right hand side rewritten, we can now write the following relationship for the macroscopic expansion coefficient:

$$\beta_{ij} = C_{ijkl}^{-1} R_{kl}$$  \hspace{1cm} (4.19)$$

**Symmetrization**

With the consideration of symmetry of the stress and strain, the stiffness tensor $C_{ijkl}$, with 81 components can be reduced to 36 components.

$$C_{\alpha\beta} = \frac{C_{ijkl} + C_{ijlk} + C_{jikl} + C_{jilk}}{4}$$  \hspace{1cm} (4.20)$$

The subscripts $\alpha$ and $\beta$ now do not follow standard index notation and range from 1 to 6. This range from 1 to 6 stands for the normal index notations 11, 22, 33, 23, 13 and 12 in this order. The non-diagonals of the hygroscopic expansion coefficient are
assumed to be symmetric as well. More specifically, with looking at equation 4.3, only the diagonals are not zero. Thus, the hygroscopic expansion coefficient can be symmetrized to:

\[
\beta = \begin{bmatrix}
\beta_{11} & \beta_{12} & \frac{\beta_{13}}{2} \\
\beta_{21} & \beta_{22} & \frac{\beta_{23}}{2} \\
\frac{\beta_{31}}{2} & \frac{\beta_{32}}{2} & \beta_{33}
\end{bmatrix}
\]  

(4.21)

The right hand side of the equation can be symmetrized as well, since we can assume a symmetry of the hygroscopic expansion coefficient \(\beta_{ij}\) and of the stiffness tensor \(k_{ik}\). This results in the right hand side having only 6 results instead of 9:

\[
R = \begin{bmatrix}
R_{11} & R_{12} & \frac{R_{13}}{2} \\
R_{21} & R_{22} & \frac{R_{23}}{2} \\
\frac{R_{31}}{2} & \frac{R_{32}}{2} & R_{33}
\end{bmatrix}
\]

(4.22)

This results in the following equation for the macro hygroscopic expansion coefficient when rewriting equation 4.12 with the symmetrization:

\[
\beta = C^{-1} \alpha R
\]

(4.23)

**Approximated solution**

Since we are interested in the approximate solution for the whole RVE in the granular micromechanics approach, the number density of the grain-pair interactions \(\rho_c\) and the inter-granular contact directional density distribution function \(\xi\) can be introduced again. With this, equations 4.11 to 4.14 can be translated to an integral form, to find the approximate solutions. For equation 4.11, this was already done in section 2.2.1, which led to equation 2.27. The same procedure will be used for equations 4.12, 4.13 and 4.14. This results in the following equations:

\[
\begin{align*}
C_{ijkl} \beta_{ij} &= l^2 \rho_c \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (K_{ik} \beta_{ij}^{m} n_j n_l) \xi \sin \theta d\phi d\theta \\
C_{ijkl} \beta_{kl} &= l^2 \rho_c \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (K_{ik} \beta_{kl}^{m} n_j n_l) \xi \sin \theta d\phi d\theta \\
C_{ijkl} \beta_{ij} \beta_{kl} &= l^2 \rho_c \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (K_{ik} \beta_{ij}^{m} \beta_{kl}^{m} n_j n_l) \xi \sin \theta d\phi d\theta
\end{align*}
\]

(4.24) (4.25) (4.26)

in these equations, the superscript \(m\) stands for the microscopic value of the particles. Appendix E has the full derivation of the approximation.
4.1.2 Homogenization based on equilibrium

Instead of starting with the principle of virtual work (PVW) and considering the energy condition where microscopic work and macroscopic work are equal, we can also consider the equilibrium of the stresses, where we consider the macroscopic stress to be equal to the volume average of the microscopic stress:

\[ \sigma_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} \sigma_{ij}^{\alpha} \]  \hspace{1cm} (4.27)

Now again the macroscopic stress can be rewritten with the macroscopic constitutive relationship, which results in the stiffness tensor and the macroscopic elastic strain. The elastic strain can then be rewritten into the total strain and the hygroscopic strain. This results in the macroscopic stress as follows:

\[ \sigma_{ij} = C_{ijkl} \varepsilon_{kl}^{\text{el}} = C_{ijkl} (\varepsilon_{kl}^{\text{tot}} - \beta_{kl} \Delta M) \]  \hspace{1cm} (4.28)

The microscopic stress can be formulated as the force and the distance between the two particle centroids. The microscopic force in contact \( \alpha \) can be rewritten with the microscopic constitutive relationship as the stiffness tensor \( (K_{ik}) \) for the contact \( \alpha \) and the relative deformation of that contact. The relative deformation can be rewritten as the displacement of the two particle centroids and the deformation due to moisture change.

\[ \frac{1}{V} \sum_{\alpha=1}^{N} \sigma_{ij}^{\alpha} = \frac{1}{V} \sum_{\alpha=1}^{N} f_{i}^{\alpha} l_{j}^{\alpha} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ik}^{\alpha} \gamma_{k}^{\alpha} l_{j}^{\alpha} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ik}^{\alpha} l_{l}^{\alpha} l_{j}^{\alpha} (\varepsilon_{kl}^{\text{tot}} - \beta_{kl} \Delta M) \]  \hspace{1cm} (4.29)

Now, we can set the macroscopic stress (equation 4.28) equal to the microscopic stress (equation 4.29). This results in the following relationships:

\[ C_{ijkl} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ik}^{\alpha} l_{l}^{\alpha} l_{j}^{\alpha} \]  \hspace{1cm} (4.30)

\[ C_{ijkl} \beta_{kl} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ik}^{\alpha} l_{l}^{\alpha} l_{j}^{\alpha} \beta_{kl} \]  \hspace{1cm} (4.31)

These two relationships are the same as were found when starting with the principle of virtual work (equations 4.11 and 4.13). Since these equations are the same as were found in the previous section, the same symmetrization (equation 4.23) and approximation (equation 4.25) apply here. When starting from the equilibrium condition of stress, equation 4.14 is not found.
5 Swelling and Mechanical behavior

In chapter 3, the calculations of the mechanical model for the hydrogel particle packing was evaluated. In chapter 4, the swelling principles were explored and derived. In this chapter, the swelling principles of chapter 4 will be investigated more and combined with the mechanical model of chapter 3. This will first be done by evaluating the homogenization relationships for the expansion coefficient, which were found in chapter 4, for different particle packings, including the particle packing which was used in chapter 3. Then swelling will be introduced on the mechanical model to see the influence on the mechanical behavior of the particle packing.

5.1 Micro-macro relationship

The homogenization relationship between the micro hygroscopic expansion coefficient (particle) and the macro hygroscopic expansion coefficient (packing) can be evaluated for different particle packings with different expansion coefficients. This can be done for equations 4.11 to 4.14 which come from the principle of virtual work and for equations 4.30 and 4.31 which come from the equilibrium of stress. Since equation 4.11 is the same as equation 4.30 and equations 4.12 and 4.13 are equal to each other and are equal to equation 4.31, we will only use four equations in the next part. For convenience, these equations will be repeated here:

\[
C_{ijkl} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ikl}^{\alpha} l_{ij}^{\alpha} \tag{5.1}
\]

\[
C_{ijkl} \beta_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ikl}^{\alpha} l_{ij}^{\alpha} \beta_{ij}^{\alpha} \tag{5.2}
\]

\[
C_{ijkl} \beta_{kl} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ikl}^{\alpha} l_{ij}^{\alpha} \beta_{kl}^{\alpha} \tag{5.3}
\]

\[
C_{ijkl} \beta_{kl} \beta_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ikl}^{\alpha} l_{ij}^{\alpha} \beta_{kl}^{\alpha} \beta_{ij}^{\alpha} \tag{5.4}
\]
The experimental particle packing with 514 mono-disperse hydrogel particles, which was also used in the mechanical model, will be used. Also, the bi-disperse experimental particle packing with 1921 hydrogel particles will be used [Barés et al., 2019]. Then a larger simulated packing with 7357 particles will be used. This last packing is used to exclude errors due to a small number of particles and to evaluate the results for different particle properties. All these particle packings consist of spherical particles, for that reason, isotropic expansion coefficients are assumed for the particles (equation 4.3).

**5.1.1 Experimental particle packing with 514 mono-disperse hydrogel particles**

First, the particle packing of 514 mono-disperse hydrogel particles, which was used for the calibration of the mechanical model, can be used. The situation where the packing starts to be loaded is used, with this, the first tangent modulus as explained in section 3.2.3 can be used. The normal and tangential grain-pair stiffness can be calculated with this tangent modulus for the kinematic constraint with equations 2.29 and 2.30. These equations can be rewritten to:

\[
k_n = \frac{E}{\rho \, (1 - 2 \nu)} \frac{1}{1 - 2 \nu} \quad (5.5)
\]

\[
k_s = \frac{E}{\rho \, (1 - 1 \nu - 2 \nu^2)} \quad (5.6)
\]

With equations 5.5 and 5.6, the properties of the particle packing, which can be used in the homogenization relationships, can be derived. These properties can be found in table 5.1. Since the kinematic method is used for a packing with a Poisson’s ratio of 0.41, a negative tangential grain-pair stiffness is found.

<table>
<thead>
<tr>
<th>Table 5.1: Material properties mono-disperse experimental particle packing</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of particles</td>
</tr>
<tr>
<td>Diameter</td>
</tr>
<tr>
<td>$k_n$</td>
</tr>
<tr>
<td>$k_s$</td>
</tr>
</tbody>
</table>

With the properties of the material as in table 5.1, the symmetrized stiffness ($C_{ij}$) of the packing can be derived (equation: 5.1):

\[
C_{ij} = \begin{bmatrix}
242.01 & 130.68 & 101.36 & -1.50 & -1.83 & -0.53 \\
130.68 & 209.28 & 85.79 & 11.02 & -0.96 & 6.26 \\
101.36 & 85.79 & 228.76 & 13.63 & -5.24 & -5.42 \\
-1.50 & 11.02 & 13.63 & -31.23 & -4.77 & -0.60 \\
-1.83 & -0.96 & -5.24 & -4.77 & -18.87 & -4.99 \\
-0.53 & 6.26 & -5.42 & -0.60 & -4.99 & -11.42
\end{bmatrix} \text{[Pa]} \quad (5.7)
\]
With the properties of the particles and the stiffness of the particle packing, different expansion coefficients for the particles can be used to find the expansion coefficient of the packing. Table 5.2 shows the result of the homogenization with a microscopic expansion coefficient ($\beta^\alpha$) of 0.01. Other examples can be found in Appendix F.1. In these tables (and following tables) the results for the macroscopic expansion coefficient that comes from equation 5.2 or equation 5.3 can be found in the second column from the left, which is labelled $\beta_{ij}$. The last column represents the outcome of equation 5.4, when the results found from equation 5.2 or equation 5.3 are filled in. This column is labelled $C_{ijkl}\beta_{ij}\beta_{kl}$. The result for the left-hand side (LHS) and the result for the right-hand side (RHS) of the equation is given, with the error between them.

The results show that with uniformly distributed hygroscopic expansion coefficients for the particles in a mono-disperse particle packing, the macroscopic (packing) hygroscopic expansion coefficient found with equation 5.2 or equation 5.3 is equal to the microscopic (particle) hygroscopic expansion coefficient. Equation 5.4 gives the same values for the left-hand side and the right-hand side, when using the results from equation 5.2 or equation 5.3. So, for a packing with spherical particles with uniformly distributed micro hygroscopic expansion coefficients, the result which comes from equilibrium and the result which comes from the principle of virtual work is the same.

Table 5.2: Micro-macro relationship mono-disperse particle packing $\beta^\alpha = 0.01$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}\beta_{ij}\beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.01</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.01</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.01</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-6.02262E-18</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>3.60617E-18</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-4.73143E-18</td>
</tr>
</tbody>
</table>

5.1.2 Experimental particle packing with 1921 bi-disperse hydrogel particles

For the bi-disperse experimental hydrogel particle packing of 1921 particles, the same thing can be done. The influence of different microscopic expansion coefficients can be evaluated. In this case, however, the particles are not mono-disperse and different expansion coefficients can be assumed for the different particles. The material of the particles is the same for both particles, which is the same as for the mono-disperse particle packing. For that reason, the same grain-pair stiffness is used. The material properties can be found in table 5.3.
This results in the following stiffness matrix \((C_{ij})\) for the bi-disperse experimental particle packing:

\[
C_{ij} = \begin{pmatrix}
482.03 & 284.85 & 202.76 & 3.58 & -4.03 & 4.98 \\
284.85 & 438.34 & 191.45 & 12.90 & 2.28 & -3.73 \\
202.76 & 191.45 & 475.79 & -5.52 & -0.18 & 2.11 \\
3.58 & 12.90 & -5.52 & -53.61 & 1.85 & 1.89 \\
-4.03 & 2.28 & -0.18 & 1.85 & -48.97 & 1.56 \\
4.98 & -3.73 & 2.11 & 1.89 & 1.56 & -12.31
\end{pmatrix} \quad [Pa] \quad (5.8)
\]

First, the same cases can be evaluated as in the mono-disperse experimental particle packing, where both particle types have the same expansion coefficient. The result of the case where \(\beta_1 = \beta_2 = 0.01\) can be found in table 5.4. Other examples can be found in appendix F.2. The macroscopic expansion coefficient which is found with equation 5.2 or equation 5.3 is equal to the microscopic expansion coefficient of the particles. These results again give no error between the left hand side and the right hand side of equation 5.4 when the result of equation 5.2 or equation 5.3 is filled in. So, the equations found from the principle of virtual work and the equations which were found from the equilibrium of stresses, give the same result.

