



Master thesis

PACKING STRUCTURE OF POWDER COMPACTS

Presenter: Aidana Boribayeva
Advisor: Boris Golman
Co-Advisor: Assiya Yermukhambetova

TABLE OF CONTENTS

01

PROBLEM STATEMENT

Importance of packing particles
and particle's parameters

02

AIM OF MASTHER THESIS

Main idea of research

03

METHODOLOGY

Description of methodologies

04

RESULTS & DISCUSSION

Results and findings of research

05

CONCLUSIONS & RECOMMENDATIONS

Important results of research and
recommendations for further research

06

REFERENCE LIST

List of used literatures

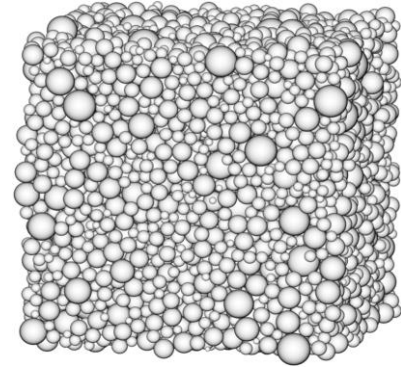
Why Packing Powder Compacts?



(<http://greenconnectionsradio.com/taking-electric-cars-mainstream/>)

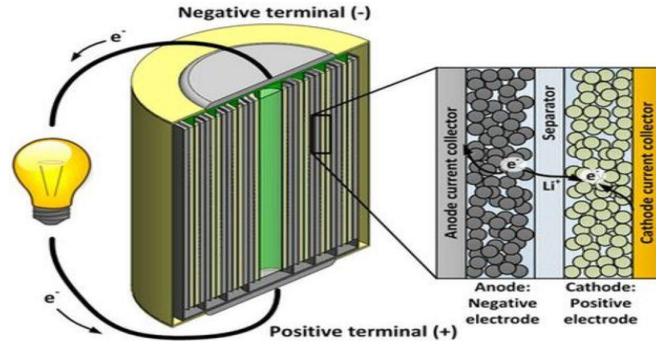
Be eco-friendly → Electro cars

My research project



(<https://pubs.rsc.org/en/content/articlehtml/2014/sm/c3sm52959b>).

Powder compact



(<https://www.bbc.com/news/magazine-26993915>).

Powerful battery

01

PACKING PARTICLES IMPORTANCE

- a wide range of applications: granular materials, composite materials, ceramics, construction materials, etc.
- minimization of the concrete pollution through modification of concrete mixture via particle packing method [1]
- microstructural arrangement of particles packing would better infer the chemical and physical properties of Portland Cement [2]

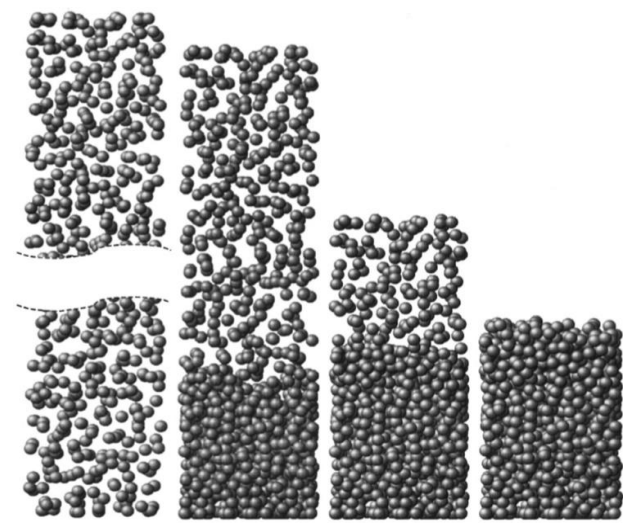


Figure 1: Simulation of packing spherical particles using DEM [5]

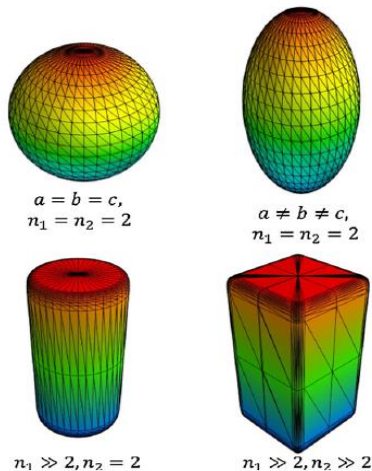


Figure 2: Superquadrics [6]