Table 5.4: Micro-macro relationship bi-disperse particle packing \(\beta_1 = \beta_2 = 0.01\)

<table>
<thead>
<tr>
<th>(\beta_1)</th>
<th>(\beta_2)</th>
<th>(C_{ijkl}\beta_{ijkl})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\beta_{11})</td>
<td>0.01</td>
<td>LHS 0.275427</td>
</tr>
<tr>
<td>(\beta_{22})</td>
<td>0.01</td>
<td>RHS 0.275427</td>
</tr>
<tr>
<td>(\beta_{33})</td>
<td>0.01</td>
<td>error 0</td>
</tr>
<tr>
<td>(\beta_{23})</td>
<td>-9.32E-18</td>
<td></td>
</tr>
<tr>
<td>(\beta_{13})</td>
<td>-6.13E-18</td>
<td></td>
</tr>
<tr>
<td>(\beta_{12})</td>
<td>-9.43E-18</td>
<td></td>
</tr>
</tbody>
</table>

Since this is a bi-disperse particle packing, it is interesting to evaluate the results for different expansion coefficients for the different particles. Tables 5.5, 5.6 and 5.7 show the results where the difference between the microscopic hygroscopic expansion coefficients \(\beta_1\) and \(\beta_2\) is a factor 2, 10 and 100.
In these tables, it can be seen that the macroscopic expansion coefficients found with equations 5.2 or 5.3 ($\beta_{ij}$) are in between the values which were used for the microscopic expansion coefficients ($\beta_{\alpha 1}$ and $\beta_{\alpha 2}$), which is what would be expected. The results lean a bit towards the microscopic hygroscopic expansion coefficient of particle type 2, this can be due to the fact that there are more particles with this expansion coefficient.

In these cases, equation 5.4, does not give the same result for the left-hand side and the right-hand side when the results from equation 5.2 or equation 5.3 are used. Since equations 5.1 to 5.4 are derived from the principle of virtual work, the best macroscopic hygroscopic expansion coefficient for the combinations of the four equations (5.1 to 5.4) should be found. This can be done with the least-squares approach, where the magnitude of the errors is minimized for the four equations combined.

The macroscopic expansion coefficient which result from this least-squares approach can also be found in tables 5.5, 5.6 and 5.7, together with the ($\text{residual})^2$ and the $R^2$-value. The $R^2$-value measures the error between the left hand side and the right hand side compared to the absolute value of the equations. The macroscopic expansion coefficients found with this least-squares approach are different from the macroscopic expansion coefficients which were found for the equilibrium condition (with equations 5.2 or 5.3). However, they are still within the range between the microscopic expansion coefficients ($\beta_{\alpha 1}$ and $\beta_{\alpha 2}$), which is physically reasonable.

When the difference between the microscopic expansion coefficients $\beta_{\alpha 1}$ and $\beta_{\alpha 2}$ is small, the error introduced with equation 5.4 is also small. When the difference between the microscopic expansion coefficients $\beta_{\alpha 1}$ and $\beta_{\alpha 2}$ becomes larger, the error in equation 5.4, when using the macroscopic expansion coefficients found with equation 5.2 or 5.3, becomes larger. Accordingly, solving equations 5.1 to 5.4 via the least-squares approach results in a more significant change in the results. This means that the influence of equation 5.4 in the principle of virtual work becomes larger when there is a larger difference in the microscopic expansion coefficient, while this influence is not there in the result found from the equilibrium condition. Also, it is visible from the $R^2$-value that these equations give a larger error between micro and macro, which results in a larger error for the principle of virtual work equation.
Table 5.5: Micro-macro relationship bi-disperse particle packing $\beta^a_1 = 0.1$ and $\beta^a_2 = 0.2$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}$ $\beta_{ij} \beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.160093</td>
<td>$\beta_{11}$ 0.160527</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.155941</td>
<td>$\beta_{22}$ 0.15646</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.161401</td>
<td>$\beta_{33}$ 0.162042</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-1.01E-03</td>
<td>$\beta_{23}$ -8.32E-04</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-1.12E-02</td>
<td>$\beta_{13}$ -1.06E-02</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-2.19E-03</td>
<td>$\beta_{12}$ -1.60E-03</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}$ $\beta_{ij} \beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>LHS 69.74104</td>
<td>$\beta_{11}$ 0.160527</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>RHS 73.24477</td>
<td>$\beta_{22}$ 0.15646</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>error 3.50373</td>
<td>$\beta_{33}$ 0.162042</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-1.01E-03</td>
<td>$\beta_{23}$ -8.32E-04</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-1.12E-02</td>
<td>$\beta_{13}$ -1.06E-02</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-2.19E-03</td>
<td>$\beta_{12}$ -1.60E-03</td>
</tr>
</tbody>
</table>

$(\text{residual})^2$ 10.6494

$R^2$ 0.999832

Table 5.6: Micro-macro relationship bi-disperse particle packing $\beta^a_1 = 0.01$ and $\beta^a_2 = 0.1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}$ $\beta_{ij} \beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.064084</td>
<td>$\beta_{11}$ 0.064252</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.060347</td>
<td>$\beta_{22}$ 0.060512</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.065261</td>
<td>$\beta_{33}$ 0.065503</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-9.10E-04</td>
<td>$\beta_{23}$ -8.06E-04</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-1.01E-02</td>
<td>$\beta_{13}$ -9.56E-03</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-1.97E-03</td>
<td>$\beta_{12}$ -1.49E-03</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}$ $\beta_{ij} \beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>LHS 11.00487</td>
<td>$\beta_{11}$ 0.064252</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>RHS 13.8429</td>
<td>$\beta_{22}$ 0.060512</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>error 2.838021</td>
<td>$\beta_{33}$ 0.065503</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-9.10E-04</td>
<td>$\beta_{23}$ -8.06E-04</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-1.01E-02</td>
<td>$\beta_{13}$ -9.56E-03</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-1.97E-03</td>
<td>$\beta_{12}$ -1.49E-03</td>
</tr>
</tbody>
</table>

$(\text{residual})^2$ 7.8634

$R^2$ 0.99923

Table 5.7: Micro-macro relationship bi-disperse particle packing $\beta^a_1 = 0.01$ and $\beta^a_2 = 1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}$ $\beta_{ij} \beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.604921</td>
<td>$\beta_{11}$ 0.666602</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.563812</td>
<td>$\beta_{22}$ 0.616886</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.617869</td>
<td>$\beta_{33}$ 0.716413</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-1.00E-02</td>
<td>$\beta_{23}$ 1.30E-03</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-1.11E-01</td>
<td>$\beta_{13}$ -1.00E-02</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-2.17E-02</td>
<td>$\beta_{12}$ 7.44E-03</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}$ $\beta_{ij} \beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>LHS 976.0845</td>
<td>$\beta_{11}$ 0.666602</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>RHS 1319.485</td>
<td>$\beta_{22}$ 0.616886</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>error 343.4006</td>
<td>$\beta_{33}$ 0.716413</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-1.00E-02</td>
<td>$\beta_{23}$ 1.30E-03</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-1.11E-01</td>
<td>$\beta_{13}$ -1.00E-02</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-2.17E-02</td>
<td>$\beta_{12}$ 7.44E-03</td>
</tr>
</tbody>
</table>

$(\text{residual})^2$ 3.47E+04

$R^2$ 0.981667

---

55 Multiscale Analysis of Swelling and Mechanical Behavior of Granular media
5.1.3 Particle packing with 7357 particles

To make sure that the difference between the principle of virtual work result and the equilibrium result which was found in the previous section was not due to the fact that the number of particles is low for these experiments, a simulated particle packing with 7357 particles is used. The particles have an E-modulus of $7.0E + 9$ Pa and a Poisson’s ratio of 0.3. First, the packing can be assumed as if all particles are the same. Then the particles in the packing are divided into two particle types. This is first done by assuming the particles only have different expansion coefficients, then also the stiffness is assumed different for the two particle types. The grain-pair stiffness which is used is based on the tangent modulus of the packing in the first loading increment of a DEM simulation of the particle packing. A tangent modulus of $E = 6.6533E + 10$ Pa is found for the first loading increment. With this, the grain-pair stiffness can be derived with equations 5.5 and 5.6.

One particle type

So first, the case where all particles are assumed to be the same is evaluated for the packing, to check if this works correctly. The properties of this particle packing can be found in table 5.8.

Table 5.8: Material properties simulated particle packing when all particles are the same

<table>
<thead>
<tr>
<th>Number of particles</th>
<th>7357</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter</td>
<td>0.0005 m</td>
</tr>
<tr>
<td>$k_n$</td>
<td>4.4E+07 N/m</td>
</tr>
<tr>
<td>$k_s$</td>
<td>-1.4E+07 N/m</td>
</tr>
</tbody>
</table>

The properties as in table 5.8 result in the stiffness matrix ($C_{ij}$) as follows:

$$
C_{ij} = \begin{pmatrix}
348.65 & 196.80 & 211.07 & -1.58 & 1.59 & 1.82 \\
196.80 & 349.86 & 212.51 & 2.13 & -2.29 & -1.90 \\
211.07 & 212.51 & 416.64 & -1.92 & -3.06 & -0.16 \\
-1.58 & 2.13 & -1.92 & 83.11 & -0.20 & -1.94 \\
1.59 & -2.29 & -3.06 & -0.20 & 81.88 & -1.51 \\
1.82 & -1.90 & -0.16 & -1.94 & -1.51 & 70.99
\end{pmatrix} E + 08 [Pa] \quad (5.9)
$$

The same cases as for the experimental packing are evaluated. The result for $\beta^a = 0.01$ can be found in table 5.9. The other results can be found in appendix F.3. These results show that for a particle packing with only one particle type, a certain microscopic expansion coefficient for the particles results in the same macroscopic expansion coefficient for the packing. Also, the principle of virtual work and the equilibrium condition is followed at the same time, since the error for equation 5.4 is
zero when the macroscopic expansion coefficient found from equation 5.2 or equation 5.3 is used. So the result which comes from equations 5.1 (the macroscopic stiffness \( C_{ij} \)) and equation 5.2 or 5.3 result in a correct result for equation 5.4. This is the same as was found for the experimental packings.

Table 5.9: Micro-macro relationship packing with 7357 particles \( \beta^\alpha = 0.01 \)

<table>
<thead>
<tr>
<th>( \beta_{ij} )</th>
<th>( C_{ijkl} \beta_{ij} \beta_{kl} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \beta_{11} )</td>
<td>0.01 LHS 23559078</td>
</tr>
<tr>
<td>( \beta_{22} )</td>
<td>0.01 RHS 23559078</td>
</tr>
<tr>
<td>( \beta_{33} )</td>
<td>0.01 error 0</td>
</tr>
<tr>
<td>( \beta_{23} )</td>
<td>2.72E-18</td>
</tr>
<tr>
<td>( \beta_{13} )</td>
<td>2.30E-19</td>
</tr>
<tr>
<td>( \beta_{12} )</td>
<td>1.36E-19</td>
</tr>
</tbody>
</table>

**Two different types of particles with equal stiffnesses**

By dividing the particle packing into two and giving them different hygroscopic expansion coefficients, the influence of this difference can be evaluated. First, the stiffness of both particles is kept the same, to evaluate only the influence of the difference in expansion coefficients. The properties of this packing can be found in table 5.10. This results in the same stiffness matrix \( (C_{ij}) \) as for the situation where only one particle type is assumed (equation 5.9), since this stiffness matrix is only dependent on the particle distribution and its contacts, and the grain-pair stiffness, which is the same as in the assumption where there is only one particle type.

Table 5.10: Material properties simulated packing with 7357 particles with two particle types with equal stiffnesses

<table>
<thead>
<tr>
<th>Particle type</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of particles</td>
<td>3679</td>
<td>3678</td>
</tr>
<tr>
<td>Diameter</td>
<td>0.0005 m</td>
<td>0.0005 m</td>
</tr>
<tr>
<td>( k_n )</td>
<td>4.4E+07 N/m</td>
<td>4.4E+07 N/m</td>
</tr>
<tr>
<td>( k_s )</td>
<td>-1.4E+07 N/m</td>
<td>-1.4E+07 N/m</td>
</tr>
</tbody>
</table>

The same cases as for the bi-disperse experimental packing are evaluated here, where the difference between the microscopic expansion coefficients \( \beta_1^\alpha \) and \( \beta_2^\alpha \) is a factor 2, 10 and 100. These results can be found in tables 5.11, 5.12 and 5.13. It can be seen that equations 5.2 and 5.3 still result in macroscopic expansion coefficients that are within the range of the microscopic expansion coefficients (between \( \beta_1^\alpha \) and \( \beta_2^\alpha \)), which is physically reasonable.

In these cases, using the results from equation 5.2 or equation 5.3, does not give the
same result for the left-hand side and the right-hand side of equation 5.4, which shows a difference between the result of the principle of virtual work and the equilibrium of stresses. The same thing which was done for the bi-disperse experimental packing should be done, the best value for the combinations of the four equations (5.1 to 5.4) should be found to find the best result for the principle of virtual work. This can be done with the least-squares approach, where the best fit of macroscopic expansion coefficients should be found. This best fit is found for the smallest errors between micro and macro in equations 5.1 to 5.4.

For the difference of a factor 2 between the microscopic expansion coefficients $\beta_1^\alpha$ and $\beta_2^\alpha$, the result of equation 5.2 or equation 5.3 give a small error in equation 5.4. For the difference of a factor 10 between the microscopic expansion coefficients $\beta_1^\alpha$ and $\beta_2^\alpha$, the results of equation 5.2 or equation 5.3 give a larger error in equation 5.4. For the case where there is a difference of a factor of 100 between the microscopic expansion coefficients $\beta_1^\alpha$ and $\beta_2^\alpha$, the result of equation 5.2 or equation 5.3 give an even larger error in equation 5.4. Accordingly, solving equations 5.1 to 5.4 via the least-squares approach results in a more significant change in the analysis results when the factor difference between the microscopic expansion coefficients $\beta_1^\alpha$ and $\beta_2^\alpha$ is larger. This also shows a larger error in the principle of virtual work equation, for a larger difference in microscopic expansion coefficients $\beta_1^\alpha$ and $\beta_2^\alpha$, as the $R^2$-value becomes lower.

To evaluate if the error in equation 5.4 is merely found due to the factor difference between the microscopic expansion coefficients $\beta_1^\alpha$ and $\beta_2^\alpha$, the same factor difference is evaluated for different absolute values. Table 5.14 shows the result which is found the case where $\beta_1^\alpha = 0.001$ and $\beta_2^\alpha = 0.1$. It can be seen that the result from equation 5.2 or 5.3 ($\beta_{ij}$) is 10 times smaller than the result which was found in table 5.13 where $\beta_1^\alpha = 0.01$ and $\beta_2^\alpha = 1$. The difference in absolute values of the microscopic expansion coefficients $\beta_1^\alpha$ and $\beta_2^\alpha$ of a factor 10 result in the error in equation 5.4 ($C_{ijkl}\beta_{ij}\beta_{kl}$) being a factor 100 different. This is due to the fact that $\beta$ is squared in equation 5.4, which results in the fact that equation 5.4 ($C_{ijkl}\beta_{ij}\beta_{kl}$) weights more for large values of $\beta$ and less for small values of $\beta$. The fact that equation 5.4 ($C_{ijkl}\beta_{ij}\beta_{kl}$) weights more for large values of $\beta$ and less for small values of $\beta$ leads to the result of the least-squares approach of equations 5.1 to 5.4 being closer to the results of equation 5.2 or equation 5.3 for smaller absolute values of the microscopic expansion coefficient. This would suggest that the result from the least-squares approach which is used with the four equations of the homogenization is depended on the scale which is used.

Thermal expansion coefficients have values which are in the order of $10^{-6}$, this means that equations 5.2 and 5.3 have this factor as $\beta$, but equation 5.4 will get $\beta\beta$, which is a factor $10^{-12}$. This results in the fact that the influence of equation 5.4 can be neglected in this case. Also, it was found with the $R^2$-values that with a larger difference between the microscopic expansion coefficients, the error in the principle of virtual work becomes larger.
In literature, similar equations as equations 5.2 and 5.3 were found, which would suggest that these equations are indeed correct [Bosco et al., 2017, Bosco et al., 2018]. The influence of equation 5.4 is not found in literature, however, from the principle of virtual work, these equations need to be followed as well. The fact that the result for the macroscopic expansion coefficient depends on the scale of the microscopic expansion coefficient and the fact that there is an error between macro and micro makes the result that comes from the principle of virtual work seem less likely. It can be that there is an additional boundary condition or assumption which applies when using the principle of virtual work, which would cancel out equation 5.4. It should be further experimentally or analytically determined whether equation 5.4 has an influence on the macroscopic expansion coefficients.

Table 5.11: Micro-macro relationship packing with 7357 particles, two particle types with equal stiffnesses $\beta_1^a = 0.1$ and $\beta_2^a = 0.2$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl} \beta_{ij} \beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.150326</td>
<td>LHS 5.32E+09</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.150568</td>
<td>RHS 5.61E+09</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.149918</td>
<td>error 2.91E+08</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>2.52E-04</td>
<td>$\beta_{23}$ 2.65E-04</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-2.97E-05</td>
<td>$\beta_{13}$ -1.23E-05</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>4.92E-04</td>
<td>$\beta_{12}$ 5.13E-04</td>
</tr>
</tbody>
</table>

(residual)$^2$ 7.46E+16

$R^2$ 0.999823

Table 5.12: Micro-macro relationship packing with 7357 particles, two particle types with equal stiffnesses $\beta_1^a = 0.01$ and $\beta_2^a = 0.1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl} \beta_{ij} \beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.055293</td>
<td>LHS 7.19E+08</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.055511</td>
<td>RHS 9.54E+08</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.054926</td>
<td>error 2.36E+08</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>2.27E-04</td>
<td>$\beta_{23}$ 2.35E-04</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-2.68E-05</td>
<td>$\beta_{13}$ -2.13E-05</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>4.43E-04</td>
<td>$\beta_{12}$ 4.59E-04</td>
</tr>
</tbody>
</table>

(residual)$^2$ 5.46E+16

$R^2$ 0.999063

59 Multiscale Analysis of Swelling and Mechanical Behavior of Granular media
Table 5.13: Micro-macro relationship packing with 7357 particles, two particle types with equal stiffnesses $\beta_1^\alpha = 0.01$ and $\beta_2^\alpha = 1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}^\alpha$</th>
<th>Least square approach</th>
<th>$\beta_{ij}$</th>
<th>LHS</th>
<th>RHS</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.508228</td>
<td></td>
<td>$\beta_{11}$</td>
<td>6.07E+10</td>
<td>6.07E+10</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.510621</td>
<td></td>
<td>$\beta_{22}$</td>
<td>8.92E+10</td>
<td>8.92E+10</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.504188</td>
<td></td>
<td>$\beta_{33}$</td>
<td>2.85E+10</td>
<td>2.85E+10</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>2.50E-03</td>
<td></td>
<td>$\beta_{23}$</td>
<td></td>
<td>1.00E-02</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-2.94E-04</td>
<td></td>
<td>$\beta_{13}$</td>
<td></td>
<td>1.00E-02</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>4.87E-03</td>
<td></td>
<td>$\beta_{12}$</td>
<td></td>
<td>1.00E-02</td>
</tr>
</tbody>
</table>

Error: 2.85E+10

$R^2$: 0.968336

Table 5.14: Micro-macro relationship packing with 7357 particles, two particle types with equal stiffnesses $\beta_1^\alpha = 0.001$ and $\beta_2^\alpha = 0.1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}^\alpha$</th>
<th>Least square approach</th>
<th>$\beta_{ij}$</th>
<th>LHS</th>
<th>RHS</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.050177</td>
<td></td>
<td>$\beta_{11}$</td>
<td>5.95E+08</td>
<td>5.95E+08</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.049938</td>
<td></td>
<td>$\beta_{22}$</td>
<td>8.8E+08</td>
<td>8.8E+08</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.050581</td>
<td></td>
<td>$\beta_{33}$</td>
<td>2.85E+08</td>
<td>2.85E+08</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-2.50E-04</td>
<td></td>
<td>$\beta_{23}$</td>
<td></td>
<td>-2.57E-04</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>2.94E-05</td>
<td></td>
<td>$\beta_{13}$</td>
<td></td>
<td>3.68E-05</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-4.87E-04</td>
<td></td>
<td>$\beta_{12}$</td>
<td></td>
<td>-5.07E-04</td>
</tr>
</tbody>
</table>

Error: 2.85E+10

$R^2$: 0.99834
Two different types of particles with different stiffnesses

The influence of having two particle types with different stiffnesses on the micro-macro relationship of the hygroscopic expansion coefficient can be evaluated. This is done by having the grain-pair stiffness of one half of the particles twice as large as the other half of the particle. So $2k_{n,1} = k_{n,2}$ and $2k_{s,1} = k_{s,2}$. The properties can be found in table 5.15.

Table 5.15: Material properties simulated packing with two particle types with different stiffnesses

<table>
<thead>
<tr>
<th>Particle type</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of particles</td>
<td>3679</td>
<td>3678</td>
</tr>
<tr>
<td>Diameter</td>
<td>0.0005 m</td>
<td>0.0005 m</td>
</tr>
<tr>
<td>$k_n$</td>
<td>4.4E+07 N/m</td>
<td>8.8E+07 N/m</td>
</tr>
<tr>
<td>$k_s$</td>
<td>-1.4E+07 N/m</td>
<td>-2.8E+07 N/m</td>
</tr>
</tbody>
</table>

This results in the stiffness matrix ($C_{ij}$) as follows:

$$
C_{ij} = \begin{pmatrix}
524.15 & 296.07 & 316.64 & -2.12 & 2.65 & 2.96 \\
296.07 & 526.09 & 319.06 & 3.28 & -3.82 & -2.60 \\
316.64 & 319.06 & 626.17 & -3.00 & -4.51 & -0.39 \\
-2.12 & 3.28 & -3.00 & 124.63 & -0.48 & -3.32 \\
2.65 & -3.82 & -4.51 & -0.48 & 122.57 & -2.01 \\
2.96 & -2.60 & -0.39 & -3.32 & -2.01 & 106.97 \\
\end{pmatrix} E + 08 [Pa]
$$

With these properties, the same factor differences can be evaluated as before. So a factor difference between the microscopic expansion coefficients $\beta_{1}^\alpha$ and $\beta_{2}^\alpha$ of 2, 10 and 100. The results can be found in tables in appendix F.3. The results of different ratio’s between the stiffness of particle type 1 and the stiffness of particle type 2 can be evaluated. The results for multiple values of $k_1/k_2$ for $\beta_{1}^\alpha = 0.01$ and $\beta_{2}^\alpha = 0.1$ can be found figure 5.1. Where the value for $k_1/k_2$ holds for both the tangential and the normal stiffness values, so $k_{n,1}/k_{n,2} = k_{s,1}/k_{s,2}$.

With both particle types having equal stiffnesses, the macroscopic expansion coefficient is almost in the middle of the two microscopic expansion coefficients. When comparing the hygroscopic expansion coefficients of the case where the stiffness is assumed not to be equal, it can be seen that the macro hygroscopic expansion coefficient shifts towards the value of the microscopic expansion coefficient of the more stiff particle type. This is what can be expected, since the more stiff particle behavior will be governing. This is the case for the results found from the equilibrium of stresses and the result found from the principle of virtual work.
Figure 5.1: Influence of the stiffness of the particles on the macroscopic hygroscopic expansion coefficient in the packing with 7357 particles.
5.2 Stress-Strain relationship

The influence of moisture on the stress-strain relationship of a particle packing such as the experimental particle packing of 514 hydrogel mono-disperse particles can be evaluated. The hygroscopic swelling can be implemented into GMA, with the force-displacement relations which were found in chapter 3 and the mechanical relationships found for swelling in section 4.1 (equations 4.4 to 4.7). Since the mechanical calculation in GMA uses averaged values to calculate a representative volume element, only one uniformly distributed hygroscopic expansion coefficient is used for the particles, thus the macroscopic expansion coefficient which comes from the homogenization is the same for both starting points.