PARTICLE PARAMETERS EFFECT

- particle size distribution which influence on either volumetric or contact properties in a packing structure [3]
- the effect of non-spherical particles packing can significantly impact to the mechanical characteristics of material [4]
- limited research on packing of non-spherical particles

The AIM of the thesis research

Objectives:

- (1) generation of powder compact with particles of various shapes using Discrete Element Method,
- (2) analysis of void spaces morphology using Voronoi Tessellation and void size distribution methodologies.

!!!

the recent works are limited to particles of spherical shape

is to ANALYZE packing structure and morphology of powder compacts made of particles of different shapes and binary mixture of spheres with fibers.

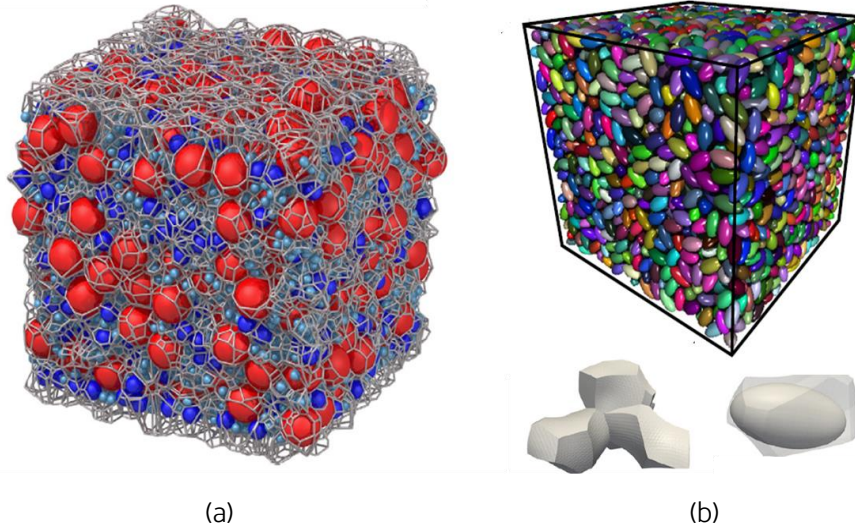


Figure 3: Application of Voronoi tessellation for spherical (a) and non-spherical (b) mixtures compact [7, 8]

STUDY 1

Effect of particle shapes on powder compact microstructure

- Generation forms of superquadrics and regarding compacts using DEM [9]

$$f(x, y, z) = \left(\left| \frac{x}{a} \right|^{n_2} + \left| \frac{y}{b} \right|^{n_2} \right)^{\frac{n_1}{n_2}} + \left| \frac{z}{c} \right|^{n_1} - 1 = 0$$

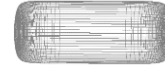
Mechanical properties	Young's modulus, [Pa]	$5 \cdot 10^6$
	Poisson ratio	0.4
	Restitution coefficient	0.6
	Friction coefficient	0.4
DEM parameters	Time-step, Δt [s]	$1 \cdot 10^{-5}$
	Gravity, g [m/s ²]	9.81
Particles physical properties	Density, kg/cm ³	2500

Preparation for analysis:

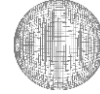
- Image analysis of cross-sections (Void size distribution)
- Voronoi diagram analysis



PILLS



CYLINDERS



SPHERES

a, m	0.004	0.004	0.0061
b, m	0.004	0.004	0.0061
c, m	0.01	0.0095	0.0061
n_1	3	10	2
n_2	3	2	2