In order to see the effect of a variation of hygroscopic expansion coefficients, a parametric study is done. Different isotropic hygroscopic expansion coefficients for the particles can be implemented with different changes in moisture content to evaluate the influence on the stress when the total strain is the same. In the following simulated experiments, the total moisture content increases linearly with the strain increments. This is done for a change in moisture content of 0, 10, 20 and 50 % at the final strain.

In figure 5.2, these increases in moisture content are combined with a hydrostatic loading. In figure 5.3, these increases in moisture content are combined with an uniaxial loading. These figures both show the results of a hygroscopic expansion coefficient of $\beta = 0.2$. Results for the stress-strain relationship with other hygroscopic expansion coefficients can be found in appendix G.

Figure 5.2: Influence of hygroscopic swelling coefficient of $\beta = 0.2$ on the stress-strain relationship for different changes in moisture content for hydrostatic compression.
The results show that the stress in the material increases due to hygroscopic swelling. The increase of this stress depends on the rate of the hygroscopic swelling. The hygroscopic swelling is dependent on the hygroscopic expansion coefficient ($\beta$) and the change in moisture content ($\Delta M$).

Figure 5.3: Influence of hygroscopic swelling coefficient of $\beta = 0.2$ on the stress-strain relationship for different changes in moisture content for uniaxial compression.

(a) In the direction of the loading

(b) Perpendicular to the loading
The goal of this research was to find an answer to the following research question: How does the swelling of individual particles influence the overall response of a granular microstructure and what is the interaction between the mechanical and the swelling response? The answer to this research question is found with theoretical research.

In order to evaluate the influence of the swelling on a particle packing and the interaction between the mechanical and the swelling response, a suitable and efficient mechanical model for a particle packing is found with the use of the granular micromechanics approach. From theory, it is found that the granular micromechanics approach is computationally less expensive than other methods which are used for the calculation of the mechanical behavior of granular material, this is because the granular micromechanics approach generalizes the contacts in all directions instead of looking at each individual direction separately. In this research, a good calibration method for the granular micromechanics approach is found, with a hydrogel particle packing. Both normal and tangential force-displacement relationships are found as exponential relationships in the form \( f = C \cdot \delta^p \). With calibrating the Granular micromechanics approach with a hydrostatic compression experiment, the best fit for the normal force-displacement relationship can be found. Then another type of loading can be used to derive the tangential force-displacement relationship. Without changing the normal and tangential force-displacement relationship, the results for the stress-strain relationship in GMA for a third type of loading is then a good assumption. The error of estimation is low and the \( R^2 \)-value is good. This resulted in an efficient and suitable mechanical model for the hydrogel particle packing. The same method of calibration can be used for other packings in the future.

The influence of swelling on a granular particle packing is found theoretically. In the case of swelling, the relative deformation between two grains not only depends on the relative displacement between two particle centroids, but also on the swelling of the particles. This results in an increase in stress due to the swelling of the particles. The rate of this increase depends on the amount of moisture that is absorbed and the particle hygroscopic swelling coefficient.
The influence of the swelling of a particle on the swelling of a granular particle packing is found with using homogenization. This can be done by starting from the principle of virtual work and by starting from the equilibrium of stresses. The influence of microscopic (particle) hygroscopic swelling coefficients on swelling of the packing could be found with the use of micro-macro relations which were found with the homogenization. Four equations are found when the homogenization starts with the principle of virtual work and two equations are found when the homogenization starts with the equilibrium of stresses. The first equation which is found for the homogenization of both starting points is the stiffness. The second equation which is found in both starting points is a relation for the macroscopic hygroscopic expansion coefficient. In the principle of virtual work two additional equations are found, the third equation found with this starting point is equal to the second equation which was found. The fourth equation is an additional equation.

When using a particle packing with just one type of microscopic expansion coefficient, the result for both principles of homogenization is the same. When the particle packing has different particle properties, the result of these two homogenization principles differs. How much it differs, depends on the difference in microscopic swelling coefficients and the absolute value of the swelling coefficients. The results which come from the equilibrium of stresses seem more likely, however, additional experimental or analytical research is needed to determine this further.
In Chapter 3, the experimental packing of hydrogel particles was used in DEM to simulate more loading paths. The simulation of the same loading as the experimental loading showed a difference between the DEM simulation and the experiment. The Hertz contact model was used and the nonlocal contact model was used. The results of both contact models differed from each other and from the experimental result. The reason for the difference of both contact models with the experimental results can be explored in further research.

This can be due to the fact that the particles are assumed frictionless in DEM. The influence of the use of a tangential contact model in DEM should be found. Doing hydrostatic loading experiments would make it possible to compare the DEM simulation of the normal contact law with the experimental data. Then another type of loading can be applied on the same experimental packing to look at the tangential contacts, which can then be researched in DEM.

The comparison between DEM and experimental results can be done in further research for more packings. Where more particle packings with the same properties should be used to look at the influence of the particle distributions. Also, the packing that is now used in the experiments is a relatively small packing, which can also cause the difference between the experimental results and the results in DEM. For that reason, the experiments should be done in the future with more particles.

In this research, the mechanical model is calibrated and validated with one experimental packing. In order to calibrate and validate better in future research, this should be done for numerous packings with the same properties. This is due to the fact that the particle distribution can have an influence on the mechanical behavior of the material. By using the mean of all samples and cancelling out the extremes, errors due to the particle distribution can be minimized.

The calculation of the hygroscopic swelling coefficient for the macroscopic packing or relative volume element in relation to the hygroscopic swelling coefficient for a particle should be experimentally or analytical further explored. The calculations can be done for micro-macro equations found with the principle of virtual work and with the equilibrium of stresses and can be compared. The influence of equation 5.4
should be explored further. Both results seem physically reasonable, however, the
results found from equilibrium seem more consistent, since scale does not influence
these results. Also, this is similar to what was found in literature, which makes the
results found from equilibrium seem more likely.

In this research, the micro-macro relation of the hygroscopic swelling of a particle
packing is explored with the kinematic constraint in the granular micromechanics
approach. We tried to do the same homogenization on the static constraint in the
granular micromechanics approach. However, due to the fact that the static constraint
is based on a relationship between force and stress, there is no direct relationship
with the hygroscopic expansion. This relationship should be found by finding the
least-squares of the relative displacement and the strain. This was done for two limits,
where there is only hygroscopic strain and where there is no hygroscopic strain. The
principle of superposition if then used for both limits and the homogenization can be
done for the micro-macro relationship of the hygroscopic expansion coefficient. The
result found for the micro-macro relationship of hygroscopic expansion coefficient in
the static constraint is not a physically possible result. For this reason, this is not
included in the thesis and this is a recommendation for further research.
Bibliography


Multiscale Analysis of Swelling and Mechanical Behavior of Granular media
Appendix
A GMA Kinematic constraint

This model was developed by Payam Poorsolhjouy and has been adapted.

Multiscale Analysis of Swelling and Mechanical Behavior of Granular media
s1 = -sin(theta.*1);
s2 = cos(theta.*1).*cos(phi.*1);
s3 = cos(theta.*1).*sin(phi.*1);
s = [s1, s2, s3];
t1 = zeros(length(theta), 1);
t2 = -sin(phi.*1);
t3 = cos(phi.*1);
t = [t1, t2, t3];

%% Apply strain
if LoadingType == 1 % Uniaxial compression
    e11s = -[0:0.001:10]'/100;
    e22s = zeros(size(e11s));
    e33s = zeros(size(e11s));
    e23s = zeros(size(e11s));
    e12s = zeros(size(e11s));
elseif LoadingType == 2 % Hydrostatic compression
    e11s = -[0:0.001:5]'/100;
    e22s = -[0:0.001:5]'/100;
    e33s = -[0:0.001:5]'/100;
    e23s = zeros(size(e11s));
    e13s = zeros(size(e11s));
    e12s = zeros(size(e11s));
elseif LoadingType == 3 % Biaxial compression
    e11s = -[0:0.001:7.5]'/100;
    e22s = -[0:0.001:7.5]'/100;
    e33s = zeros(size(e11s));
    e23s = zeros(size(e11s));
    e13s = zeros(size(e11s));
    e12s = zeros(size(e11s));
end

%% Solve for all steps
s11_int = zeros(size(e11s)); s22_int = zeros(size(e11s));...
s33_int = zeros(size(e11s));
s23_int = zeros(size(e11s)); s13_int = zeros(size(e11s));...
s12_int = zeros(size(e11s));
s11_ext = zeros(size(e11s)); s22_ext = zeros(size(e11s));...
s33_ext = zeros(size(e11s));
s23_ext = zeros(size(e11s)); s13_ext = zeros(size(e11s));...
s12_ext = zeros(size(e11s));
all_fn = zeros(ntheta, length(e11s));...
Appendix

```matlab
all_fw=zeros(ntheta,length(e11s));
all_dn=zeros(ntheta,length(e11s));
all_dw=zeros(ntheta,length(e11s));

for inc=2:length(e11s)
e11=e11s(inc); e22=e22s(inc); e33=e33s(inc);
e13=e13s(inc); e23=e23s(inc); e12=e12s(inc);

L0*(e11*n1+e12*n2+e13*n3);  % Delta 1
L0*(e12*n1+e22*n2+e23*n3);  % Delta 2
L0*(e13*n1+e23*n2+e33*n3);  % Delta 3

Delta_n=Delta_1.*n1+Delta_2.*n2+Delta_3.*n3;
Delta_s=Delta_1.*s1+Delta_2.*s2+Delta_3.*s3;
Delta_t=Delta_1.*t1+Delta_2.*t2+Delta_3.*t3;

Delta_w=(Delta_s.^2+Delta_t.^2).^0.5;
all_dn(:,inc)=Delta_n; all_dw(:,inc)=Delta_w;

if MaterialType==1
    [sn,sw,swn,dn,dw,v]=Local_Const_linear(forcen,forcew);
elseif MaterialType==2
    [sn,sw,swn,dn,dw,v]=Local_Const_new(forcen,forcew);
end

all_fn(:,inc)=fn; all_fw(:,inc)=fw;
fs=zeros(length(theta),1);
ft=zeros(length(theta),1);
for dw_check=1:length(theta)
    if abs(Delta_w(dw_check))>10^(-14)
        fs(dw_check)=fw(dw_check)*Delta_s(dw_check)/Delta_w(dw_check);
        ft(dw_check)=fw(dw_check)*Delta_t(dw_check)/Delta_w(dw_check);
    end
end

f1=fn.*n1+fs.*s1+ft.*t1;
f2=fn.*n2+fs.*s2+ft.*t2;
f3=fn.*n3+fs.*s3+ft.*t3;

s11_int(inc)=sum(f1.*n1.*xi)*L0*Np;  % S11
s22_int(inc)=sum(f2.*n2.*xi)*L0*Np;  % S22
s33_int(inc)=sum(f3.*n3.*xi)*L0*Np;  % S33
s23_int(inc)=sum(f2.*n3.*xi)*L0*Np;  % S23
s13_int(inc)=sum(f1.*n3.*xi)*L0*Np;  % S13
s12_int(inc)=sum(f1.*n2.*xi)*L0*Np;  % S12
k11=kn.*n1.*n1+kw.*(s1.*s1+t1.*t1);
```

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k12 = kn.*n1.*n2 + kw.*(s1.*s2 + t1.*t2);
k13 = kn.*n1.*n3 + kw.*(s1.*s3 + t1.*t3);
k21 = kn.*n2.*n1 + kw.*(s2.*s1 + t2.*t1);
k22 = kn.*n2.*n2 + kw.*(s2.*s2 + t2.*t2);
k23 = kn.*n2.*n3 + kw.*(s2.*s3 + t2.*t3);
k31 = kn.*n3.*n1 + kw.*(s3.*s1 + t3.*t1);
k32 = kn.*n3.*n2 + kw.*(s3.*s2 + t3.*t2);
k33 = kn.*n3.*n3 + kw.*(s3.*s3 + t3.*t3);

k = [k11 k12 k13; k21 k22 k23; k31 k32 k33];

% Calling Stiffness_Matrix function
[Cij,Cijkl] = Stiffness_Matrix(L2Np, k11, k12, k13, k21, k22, ... k23, k31, k32, k33, n1, n2, n3, xi);