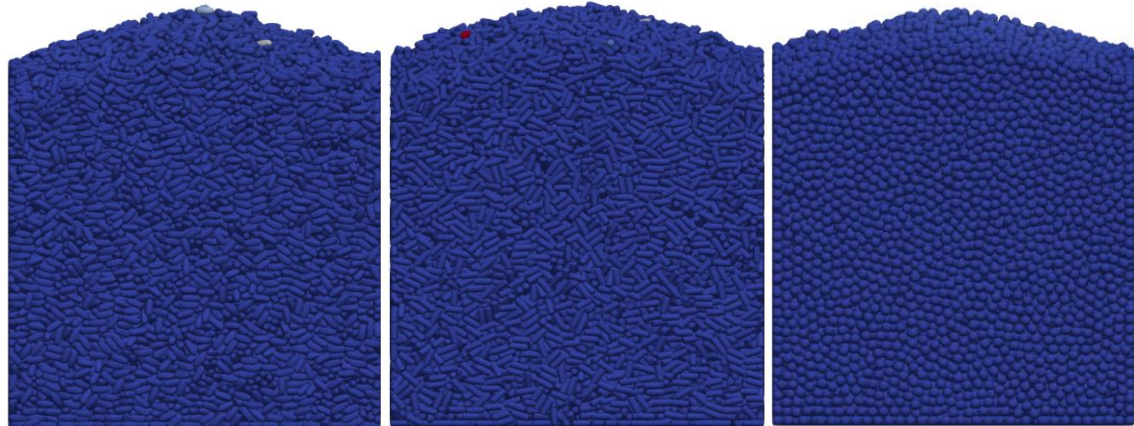
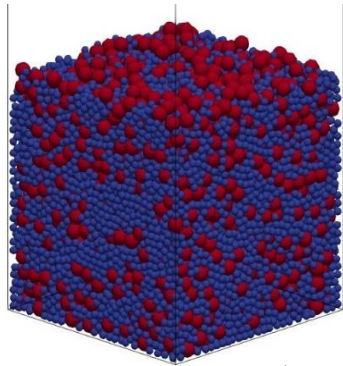


Figure 4: Visualization of packed compacts

STUDY 2

Effect of non-spherical particles inclusion into spherical powder compact mixture

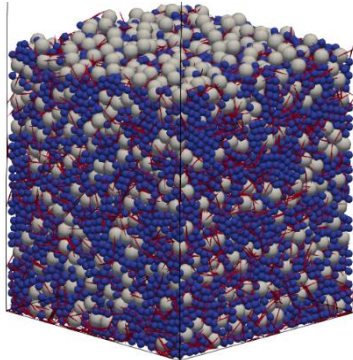
- Generation forms of superquadrics and their compacts using DEM



Binary mixture of spherical particles

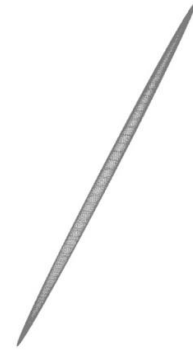
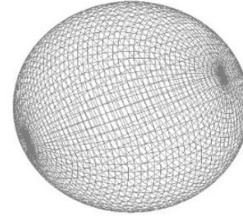


Binary mixture with fibers



Preparation for analysis:

- Image analysis of cross-sections (Void size distribution)



	Fine spherical	Coarse spherical	Fibers
a, m	0.002	0.004	0.0002875
b, m	0.002	0.004	0.0002875
c, m	0.002	0.004	0.006
n_1	2	2	2
n_2	2	2	2

Simulation	Fine	Coarse	Fiber
1	63	37	0
2	62	37	1
3	40	60	0
4	40	59	1

Figure 5: The images of packing structure

- Void size distribution analysis based on the cross-sectional images analysis

STUDY 1 Effect of particle shapes on compact morphology

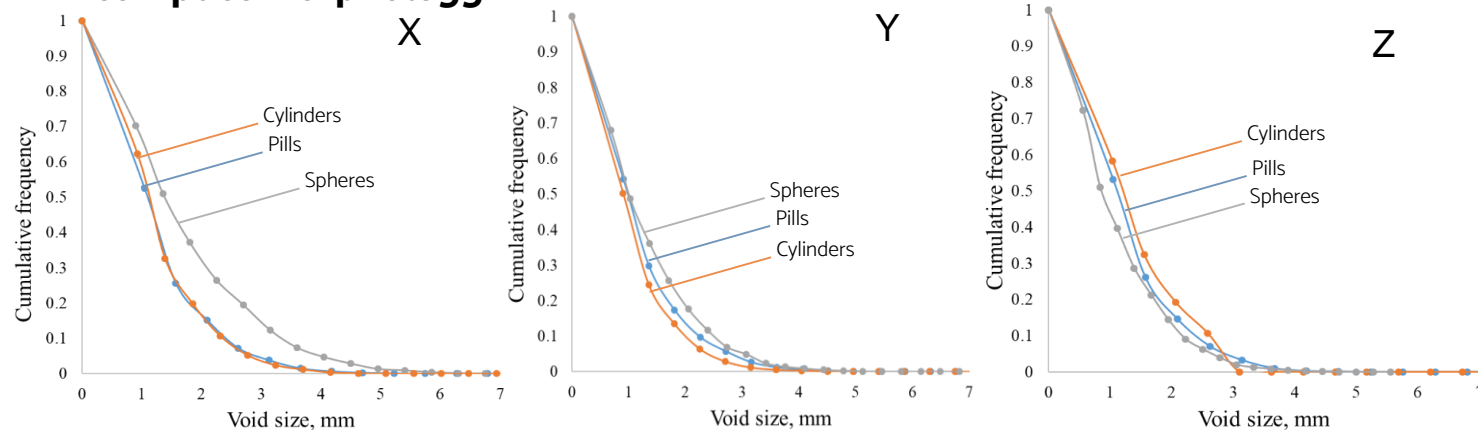


Figure 6:
Normalized VSDs
of three samples

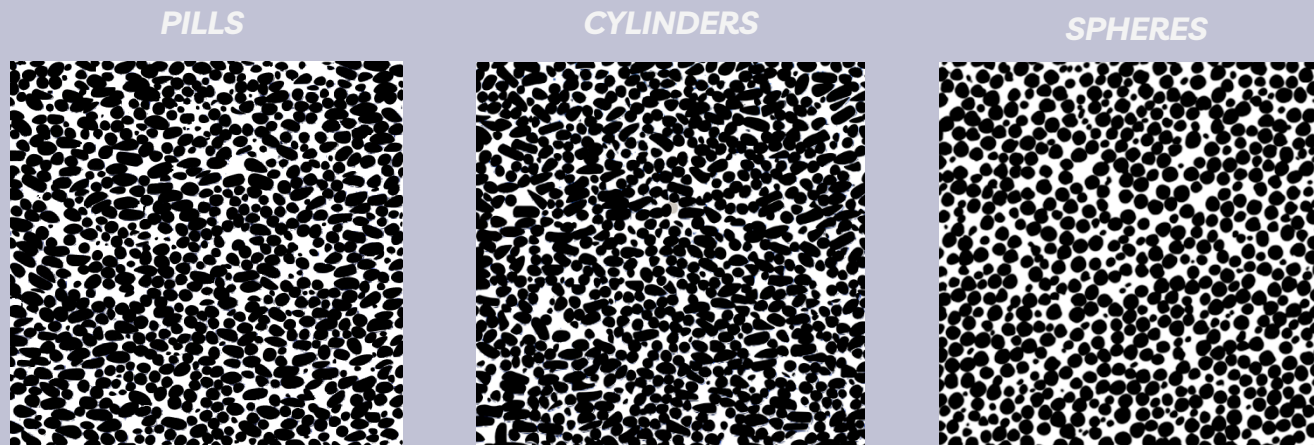
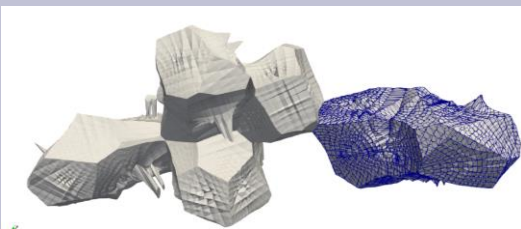