Cijkl_inv = inv(Cijkl);

de11 = e11 - e11s*(inc-1); de22 = e22 - e22s*(inc-1); ...
de33 = e33 - e33s*(inc-1);
de23 = e23 - e23s*(inc-1); de13 = e13 - e13s*(inc-1); ...
de12 = e12 - e12s*(inc-1);

ds = Cij*[de11; de22; de33; 2*de23; 2*de13; 2*de12];

s11_ext(inc) = s11_ext(inc-1) + ds(1); ...
s22_ext(inc) = s22_ext(inc-1) + ds(2); ...
s33_ext(inc) = s33_ext(inc-1) + ds(3);
s23_ext(inc) = s23_ext(inc-1) + ds(4); ...
s13_ext(inc) = s13_ext(inc-1) + ds(5); ...
s12_ext(inc) = s12_ext(inc-1) + ds(6);
end
figure;
plot(e11s, s11_int,'o'); hold on;
plot(e11s, s11_ext,'.');
title('s11 kinematic constraint');
xlabel('Strain','FontName','Times New Roman','Interpreter','latex')
ylabel('Stress','FontName','Times New Roman','Interpreter','latex')
lgd1 = legend('external', 'internal');
set(lgd1,'Location','Southeast','FontSize',18,'FontName','Times New Roman');
set(gca,'FontSize',20,'FontName','Times New Roman')
grid on
figure;
plot(all_fn,'o');
xlabel('increment','FontName','Times New Roman','Interpreter','latex')
% Label the y-axis
ylabel('normal force (f_n)', 'FontName', 'Times New Roman')

% Set font size and name for the graph
set(gca, 'FontSize', 20, 'FontName', 'Times New Roman')

% Grid on the graph
grid on

toc

%% Function(s) Starting
%% Calculate forces

function [kn, kw, fn, fw] = Local_Const_linear(Δn, Δw)

kn = zeros(size(forcen));
kw = zeros(size(forcen));
fn = zeros(size(forcen));
fw = zeros(size(forcew));

for ctc = 1:length(Δn)
    dn = Δn(ctc); dw = Δw(ctc);
    if dn > 0  % tension
        coefn = 10;
        fn(ctc) = coefn * dn;
        kn(ctc) = coefn;
    else  % compression
        coefn = 10;
        fn(ctc) = coefn * dn;
        kn(ctc) = coefn;
    end

    coefw = 1/10;
    fw(ctc) = coefw * dw;
    kw(ctc) = coefw;
end

function [sn, sw, swn, dn, dw, v] = Local_Const_new(forcen, forcew)
This model is based on the model for the kinematic approach which was developed by Payam Poorsolhjouy.

```matlab
1 clear
2 close all
3 clc
4 tic
5
6 L0=0.021; % [m]
7 NumDens_Particles=514/(0.165654561787257+0.165906817693379 ...
  *[0.167365141711893]); % [1/m3]
8 MeanCoord=8;
9 Np=NumDens_Particles*MeanCoord/2; % number density of contacts ...
  [1/m3]
10 L2Np=L0^2*Np;
11
12 MaterialType=2;
13 %%% Linear material: 1
14 %%% new: 2
15
16 LoadingType=1;
17 %%% Uniaxial compression: 1
18 %%% Hydrostatic compression: 2
19 %%% Biaxial compression: 3
20
21 % Finding integration points
22 % [ xLEB, yLEB, zLEB, wLEB ] = ld0110 ( );
23 [ xLEB, yLEB, zLEB, wLEB ] = ld0590 ( );
24 % [ xLEB, yLEB, zLEB, wLEB ] = ld0006 ( );
25 % [ xLEB, yLEB, zLEB, wLEB ] = ld0974 ( );
26 % [ xLEB, yLEB, zLEB, wLEB ] = ld1202 ( );
27 theta=acos(zLEB);
28 phi = atan2(yLEB,xLEB);
29 a20=0;
30 a40=0;
31 xi_distribution=(1+(1/4)*a20*(3*cos(2*theta.*1)+1)+a40/8 ...
  *(35*(cos(theta)).^4-30*(cos(theta)).^2+3));
32 xi=xidistribution.*wLEB;
33 da20=0;
34 da40=0;
35 dxidistribution=(1+(1/4)*da20*(3*cos(2*theta.*1)+1)+da40/8 ...
  *(35*(cos(theta)).^4-30*(cos(theta)).^2+3));
```

B GMA Static constraint
dxidxidistribution.*wLEB;

ntheta=length(theta);

%%% direction cosines
n1=cos(theta.*1);
n2=sin(theta.*1).*cos(phi.*1);
n3=sin(theta.*1).*sin(phi.*1);
n=[n1,n2,n3];

s1=-sin(theta.*1);
s2=cos(theta.*1).*cos(phi.*1);
s3=cos(theta.*1).*sin(phi.*1);
s=[s1,s2,s3];

t1=zeros(length(theta),1);
t2=-sin(phi.*1);
t3=cos(phi.*1);
t=[t1,t2,t3];

%%% Fabric tensor
[Nij]=Fabric_tensor(L2Np, n1, n2, n3, s1, s2, s3, t1, t2, t3, dxid);

N11=Nij(1,1); N12=Nij(1,2); N13=Nij(1,3);
N21=Nij(2,1); N22=Nij(2,2); N23=Nij(2,3);
N31=Nij(3,1); N32=Nij(3,2); N33=Nij(3,3);

invNij=inv(Nij);

invN11=invNij(1,1); invN12=invNij(1,2); invN13=invNij(1,3);
invN21=invNij(2,1); invN22=invNij(2,2); invN23=invNij(2,3);
invN31=invNij(3,1); invN32=invNij(3,2); invN33=invNij(3,3);

%%% Apply strain
if LoadingType==1 %%% Uniaxial compression
    e11s=[0:0.001:10]'/100;
e22s=zeros(size(e11s));
e33s=zeros(size(e11s));
e23s=zeros(size(e11s));
e13s=zeros(size(e11s));
e12s=zeros(size(e11s));
elseif LoadingType==2 %%% Hydrostatic compression
    e11s=[0:0.001:5]'/100;
e22s=[0:0.001:5]'/100;
e33s=[0:0.001:5]'/100;
e23s=zeros(size(e11s));
e13s=zeros(size(e11s));
e12s=zeros(size(e11s));
elseif LoadingType==3 %%% Biaxial compression

```matlab
ell_s=[0:0.001:7.5]/100;
e22_s=[0:0.001:7.5]/100;
e33s=zeros(size(ell_s));
e23s=zeros(size(ell_s));
e13s=zeros(size(ell_s));
e12s=zeros(size(ell_s));
end

%% Solve for all steps
s11s=zeros(size(ell_s)); s22s=zeros(size(ell_s)); ... s33s=zeros(size(ell_s));
s23s=zeros(size(ell_s)); s13s=zeros(size(ell_s)); ... s12s=zeros(size(ell_s));
e11_int=zeros(size(ell_s)); e22_int=zeros(size(ell_s)); ... e33_int=zeros(size(ell_s));
e23_int=zeros(size(ell_s)); e13_int=zeros(size(ell_s)); ... e12_int=zeros(size(ell_s));

all_fn=zeros(ntheta,length(e11s));... all_fw=zeros(ntheta,length(e11s));
all_dn=zeros(ntheta,length(e11s));... all_dw=zeros(ntheta,length(e11s));

fn_max_T=zeros(ntheta,1);
fn_max_C=zeros(ntheta,1);

for inc=2:length(e11s)
    s11=s11s(inc-1); s22=s22s(inc-1); s33=s33s(inc-1);
    s23=s23s(inc-1); s13=s13s(inc-1); s12=s12s(inc-1);
    e11=e11s(inc); e22=e22s(inc); e33=e33s(inc);
    e23=e23s(inc); e13=e13s(inc); e12=e12s(inc);
    force1=L0*(s11*(invN11*n1)+s12*(invN22*n2)+s13*(invN33*n3));
    force2=L0*(s12*(invN11*n1)+s22*(invN22*n2)+s23*(invN33*n3));
    force3=L0*(s13*(invN11*n1)+s23*(invN22*n2)+s33*(invN33*n3));
    forcen=force1.*n1+force2.*n2+force3.*n3;
    forces=force1.*s1+force2.*s2+force3.*s3;
    forcen=force1.*t1+force2.*t2+force3.*t3;
    forcew=(forces.^2+forcen.^2).^.5;
    all_fn(:,inc)=forcen; all_fw(:,inc)=forcew;
    if MaterialType==1
        [sn,sw,swn,dn,dw,v]=Local_Const_linear(forcen,forcew);
    end
end
```
elseif MaterialType==2
    [sn, sw, swn, dn, dw, v] = LocalConst_new(forcen, forcew);
end

all_dn(:, inc) = dn; all_dw(:, inc) = dw;
ds = zeros(length(theta), 1);
dt = zeros(length(theta), 1);
for fw_check = 1:length(theta)
    if abs(forcew(fw_check)) > 10^(-14)
        ds(fw_check) = dw(fw_check) .* forces(fw_check) ./ forcew(fw_check);
dt(fw_check) = dw(fw_check) .* forcet(fw_check) ./ forcew(fw_check);
    end
end
d1 = dn .* n1 + ds .* s1 + dt .* t1;
d2 = dn .* n2 + ds .* s2 + dt .* t2;
d3 = dn .* n3 + ds .* s3 + dt .* t3;
e11_int(inc) = sum(d1 .* n1 .* xi) * L0 * Np * (invN11);
e22_int(inc) = sum(d2 .* n2 .* xi) * L0 * Np * (invN22);
e33_int(inc) = sum(d3 .* n3 .* xi) * L0 * Np * (invN33);
e23_int(inc) = sum(d2 .* n3 .* xi) * L0 * Np * (invN33);
e13_int(inc) = sum(d1 .* n3 .* xi) * L0 * Np * (invN33);
e12_int(inc) = sum(d1 .* n2 .* xi) * L0 * Np * (invN22);
comp11 = sn .* n1 .* n1 + sw .* ((s1 .* s1 + t1 .* t1) + swn .* (n1 .* s1 + n1 .* t1));
comp12 = sn .* n1 .* n2 + sw .* ((s1 .* s2 + t1 .* t2) + swn .* (n1 .* s2 + n1 .* t2));
comp13 = sn .* n1 .* n3 + sw .* ((s1 .* s3 + t1 .* t3) + swn .* (n1 .* s3 + n1 .* t3));
comp21 = sn .* n2 .* n1 + sw .* ((s2 .* s1 + t2 .* t1) + swn .* (n1 .* s2 + n1 .* t2));
comp22 = sn .* n2 .* n2 + sw .* ((s2 .* s2 + t2 .* t2) + swn .* (n2 .* s2 + n2 .* t2));
comp23 = sn .* n2 .* n3 + sw .* ((s2 .* s3 + t2 .* t3) + swn .* (n3 .* s2 + n2 .* t2));
comp31 = sn .* n3 .* n1 + sw .* ((s3 .* s1 + t3 .* t1) + swn .* (n1 .* s3 + n1 .* t3));
comp32 = sn .* n3 .* n2 + sw .* ((s3 .* s2 + t3 .* t2) + swn .* (n2 .* s3 + n2 .* t3));
comp33 = sn .* n3 .* n3 + sw .* ((s3 .* s3 + t3 .* t3) + swn .* (n3 .* s3 + n3 .* t3));

%Calling Compliance_tensor function
[Sij, Sijkl] = Compliance_tensor(L2Np, v, comp11, comp12, ...
    comp13, comp21, comp22, comp23, comp31, comp32, comp33, ...
    n1, n2, n3, s1, s2, s3, t1, t2, t3, xi, N11, N12, N13, ...
    N21, N22, N23, N31, N32, N33);
de11 = e11 - e11s(inc - 1); de22 = e22 - e22s(inc - 1); ...
    de33 = e33 - e33s(inc - 1);
de23 = e23 - e23s(inc - 1); de13 = e13 - e13s(inc - 1); ...
    de12 = e12 - e12s(inc - 1);
dss = Sij \ [de11; de22; de33; 2*de23; 2*de13; 2*de12];
% calculate stresses
s11s(inc,1)=s11+dss(1); s22s(inc,1)=s22+dss(2); ...  
   s33s(inc,1)=s33+dss(3);
  s23s(inc,1)=s23+dss(4); s13s(inc,1)=s13+dss(5); ...  
  s12s(inc,1)=s12+dss(6);
end