Figure 7:
Colored cross-sectional images
of three samples
normal to X

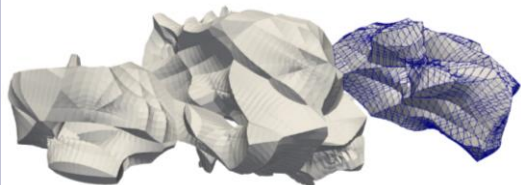
STUDY 1

Effect of particle shapes on compact morphology

PILLS



CYLINDERS



SPHERES

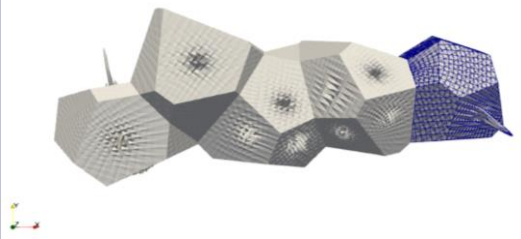


Figure 8: Visualization of five selected voronoi cells for each sample

- Voronoi tessellation analysis

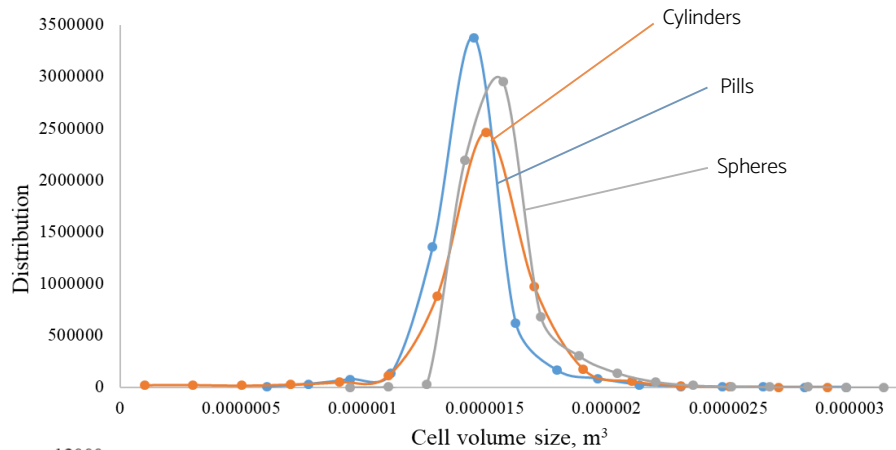


Figure 9: Normalized Voronoi cells volume correlation

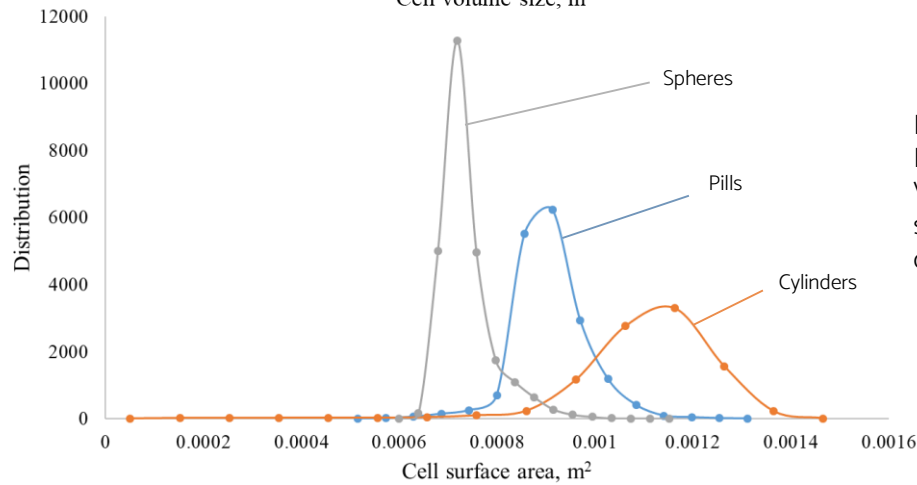


Figure 10: Normalized Voronoi cells surface area correlation

STUDY 2

Effect of non-spherical particles inclusion into spherical powder compact mixture