%% plot data
% adapt to loading type
figure;  
plot(e11_int, s22s,'bo');
hold on;
plot(e11s, s22s,'r.');
title('s22');
ylabel('Stress','FontName','Times New Roman','Interpreter','latex')
lgd1 = legend('internal','external');
set(lgd1,'Location','Southeast','FontSize',18,'FontName','Times New Roman');
set(gca,'FontSize',20,'FontName','Times New Roman')
grid on

figure;  
plot(e11_int, s11s,'bo');
hold on;
plot(e11s, s11s,'r.');  
title('s11');
ylabel('Stress','FontName','Times New Roman','Interpreter','latex')
lgd1 = legend('internal','external');
set(lgd1,'Location','Southeast','FontSize',18,'FontName','Times New Roman');
set(gca,'FontSize',20,'FontName','Times New Roman')
grid on

figure;  
plot(e11_int, s22s,'bo');
hold on;
plot(e11s, s22s,'r.');
title('s22');
ylabel('Stress','FontName','Times New Roman','Interpreter','latex')
lgd1 = legend('internal','external');
set(lgd1,'Location','Southeast','FontSize',18,'FontName','Times New Roman');
set(gca,'FontSize',20,'FontName','Times New Roman')
grid on

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Appendix

```matlab
figure;
plot(all_dn',all_fn');
title('Force − Displacement')
xlabel('Displacement','FontName','Times New Roman','Interpreter','latex')
ylabel('Force','FontName','Times New Roman','Interpreter','latex')
lgd1 = legend('Normal');
set(lgd1,'Location','Southeast','FontSize',18,'FontName','Times New Roman');
set(gca,'FontSize',20,'FontName','Times New Roman')
grid on

%% material functions
function [sn,sw,swn,dn,dw,v]=Local_Const_linear(forcen,forcew);
v=0.5; %poissons ratio
	dn=zeros(size(forcen)); dw=zeros(size(forcen));
    sn=zeros(size(forcen)); sw=zeros(size(forcen));
    swn=zeros(size(forcen));

    for ctc=1:length(forcen)
        fn=forcen(ctc); fw=forcew(ctc);
        if fn>0 %tension
            coefn=1/100;
            dn(ctc)=coefn*fn;
            sn(ctc)=coefn;
        else %compression
            coefn=1/100;
            dn(ctc)=coefn*fn;
            sn(ctc)=coefn;
        end
    end
    coefw=1/10;
    dw(ctc)=coefw*fw;
    sw(ctc)=coefw;
end

function [sn,sw,swn,dn,dw,v]=Local_Const_new(forcen,forcew)
end

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```
C Displacement-force relationship GMA

function [sn, sw, swn, dn, dw, v]=Local_Const_sqrt(forcen, forcew)
  %poissons ratio
  v=0.5;
  dn=zeros(size(forcen)); dw=zeros(size(forcen));
  sn=zeros(size(forcen)); sw=zeros(size(forcen));
  swn=zeros(size(forcen));
  for ctc=1:length(forcen)
    fn=forcen(ctc); fw=forcew(ctc);
    if fn>0 %tension
      pn=2;
      coefn=10000;
      fnthresh=0.0000001;
      dn(ctc)=coefn*(fn+fnthresh)^(pn);
      sn(ctc)=coefn*pw*(fn+fnthresh)^(pn−1);
    else %compression
      pn=1/1.65;
      coefn=1/225;
      fnthresh=1/10000000000000000000000000000000000000;
      dn(ctc)=−coefn*(abs(fn)+fnthresh)^(pn);
      sn(ctc)=coefn*pw*(abs(fn)+fnthresh)^(pn−1);
    end
  pw=1/1.5;
  coefw=1/35;
  fwthresh=1/10000000000000000000000000000000000000;
  dw(ctc)=coefw*(fw+fwthresh)^(pw);
  sw(ctc)=coefw*pw*(fw+fwthresh)^(pw−1);
end
end
The macroscopic work can be expressed by the macroscopic stress and the macroscopic elastic strain.

\[ W = \sigma_{ij} \varepsilon_{el}^{ij} \] (D.1)

The macroscopic stress is defined by the macroscopic constitutive relation, which is the stiffness tensor and the macroscopic elastic strain. This results in:

\[ W = C_{ijkl} \varepsilon_{el}^{kl} \varepsilon_{el}^{ij} \] (D.2)

The macroscopic elastic strain can be rewritten as the total strain and the hygroscopic strain.

\[ W = C_{ijkl} (\varepsilon_{kl}^{tot} - \beta_{kl} \Delta M) (\varepsilon_{ij}^{tot} - \beta_{ij} \Delta M) \] (D.3)

\[ W = C_{ijkl} (\varepsilon_{kl}^{tot} \varepsilon_{ij}^{tot} + \beta_{kl} \beta_{ij} \Delta M^2 - \varepsilon_{kl}^{tot} \beta_{ij} \Delta M - \varepsilon_{ij}^{tot} \beta_{kl} \Delta M) \] (D.4)

The microscopic work is the volume average of the force and the displacement.

\[ W = \frac{1}{V} \sum_{\alpha=1}^{N} f_{i}^{\alpha} \gamma_{i}^{\alpha} \] (D.6)

The force can be defined by the stiffness and the relative displacement.

\[ W = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ik}^{\alpha} \gamma_{k}^{\alpha \alpha} \gamma_{i}^{\alpha} \] (D.7)

The relative displacement can be filled in with the kinematic constraint.

\[ W = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ikl}^{\alpha} \gamma_{l}^{\alpha \alpha} \varepsilon_{el}^{ij} \varepsilon_{el}^{kl} \] (D.8)

Elastic strain can be replaced by the total strain and the hygroscopic strain.

\[ W = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ikl}^{\alpha} \gamma_{l}^{\alpha} (\varepsilon_{kl}^{tot} - \beta_{kl}^{\alpha} \Delta M) (\varepsilon_{ij}^{tot} - \beta_{ij}^{\alpha} \Delta M) \] (D.9)
The equation can be rewritten:

\[ W = \frac{1}{V} \sum_{a=1}^{N} K_{ikl}^{\alpha} p_a^{\alpha} (\varepsilon_{kl}^{\text{tot}} \varepsilon_{ij}^{\text{tot}} + \beta_{kl}^{\alpha} \beta_{ij}^{\alpha} \Delta M^2 - \varepsilon_{kl}^{\text{tot}} \beta_{ij}^{\alpha} \Delta M - \varepsilon_{ij}^{\text{tot}} \beta_{kl}^{\alpha} \Delta M) \]  

(D.10)  

\[ W = \left( \frac{1}{V} \sum_{a=1}^{N} K_{ikl}^{\alpha} p_a^{\alpha} \right) \varepsilon_{kl}^{\text{tot}} \varepsilon_{ij}^{\text{tot}} + \left( \frac{1}{V} \sum_{a=1}^{N} K_{ikl}^{\alpha} p_a^{\alpha} \beta_{ij}^{\alpha} \right) \Delta M^2 
- \left( \frac{1}{V} \sum_{a=1}^{N} K_{ikl}^{\alpha} p_a^{\alpha} \beta_{kl}^{\alpha} \right) \varepsilon_{ij}^{\text{tot}} \Delta M \]  

(D.11)  

With the use of the principle of virtual work, the micro and macro work can be set equal to each other.

\[ \sigma_{ij} \varepsilon_{ij} = \sum_{a=1}^{N} f_i^{\alpha} \gamma_i^{\alpha} \]  

(D.12)  

Having this micro-macro relationship for equations D.5 and D.11 gives the following relationships:

\[ C_{ijkl} \varepsilon_{kl}^{\text{tot}} \varepsilon_{ij}^{\text{tot}} = \left( \frac{1}{V} \sum_{a=1}^{N} K_{ikl}^{\alpha} p_a^{\alpha} \right) \varepsilon_{kl}^{\text{tot}} \varepsilon_{ij}^{\text{tot}} \]  

(D.13)  

\[ C_{ijkl} \varepsilon_{kl} \beta_{ij} \Delta M = \left( \frac{1}{V} \sum_{a=1}^{N} K_{ikl}^{\alpha} p_a^{\alpha} \beta_{ij}^{\alpha} \right) \varepsilon_{kl} \Delta M \]  

(D.14)  

\[ C_{ijkl} \varepsilon_{ij} \beta_{kl} \Delta M = \left( \frac{1}{V} \sum_{a=1}^{N} K_{ikl}^{\alpha} p_a^{\alpha} \beta_{kl}^{\alpha} \right) \varepsilon_{ij} \Delta M \]  

(D.15)  

\[ C_{ijkl} \beta_{kl} \beta_{ij} \Delta M^2 = \left( \frac{1}{V} \sum_{a=1}^{N} K_{ikl}^{\alpha} p_a^{\alpha} \beta_{kl}^{\alpha} \right) \beta_{ij} \Delta M^2 \]  

(D.16)  

With assuming that the total strain microscopically is equal to the total strain macroscopically, this results into:

\[ C_{ijkl} = \frac{1}{V} \sum_{a=1}^{N} K_{ikl}^{\alpha} p_a^{\alpha} \]  

(D.17)  

\[ C_{ijkl} \beta_{ij} = \frac{1}{V} \sum_{a=1}^{N} K_{ikl}^{\alpha} p_a^{\alpha} \beta_{ij}^{\alpha} \]  

(D.18)  

\[ C_{ijkl} \beta_{kl} = \frac{1}{V} \sum_{a=1}^{N} K_{ikl}^{\alpha} p_a^{\alpha} \beta_{kl}^{\alpha} \]  

(D.19)  

\[ C_{ijkl} \beta_{kl} \beta_{ij} = \frac{1}{V} \sum_{a=1}^{N} K_{ikl}^{\alpha} p_a^{\alpha} \beta_{kl}^{\alpha} \beta_{ij}^{\alpha} \]  

(D.20)
Where equations D.18 and D.19 can be rewritten into equations for the macro hygroscopic expansion coefficients:

\[ C_{ijkl} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ikl}^{\alpha} l_{ij}^{\alpha} \]  

(D.21)

\[ \beta_{ij} = C_{ijkl}^{-1} \frac{1}{V} \sum_{\alpha=1}^{N} K_{mkl}^{\alpha} l_{i}^{\alpha} \beta_{mn}^{\alpha} \]  

(D.22)

\[ \beta_{kl} = C_{ijkl}^{-1} \frac{1}{V} \sum_{\alpha=1}^{N} K_{imn}^{\alpha} l_{j}^{\alpha} \beta_{mn}^{\alpha} \]  

(D.23)

\[ C_{ijkl} \beta_{kl} \beta_{ij} = \frac{1}{V} \sum_{\alpha=1}^{N} K_{ikl}^{\alpha} l_{ij}^{\alpha} \beta_{kl}^{\alpha} \beta_{ij}^{\alpha} \]  

(D.24)
E Approximate solution homogenization kinematic approach

E.1 Equation 4.24

To get the approximate solution, the summation is changed to an integration over all directions [Poorsolhjouy, 2016]. This is done by rewriting equation D.18 into the normal and tangential components for the grain-pair stiffness tensor:

\[ C_{ijkl}^{\beta_{ij}} = \frac{1}{V} \sum_{\alpha=1}^{N} \left( (l^\alpha)^2 K_{n}^{\alpha} \beta_{n}^{\alpha} n_i^{\alpha} n_j^{\alpha} n_k^{\alpha} n_l^{\alpha} + (l^\alpha)^2 K_{s}^{\alpha} \beta_{s}^{\alpha} s_i^{\alpha} s_j^{\alpha} s_k^{\alpha} s_l^{\alpha} n_i^{\alpha} n_j^{\alpha} + (l^\alpha)^2 K_{t}^{\alpha} \beta_{t}^{\alpha} t_i^{\alpha} t_j^{\alpha} t_k^{\alpha} t_l^{\alpha} n_i^{\alpha} n_j^{\alpha} \right) \]  \hspace{1cm} (E.1)

Where in this equation, the terms in the summation are products of the directions as in figure 2.4. The summation can be changed from a summation over the total number of contacts into a summation over all directions (\( \theta \) and \( \phi \)) followed by a summation over all contacts (\( \rho \)) in each given direction:

\[ C_{ijkl} = \frac{1}{V} \sum_{\theta} \sum_{\phi} \left[ \left( \sum_{\rho} (l^\rho)^2 K_{n}^{\rho} \beta_{n}^{\rho} \right) n_i n_j n_k n_l \right. \]  
\[ + \left. \left( \sum_{\rho} (l^\rho)^2 K_{s}^{\rho} \beta_{s}^{\rho} \right) s_i s_j s_k n_i n_j \right. \]  
\[ + \left. \left( \sum_{\rho} (l^\rho)^2 K_{t}^{\rho} \beta_{t}^{\rho} \right) t_i t_j t_k n_i n_j \right] \]  \hspace{1cm} (E.2)

where \( N^\rho(\theta, \phi) \) is the number of grain-pair contacts for a given solid angle. The total number of contacts (\( N \)) in the packing is defined as:

\[ N = \sum_{\theta} \sum_{\phi} N^\rho(\theta, \phi) \]  \hspace{1cm} (E.3)

Considering, as an example, the first term in equation E.2, it is clear that the directional density distribution of \( l^2 k_{\alpha} \beta_{\alpha} \) can be defined as:

\[ \xi(\theta, \phi) = \frac{\sum_{\rho} (l^\rho)^2 K_{n}^{\rho} \beta_{n}^{\rho}}{\sum_{\alpha=1}^{N} (l^\alpha)^2 K_{n}^{\alpha} \beta_{n}^{\alpha}} \]  \hspace{1cm} (E.4)
which also guarantees that $\sum_\theta \sum_\phi \xi = 1$, an essential property of a probability distribution function. The average value of the term $l^2 k_n \beta_n$ is defined as:

$$\overline{P K_n^{\beta_m}} = \frac{\sum_{\alpha=1}^{N} (l^\alpha)^2 K_n^{\alpha} \beta_n^{\alpha}}{N}$$  \hspace{1cm} (E.5)$$

where the total number of contacts ($N$) in the material point can be defined as follows:

$$N = V \rho_c$$  \hspace{1cm} (E.6)$$

where $\rho_c$ is the number density of grain-pair interactions. Substituting equations E.4 and E.5 yields:

$$\sum_\rho (l^\rho)^2 K_n^{\rho} \beta_n^{\rho} = \xi(\theta, \phi) N \overline{P K_n^{\beta_m}}$$  \hspace{1cm} (E.7)$$

where $\xi$ represent the directional distribution of contact size and stiffness coefficients and enables the analysis of materials with different levels of anisotropy. For isotropic materials, as the directional distribution of contact properties should be uniform, naturally $\xi$ reduces to a mere normalization coefficient equal to $\frac{1}{4\pi}$, which ensures that $\int_\theta^\pi \int_\phi^{2\pi} \xi(\theta, \phi) \sin \theta d\phi d\theta = 1$.

These steps can be done for the tangential terms in equation E.2 as well and then the average with the density distribution function can be filled in and equation E.2 can be rewritten into an integration.

$$C_{ijkl} \beta_{ij} = l^2 \rho_c \int_\theta^\pi \int_\phi^{2\pi} (K_{ik} \beta_{ij} n_i n_j) \xi \sin \theta d\phi d\theta$$  \hspace{1cm} (E.8)$$

E.2 Equation 4.25

The same thing is done for equation D.19, which results in the following:

$$C_{ijkl} \beta_{kl} = l^2 \rho_c \int_\theta^\pi \int_\phi^{2\pi} (K_{ik} \beta_{kl} n_i n_j) \xi \sin \theta d\phi d\theta$$  \hspace{1cm} (E.9)$$

E.3 Equation 4.26

To get the approximate solution, the summation is changed to an integration over all directions [Poorsollijouy, 2016]. This is done by rewriting equation D.20 into the normal and tangential components for the grain-pair stiffness tensor.
Where in this equation, the terms in the summation are products of the directions as in figure 2.4. The summation can be changed from a summation over the total number of contacts into a summation over all directions ($\theta$ and $\phi$) followed by a summation over all contacts ($\rho$) in each given direction:

\[
C_{ijkl} = \frac{1}{V} \sum_{\alpha=1}^{N} \left( \sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}\right)
\]

Considering, as an example, the first term in equation E.11, it is clear that the directional density distribution of $l^{2}K_{n}\beta_{n}\beta_{n}$ can be defined as:

\[
\xi(\theta, \phi) = \frac{\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}}{\sum_{\alpha=1}^{N}(l^{\alpha})^{2}K_{\alpha}^{\alpha}\beta_{\alpha}^{\alpha}}
\]

which also guarantees that $\sum_{\theta}\sum_{\phi} \xi = 1$, an essential property of a probability distribution function. The average value of the term $l^{2}K_{n}\beta_{n}\beta_{n}$ is defined as:

\[