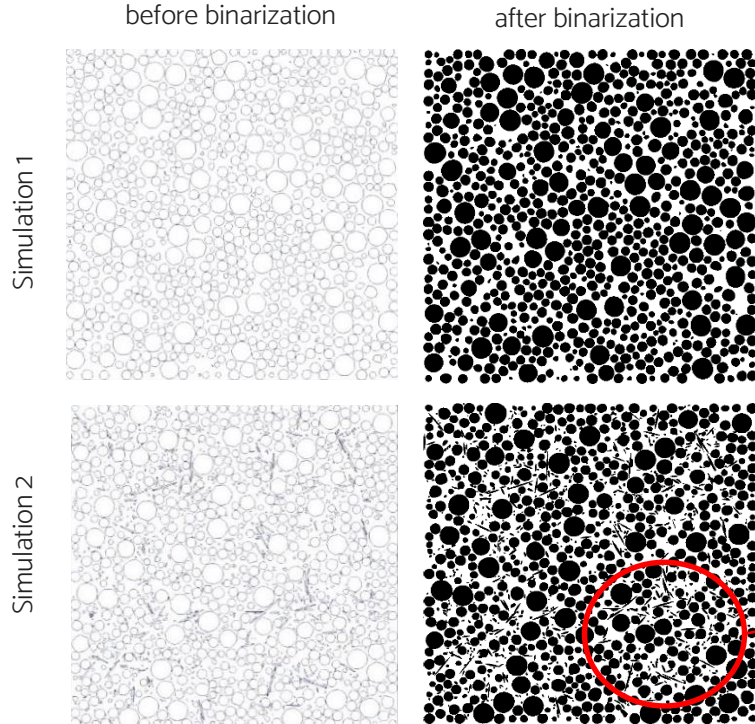
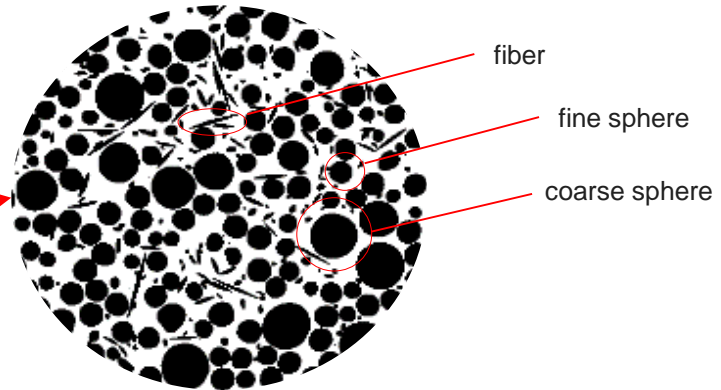
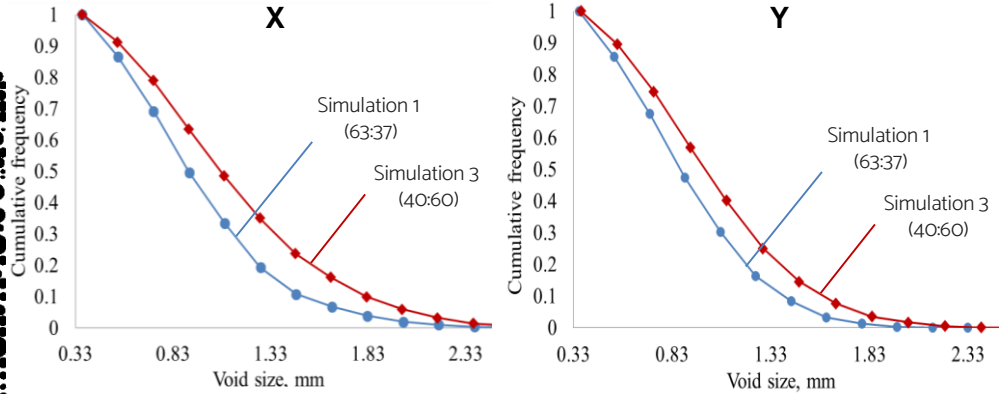


Figure 11: Images of compact cuts from DEM normal to Z direction

Figure 12: VSD for simulations of binary mixtures of spherical particles



STUDY 2

Effect of non-spherical particles inclusion into spherical powder compact mixture

Parameters of void size distribution

Parameters		d_{50}	d_{90}	d_{10}	d_{90}/d_{10}
Simulation 1 (63:37)	x	0.914	0.500	1.475	2.950
	y	0.864	0.490	1.390	2.837
	z	0.930	0.485	1.626	3.353
Simulation 2 (62:37:1)	x	0.940	0.528	1.530	3.211
	y	0.900	0.500	1.457	2.944
	z	0.795	0.437	1.268	3.109
Simulation 3 (40:60)	x	1.068	0.570	1.830	2.898
	y	0.998	0.540	1.590	2.914
	z	0.984	0.533	1.657	2.949
Simulation 4 (40:59:1)	x	0.960	0.540	1.550	2.870
	y	0.965	0.540	1.515	2.806
	z	0.870	0.475	1.380	2.905