[l^{2}K_{n}\beta_{n}\beta_{n}] = \frac{\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}\sum_{\rho}(l^{\rho})^{2}K_{\rho}^{\alpha}\beta_{\rho}^{\alpha}}{N}
\]

where the total number of contacts ($N$) in the material point can be defined as follows:

\[
N = V_{\rho c}
\]
where $\rho_c$ is the number density of grain-pair interactions. Substituting equations E.13 and E.14 yields:

$$\sum_p (l^p)^2 K_{n}^p \beta_n^p \beta_n^p = \xi(\theta, \phi) N^2 K_{n}^{m} \beta_n^m \beta_n^m$$

(E.16)

where $\xi$ represent the directional distribution of contact size and stiffness coefficients and enables the analysis of materials with different levels of anisotropy. For isotropic materials, as the directional distribution of contact properties should be uniform, naturally $\xi$ reduces to a mere normalization coefficient equal to $\frac{1}{4\pi}$, which ensures that $\int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \xi(\theta, \phi) \sin \theta d\theta d\phi = 1$.

These steps can be done for the tangential terms in equation E.11 as well and then the average with the density distribution function can be filled in and equation E.11 can be rewritten into an integration.

$$C_{ijkl} \beta_{ij} \beta_{kl} = l^2 \rho_c \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (K_{ik} \beta_{ij}^m \beta_{kl}^m \beta_{ij}^m) \xi \sin \theta d\phi d\theta$$

(E.17)
F Results swelling Micro-Macro

F.1 Experimental particle packing with 514 mono-disperse hydrogel particles

Table F.1: Micro-macro relationship mono-disperse particle packing $\beta^\alpha = 0.001$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$\beta_{ij} \cdot C_{ijkl} \cdot \beta_{ij} \cdot \beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.001</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.001</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.001</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-2.28E-19</td>
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<tr>
<td>$\beta_{13}$</td>
<td>3.89E-19</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-4.52E-19</td>
</tr>
</tbody>
</table>

Table F.2: Micro-macro relationship mono-disperse particle packing $\beta^\alpha = 0.01$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$\beta_{ij} \cdot C_{ijkl} \cdot \beta_{ij} \cdot \beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.01</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.01</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.01</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-6.02262E-18</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>3.60617E-18</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-4.73143E-18</td>
</tr>
</tbody>
</table>

Table F.3: Micro-macro relationship mono-disperse particle packing $\beta^\alpha = 0.1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$\beta_{ij} \cdot C_{ijkl} \cdot \beta_{ij} \cdot \beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.1</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.1</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.1</td>
</tr>
<tr>
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<td>-1.94547E-17</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>3.19702E-17</td>
</tr>
</tbody>
</table>
Appendix

Table F.4: Micro-macro relationship mono-disperse particle packing $\beta^a = 1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}\beta_{ij}\beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>1 LHS 1315.725</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>1 RHS 1315.725</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>1 error 0</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-2.19057E-17</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>5.48856E-18</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
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</tr>
</tbody>
</table>

Table F.5: Micro-macro relationship mono-disperse particle packing $\beta^a = 10$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}\beta_{ij}\beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>10 LHS 131572.5</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>10 RHS 131572.5</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>10 error 0</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-5.31885E-15</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-2.26125E-15</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-2.80471E-15</td>
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</table>
F.2 Experimental particle packing with 1921 bi-disperse hydrogel particles

Table F.6: Micro-macro relationship bi-disperse particle packing $\beta_1^\alpha = \beta_2^\alpha = 0.001$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$\beta_{ij}^\alpha = 0.001$</th>
<th>$\beta_{ij}^\alpha = 0.001$</th>
<th>$C_{ijkl}\beta_{ij}\beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.001</td>
<td>LHS</td>
<td>0.002754</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.001</td>
<td>RHS</td>
<td>0.002754</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.001</td>
<td>error</td>
<td>0</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-3.44E-19</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-2.03E-19</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>6.52E-19</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table F.7: Micro-macro relationship bi-disperse particle packing $\beta_1^\alpha = \beta_2^\alpha = 0.01$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$\beta_{ij}^\alpha = 0.01$</th>
<th>$\beta_{ij}^\alpha = 0.01$</th>
<th>$C_{ijkl}\beta_{ij}\beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.01</td>
<td>LHS</td>
<td>0.275427</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.01</td>
<td>RHS</td>
<td>0.275427</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.01</td>
<td>error</td>
<td>0</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-9.32E-18</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-6.13E-18</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-9.43E-18</td>
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</tr>
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</table>

Table F.8: Micro-macro relationship bi-disperse particle packing $\beta_1^\alpha = \beta_2^\alpha = 0.1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$\beta_{ij}^\alpha = 0.1$</th>
<th>$\beta_{ij}^\alpha = 0.1$</th>
<th>$C_{ijkl}\beta_{ij}\beta_{kl}$</th>
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<tr>
<td>$\beta_{11}$</td>
<td>0.1</td>
<td>LHS</td>
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<tr>
<td>$\beta_{22}$</td>
<td>0.1</td>
<td>RHS</td>
<td>27.5427</td>
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<tr>
<td>$\beta_{33}$</td>
<td>0.1</td>
<td>error</td>
<td>0</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>1.56E-17</td>
<td></td>
<td></td>
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<tr>
<td>$\beta_{13}$</td>
<td>-2.03E-17</td>
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<td></td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>1.29E-17</td>
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</table>
### Table F.9: Micro-macro relationship bi-disperse particle packing $\beta_1^\alpha = \beta_2^\alpha = 1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}\beta_{ij}\beta_{kl}$</th>
<th>LHS 2754.27</th>
<th>RHS 2754.27</th>
<th>error 0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
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</tr>
<tr>
<td>$\beta_{22}$</td>
<td>1</td>
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<td></td>
<td></td>
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<tr>
<td>$\beta_{33}$</td>
<td>1</td>
<td></td>
<td></td>
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<tr>
<td>$\beta_{23}$</td>
<td>1.43E-16</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>$\beta_{13}$</td>
<td>6.36E-17</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\beta_{12}$</td>
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</tbody>
</table>

### Table F.10: Micro-macro relationship bi-disperse particle packing $\beta_1^\alpha = \beta_2^\alpha = 10$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}\beta_{ij}\beta_{kl}$</th>
<th>LHS 275427</th>
<th>RHS 275427</th>
<th>error 0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>10</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>10</td>
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<tr>
<td>$\beta_{33}$</td>
<td>10</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-2.95E-15</td>
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<tr>
<td>$\beta_{13}$</td>
<td>1.47E-15</td>
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<td></td>
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</tr>
<tr>
<td>$\beta_{12}$</td>
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</tbody>
</table>

### Table F.11: Micro-macro relationship bi-disperse particle packing $\beta_1^\alpha = 0.1$ and $\beta_2^\alpha = 0.2$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}\beta_{ij}\beta_{kl}$</th>
<th>LHS 69.74104</th>
<th>RHS 73.24477</th>
<th>error 3.50373</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.160093</td>
<td></td>
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<td>$\beta_{11}$ 0.160527</td>
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<tr>
<td>$\beta_{22}$</td>
<td>0.155941</td>
<td></td>
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<td>$\beta_{22}$ 0.15646</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.161401</td>
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<td>$\beta_{33}$ 0.162042</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
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<td></td>
<td>$\beta_{23}$ -8.32E-04</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
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<td></td>
<td></td>
<td>$\beta_{13}$ -1.06E-02</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-2.19E-03</td>
<td></td>
<td></td>
<td></td>
<td>$\beta_{12}$ -1.60E-03</td>
</tr>
</tbody>
</table>

$(residual)^2$ 10.6494  
$R^2$ 0.999832

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Table F.12: Micro-macro relationship bi-disperse particle packing $\beta_1^\alpha = 0.01$ and $\beta_2^\alpha = 0.1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}\beta_{ij}\beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.064084</td>
<td>LHS 11.00487</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.060347</td>
<td>RHS 13.8429</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
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<td>error 2.838021</td>
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<tr>
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<td>$\beta_{13}$</td>
<td>-1.01E-02</td>
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<tr>
<td>$\beta_{12}$</td>
<td>-1.97E-03</td>
<td>$\beta_{12}$</td>
</tr>
</tbody>
</table>

$\sum (\text{residual})^2 = 7.8634$

$R^2 = 0.99923$

Table F.13: Micro-macro relationship bi-disperse particle packing $\beta_1^\alpha = 0.01$ and $\beta_2^\alpha = 1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}\beta_{ij}\beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.604921</td>
<td>LHS 976.0845</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.563812</td>
<td>RHS 1319.485</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.617869</td>
<td>error 343.4006</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-1.00E-02</td>
<td>$\beta_{23}$</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-1.11E-01</td>
<td>$\beta_{13}$</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-2.17E-02</td>
<td>$\beta_{12}$</td>
</tr>
</tbody>
</table>

$\sum (\text{residual})^2 = 3.47E+04$

$R^2 = 0.981667$
## Appendix

### F.3 Particle packing with 7357 particles

#### One particle type

Table F.14: Micro-macro relationship packing with 7357 particles $\beta^a = 0.001$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl} \beta_{ij} \beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.001</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.001</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.001</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>8.49E-20</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>5.84E-20</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>7.52E-20</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl} \beta_{ij} \beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>LHS 235590.8</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>RHS 235590.8</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>error 0</td>
</tr>
</tbody>
</table>

Table F.15: Micro-macro relationship packing with 7357 particles $\beta^a = 0.01$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl} \beta_{ij} \beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.01</td>