*the densest packed compact was obtained for ternary mixture with $f_{\text{fine}}:f_{\text{coarse}}:f_{\text{fiber}}$ 63:37:1, the smallest voids median size $d_{50}=0.795$ mm and the most uniform voids distribution

- Void size distribution analysis based on the cross-sectional images analysis

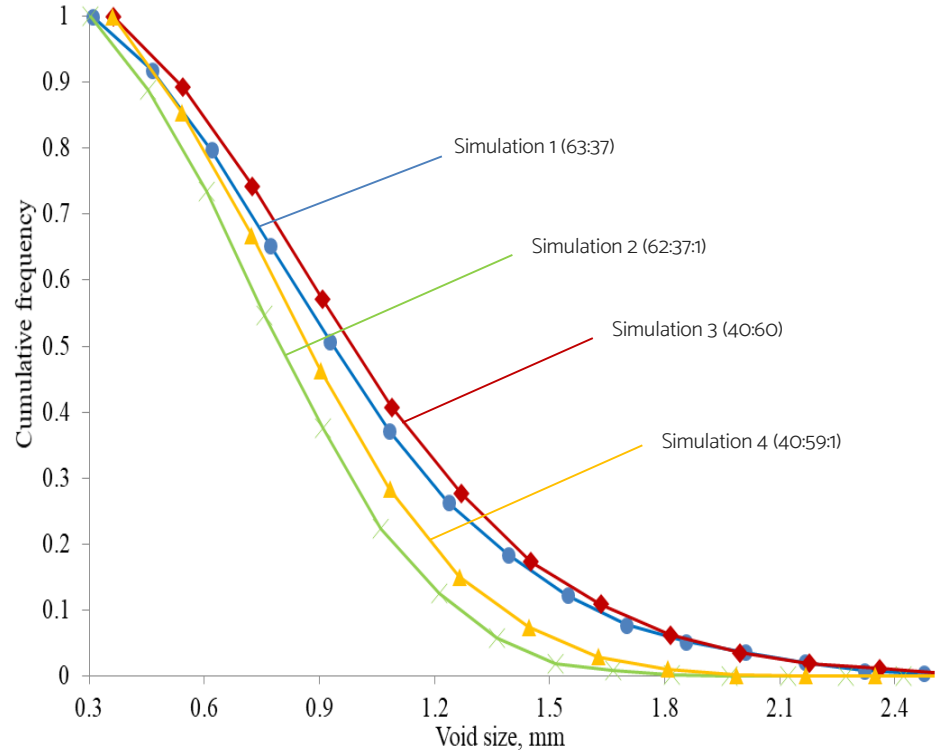


Figure 11:
VSD for all simulations in z direction



Study 1 on the effect of differently shaped particles compacts

Non-spherical form

the non-spherical form influences on the packing structure

Void size distribution

more uniform voids size distribution with small voids for pills and cylinders

Voronoi Tessellation

- more smooth voronoi cells for pills and cylinders
- sharpness of cylinder shape represented => wider range of voronoi cell volumes and surface area
- spheres => wider range of voronoi volume cells and less range of voronoi cell surface area



Study 2 on the effect of fiber inclusion into spherical particles mixture

Addition of non-spherical particles

addition of fibers into spherical particles mixture positively affected to the increase of packing

Void size distribution

the most packed compact

$$f_{\text{fine}} : f_{\text{coarse}} : f_{\text{fiber}} = 62 : 37 : 1$$

- the smallest voids with median size $d_{50} = 0.795 \text{ mm}$
- the most uniform voids distribution

Recommendations



- further research on the evaluation of other superquadric forms
- extension of VT to analyze packing microstructure of complex bodies of superquadric compacts and mixtures of non-spherical particles
- Implementation of superquadrics with different aspect ratios and sharpness to analyze in two-dimensional and three-dimensional analyses