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<tr>
<td>$\beta_{22}$</td>
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</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.01</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>2.72E-18</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>2.30E-19</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>1.36E-19</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl} \beta_{ij} \beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>LHS 23559078</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>RHS 23559078</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>error 0</td>
</tr>
</tbody>
</table>

Table F.16: Micro-macro relationship packing with 7357 particles $\beta^a = 0.1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl} \beta_{ij} \beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
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</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.1</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.1</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>1.79E-17</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-4.14E-17</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-2.19E-17</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl} \beta_{ij} \beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>LHS 2.36E+09</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>RHS 2.36E+09</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>error 0</td>
</tr>
</tbody>
</table>

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Table F.17: Micro-macro relationship packing with 7357 particles $\beta^a = 1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl} \beta_{ij} \beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>LHS 2.36E+11</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>RHS 2.36E+11</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>error 0</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>3.25E-17</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-2.22E-17</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-1.73E-17</td>
</tr>
</tbody>
</table>

Table F.18: Micro-macro relationship packing with 7357 particles $\beta^a = 10$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl} \beta_{ij} \beta_{kl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>LHS 2.36E+13</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>RHS 2.36E+13</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>error 0</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>2.85E-15</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-1.09E-15</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-2.11E-15</td>
</tr>
</tbody>
</table>

Two different types of particles with equal stiffnesses

Table F.19: Micro-macro relationship packing with 7357 particles, two particle types with equal stiffnesses $\beta^a_1 = 0.1$ and $\beta^a_2 = 0.2$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl} \beta_{ij} \beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>LHS 5.32E+09</td>
<td>$\beta_{11}$ 0.150906</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>RHS 5.61E+09</td>
<td>$\beta_{22}$ 0.151144</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>error 2.91E+08</td>
<td>$\beta_{33}$ 0.150254</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>2.52E-04</td>
<td>$\beta_{23}$ 2.65E-04</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-2.97E-05</td>
<td>$\beta_{13}$ -1.23E-05</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>4.92E-04</td>
<td>$\beta_{12}$ 5.13E-04</td>
</tr>
</tbody>
</table>

(residual)$^2$ 7.46E+16

$R^2$ 0.999823

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Appendix

Table F.20: Micro-macro relationship packing with 7357 particles, two particle types with equal stiffnesses \( \beta_1^a = 0.01 \) and \( \beta_2^a = 0.1 \)

<table>
<thead>
<tr>
<th>( \beta_{ij} )</th>
<th>( C_{ijkl} \beta_{ij} \beta_{kl} )</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \beta_{11} )</td>
<td>0.055293</td>
<td>LHS 7.19E+08</td>
</tr>
<tr>
<td>( \beta_{22} )</td>
<td>0.055511</td>
<td>RHS 9.54E+08</td>
</tr>
<tr>
<td>( \beta_{33} )</td>
<td>0.054926</td>
<td>error 2.36E+08</td>
</tr>
<tr>
<td>( \beta_{23} )</td>
<td>2.27E-04</td>
<td></td>
</tr>
<tr>
<td>( \beta_{13} )</td>
<td>-2.68E-05</td>
<td></td>
</tr>
<tr>
<td>( \beta_{12} )</td>
<td>4.43E-04</td>
<td></td>
</tr>
</tbody>
</table>

\((\text{residual})^2\) 5.46E+16

\( R^2 \) 0.999063

Table F.21: Micro-macro relationship packing with 7357 particles, two particle types with equal stiffnesses \( \beta_1^a = 0.01 \) and \( \beta_2^a = 1 \)

<table>
<thead>
<tr>
<th>( \beta_{ij} )</th>
<th>( C_{ijkl} \beta_{ij} \beta_{kl} )</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \beta_{11} )</td>
<td>0.508228</td>
<td>LHS 6.07E+10</td>
</tr>
<tr>
<td>( \beta_{22} )</td>
<td>0.510621</td>
<td>RHS 8.92E+10</td>
</tr>
<tr>
<td>( \beta_{33} )</td>
<td>0.504188</td>
<td>error 2.85E+10</td>
</tr>
<tr>
<td>( \beta_{23} )</td>
<td>2.50E-03</td>
<td></td>
</tr>
<tr>
<td>( \beta_{13} )</td>
<td>-2.94E-04</td>
<td></td>
</tr>
<tr>
<td>( \beta_{12} )</td>
<td>4.87E-03</td>
<td></td>
</tr>
</tbody>
</table>

\((\text{residual})^2\) 2.93E+20

\( R^2 \) 0.968336

Table F.22: Micro-macro relationship packing with 7357 particles, two particle types with equal stiffnesses \( \beta_1^a = 0.001 \) and \( \beta_2^a = 0.1 \)

<table>
<thead>
<tr>
<th>( \beta_{ij} )</th>
<th>( C_{ijkl} \beta_{ij} \beta_{kl} )</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \beta_{11} )</td>
<td>0.050177</td>
<td>LHS 5.95E+08</td>
</tr>
<tr>
<td>( \beta_{22} )</td>
<td>0.049938</td>
<td>RHS 8.8E+08</td>
</tr>
<tr>
<td>( \beta_{33} )</td>
<td>0.050581</td>
<td>error 2.85E+08</td>
</tr>
<tr>
<td>( \beta_{23} )</td>
<td>-2.50E-04</td>
<td></td>
</tr>
<tr>
<td>( \beta_{13} )</td>
<td>2.94E-05</td>
<td></td>
</tr>
<tr>
<td>( \beta_{12} )</td>
<td>-4.87E-04</td>
<td></td>
</tr>
</tbody>
</table>

\((\text{residual})^2\) 8.02E+16

\( R^2 \) 0.99834

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Two different types of particles with different stiffnesses

Table F.23: Micro-macro relationship packing with 7357 particles, two particle types with different stiffnesses $\beta_1^\alpha = 0.1$ and $\beta_2^\alpha = 0.2$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}\beta_{ij}\beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.15859</td>
<td>$\beta_{11}$ 0.159159</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.15865</td>
<td>$\beta_{22}$ 0.159213</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.158229</td>
<td>$\beta_{33}$ 0.158563</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>1.47E-04</td>
<td>$\beta_{23}$ 1.55E-04</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>2.05E-04</td>
<td>$\beta_{13}$ 2.30E-04</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>7.39E-04</td>
<td>$\beta_{12}$ 7.65E-04</td>
</tr>
</tbody>
</table>

$LHS = 8.89E+09$, $RHS = 9.3E+09$, error = 4.13E+08

$(\text{residual})^2 = 1.48E+17$, $R^2 = 0.99986$

---

Table F.24: Micro-macro relationship packing with 7357 particles, two particle types with different stiffnesses $\beta_1^\alpha = 0.2$ and $\beta_2^\alpha = 0.1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}\beta_{ij}\beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.14141</td>
<td>$\beta_{11}$ 0.141929</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.14135</td>
<td>$\beta_{22}$ 0.14186</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.141771</td>
<td>$\beta_{33}$ 0.142083</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-1.47E-04</td>
<td>$\beta_{23}$ -1.49E-04</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-2.05E-04</td>
<td>$\beta_{13}$ -1.95E-04</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-7.39E-04</td>
<td>$\beta_{12}$ -7.66E-04</td>
</tr>
</tbody>
</table>

$LHS = 7.09E+09$, $RHS = 7.5E+09$, error = 4.13E+08

$(\text{residual})^2 = 1.52E+17$, $R^2 = 0.99982$
### Table F.25: Micro-macro relationship packing with 7357 particles, two particle types with different stiffnesses $\beta_1^\alpha = 0.01$ and $\beta_2^\alpha = 0.1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}^\beta_{ij}\beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.062731</td>
<td>LHS 1.39E+09</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.062785</td>
<td>RHS 1.72E+09</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.062407</td>
<td>error 3.34E+08</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>1.32E-04</td>
<td></td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>1.85E-04</td>
<td></td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>6.65E-04</td>
<td></td>
</tr>
</tbody>
</table>

(residual)$^2$: 1.09E+17

$R^2$: 0.999353

### Table F.26: Micro-macro relationship packing with 7357 particles, two particle types with different stiffnesses $\beta_1^\alpha = 0.1$ and $\beta_2^\alpha = 0.01$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}^\beta_{ij}\beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.047269</td>
<td>LHS 7.94E+08</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.047215</td>
<td>RHS 1.13E+09</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.047593</td>
<td>error 3.34E+08</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-1.32E-04</td>
<td></td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-1.85E-04</td>
<td></td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-6.65E-04</td>
<td></td>
</tr>
</tbody>
</table>

(residual)$^2$: 1.10E+17

$R^2$: 0.998866

### Table F.27: Micro-macro relationship packing with 7357 particles, two particle types with different stiffnesses $\beta_1^\alpha = 0.01$ and $\beta_2^\alpha = 1$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}^\beta_{ij}\beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.590046</td>
<td>LHS 1.23E+11</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.590639</td>
<td>RHS 1.63E+11</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.586472</td>
<td>error 4.04E+10</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>1.45E-03</td>
<td></td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>2.03E-03</td>
<td></td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>7.32E-03</td>
<td></td>
</tr>
</tbody>
</table>

(residual)$^2$: 4.92E+20

$R^2$: 0.983506

---

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Table F.28: Micro-macro relationship packing with 7357 particles, two particle types with different stiffnesses $\beta_1^\alpha = 1$ and $\beta_2^\alpha = 0.01$

<table>
<thead>
<tr>
<th>$\beta_{ij}$</th>
<th>$C_{ijkl}/\beta_{ij}\beta_{kl}$</th>
<th>Least square approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{11}$</td>
<td>0.419954</td>
<td>$\beta_{11}$ 0.524499</td>
</tr>
<tr>
<td>$\beta_{22}$</td>
<td>0.419361</td>
<td>$\beta_{22}$ 0.520038</td>
</tr>
<tr>
<td>$\beta_{33}$</td>
<td>0.423528</td>
<td>$\beta_{33}$ 0.439607</td>
</tr>
<tr>
<td>$\beta_{23}$</td>
<td>-1.45E-03</td>
<td>$\beta_{23}$ -1.00E-02</td>
</tr>
<tr>
<td>$\beta_{13}$</td>
<td>-2.03E-03</td>
<td>$\beta_{13}$ 1.00E-02</td>
</tr>
<tr>
<td>$\beta_{12}$</td>
<td>-7.32E-03</td>
<td>$\beta_{12}$ -1.00E-02</td>
</tr>
</tbody>
</table>

(Residual)$^2$ 7.26E+20

$R^2$ 0.944878
G  Swelling of particles GMA Kinematic approach

Figure G.1: Influence of a change in moisture content of $\Delta M = 10\%$ on the stress-strain relationship for different hygroscopic swelling coefficients for hydrostatic compression

Figure G.2: Influence of hygroscopic swelling coefficient of $\beta = 0.05$ on the stress-strain relationship for different changes in moisture content for hydrostatic compression
Figure G.3: Influence of hygroscopic swelling coefficient of $\beta = 0.1$ on the stress-strain relationship for different changes in moisture content for hydrostatic compression.

Figure G.4: Influence of hygroscopic swelling coefficient of $\beta = 0.2$ on the stress-strain relationship for different changes in moisture content for hydrostatic compression.
(a) In the direction of the loading

(b) Perpendicular to the loading

Figure G.5: Influence of hygroscopic swelling coefficient of $\beta = 0.05$ on the stress-strain relationship for different changes in moisture content for uniaxial compression.
Figure G.6: Influence of hygroscopic swelling coefficient of $\beta = 0.1$ on the stress-strain relationship for different changes in moisture content for uniaxial compression.
Appendix

Figure G.7: Influence of hygroscopic swelling coefficient of $\beta = 0.2$ on the stress-strain relationship for different changes in moisture content for uniaxial compression.

(a) In the direction of the loading

(b) Perpendicular to the loading