Publications and conference proceeding of author *based on the research*

ICBMC 2020 IOP Publishing
 IOP Conf. Series: Materials Science and Engineering **829** (2020) 012020 doi:10.1088/1757-899X/829/1/012020

Packing Structure of Binary Particle Compacts with Fibers

A Boribayeva, A Zharbossyn, Z Berkinova, A Yermukhambetova, B Golman*

Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan, Kazakhstan


Analysis of Tortuosity in Compacts of Ternary Mixtures of Spherical Particles

Assem Zharbossyn ^{1,2}, Zhazira Berkinova ^{1,2}, Aidana Boribayeva ^{1,2}, Assiya Yermukhambetova ^{1,*} and Boris Golman ^{1,2}

¹ Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan 010000, Kazakhstan; assem.zharbossyn@nu.edu.kz (A.Z.); zhazira.berkinova@nu.edu.kz (Z.B.); aidana.boribayeva@nu.edu.kz (A.B.); boris.golman@nu.edu.kz (B.G.)

² National Laboratory Astana, Nazarbayev University, Nur-Sultan 010000, Kazakhstan

* Correspondence: ayermukhambetova@nu.edu.kz; Tel.: +7-717-269-4606




CHEMICAL ENGINEERING TRANSACTIONS

VOL. 74, 2019

Guest Editors: Sauro Pierucci, Jiří Jaromír Klemes, Laura Piazza
 Copyright © 2019, AIDIC Servizi S.r.l.
 ISBN 978-88-95608-71-6; ISSN 2283-9216

A publication of



The Italian Association of Chemical Engineering
 Online at www.cetjournal.it

DOI: 10.3303/CET1974065

Microstructural Features of Ternary Powder Compacts

Zhanibek Akhmetov^a, Aidana Boribayeva^a, Zhazira Berkinova^{a,b}, Assiya Yermukhambetova^{a,b}, Boris Golman^{a*}

^aDepartment of Chemical and Materials Engineering, School of Engineering, Nazarbayev University, 53 Kabanbay Batyr Ave., Astana, 010000, Kazakhstan
^bNational Laboratory Astana, Nazarbayev University, 53 Kabanbay Batyr Ave., Astana, 010000, Kazakhstan
 boris.golman@nu.edu.kz

Reference list

1. Fennis, S. A., & Walraven, J. C. (2012). Using particle packing technology for sustainable concrete mixture design. *Heron*, 57, 2 73-101. Retrieved from: <http://heronjournal.nl/>
2. Wang, M., Al-Tabbaa, A., & Wang, W. (2019). Improving discrete particle packing models for the microstructural formation simulation of Portland cement. *Construction and Building Materials*, 229, 116841.
3. Shen S, Yu H. Characterize packing of aggregate particles for paving materials: particle size impact. *Constr Build Mater* 2011;25:1362–8.
4. Soltanbeigi, B., Podlozhnyuk, A., Papanicolopoulos, S. A., Kloss, C., Pirker, S., & Ooi, J. Y. (2018). DEM study of mechanical characteristics of multi-spherical and superquadric particles at micro and macro scales. *Powder Technology*, 329, 288-303.
5. Yang, R. Y., Zou, R. P., & Yu, A. B. (2000). Computer simulation of the packing of fine particles. *Physical review E*, 62(3), 3900.
6. Podlozhnyuk, A., Pirker, S., & Kloss, C. (2017). Efficient implementation of superquadric particles in Discrete Element Method within an open-source framework. *Computational Particle Mechanics*, 4(1), 101-118.
7. Yi, L. Y., Dong, K. J., Zou, R. P., & Yu, A. B. (2011). Coordination number of the packing of ternary mixtures of spheres: DEM simulations versus measurements. *Industrial & engineering chemistry research*, 50(14), 8773-8785
8. Zhao, S., Evans, T. M., & Zhou, X. (2018). Three-dimensional Voronoi analysis of monodisperse ellipsoids during triaxial shear. *Powder Technology*, 323, 323-336.
9. Soltanbeigi, B., Podlozhnyuk, A., Papanicolopoulos, S. A., Kloss, C., Pirker, S., & Ooi, J. Y. (2018). DEM study of mechanical characteristics of multi-spherical and superquadric particles at micro and macro scales. *Powder Technology*, 329, 288-303.