CHoPS2022

10th International Conference on Conveying and Handling of Particulate Solids

Salerno (Italy), 5-9 July 2022

BOOK OF ABSTRACTS

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UNIVERSITÀ DEGLI STUDI DI SALERNO

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UNIVERSITÀ DEGLI STUDI DI SALERNO

ORGANIZING SECRETARIAT

EVENTI E CONGRESSI

Rione Sirignano, 5
80121 Naples (Italy)
Ph. +39 081 7611085 – 668774
info@mcmcongressi.it

The International Conference on Conveying and Handling of Particulate Solids (CHoPS) is now at its 10th edition, since it started in Israel in 1995. This conference is the place where the opportunities coming from the advances in the scientific fundamentals of particle mechanics and technology can meet the industrial needs related to storage and handling of particulates, for all fields and possible scales, ranging from handling of bulky particulate materials to precision dosage of fine powders. The timely theme of this Conference edition is "New horizons for particle mechanics and solids handling in the smart manufacturing revolution".

The scope of the Conference includes the science and technology for the production, transformation and handling of any particulate material such as, but not limited to, chemicals, minerals, ceramic, pharmaceuticals, foods and health products, conventional and biomass fuels, wastes, particles for 3d-printing and includes also the mechanics of particulates relevant to environment preservation and care.

This is a unique forum to promote the exchange of technical and scientific information in the academic and industrial sectors in the fields of solids flow, mechanical behavior of bulk materials, powder testing, mixing and segregation, modelling, etc. It is also designed to foster business and collaboration opportunities around the world.

The conference is gathering more than 190 participants. The programme includes 7 plenaries 26 keynotes and about 150 presentations and posters. The participants come from all over the world, even if intercontinental participation has been greatly affected by the pandemic situation

The conference hosts also the MATHEGRAM Symposium and the TUSAIL Symposium.

MATHEGRAM (Multiscale analysis of thermomechanical behaviour of granular materials) has received since 2018 funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Innovative Training Network grant agreement MATHEGRAM No 813202. The project is now approaching at its end, and the MATHEGRAM Symposium is an occasion for drawing some conclusions and disseminate the so far reached results of the research work of its 14 Early-Stage Researchers in the hosting institutions.

TUSAIL (Training in Upscaling particle Systems: Advancing Industry across Length-scales) has received since 2021 funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Innovative Training Network grant agreement TUSAIL No 955661. The 15 Early-Stage Researchers of the project have started their activity since few months and the Symposium is a chance for meeting among them and with the experts of the External Advisory Board.

The conference venue is the Grand Hotel Salerno.

Massimo Poletto and Diego Barletta

Conference Chairs

LOCAL ORGANIZING COMMITTEE

Massimo Poletto (Co-Chair), *University of Salerno*
Diego Barletta(Co-Chair), *University of Salerno*
Andrea Benassi, *Chiesi Farmaceutici S.p.A.*
Giuseppe Bonifazi, *Sapienza – University of Rome*
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Balaji Soundarajan, *University of Salerno*
Sina Zinatlou Ajabshir, *University of Salerno*

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Avi Levy, *Ben Gurion University (Israel)*
Stefan Luding, *University of Twente (Netherlands)*
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Vadim Mizonov, *Ivanovo University (Russia)*
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Tomasz Olejnik, *Lodz University of Technology (Poland)*
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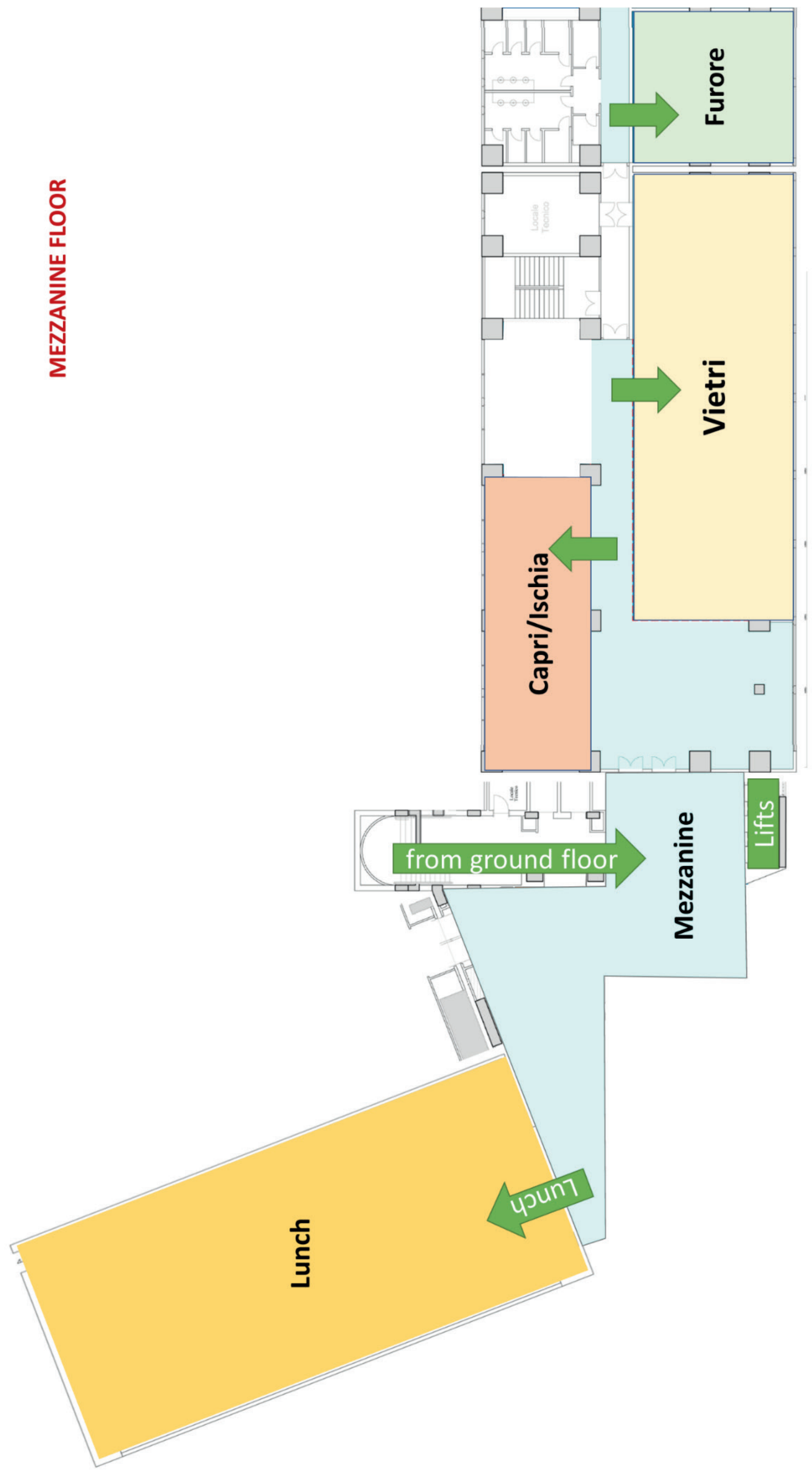
VENUE MAP

GROUND FLOOR

MEZZANINE FLOOR



CONFERENCE PROGRAM

Tuesday, 5 July 2022

16.30-19.00	**Exhibition Hall** **Conference registration**
19.00-21.30	**Roof Terrace (Specchio di Mare & Le Divine Costiere)** **Welcome reception**

Wednesday, 6 July 2022 - morning

	Room Tafuri	Room Vietri
8.00-8.30	Exhibition Hall	
08.30-09.30	**Plenary: Room Tafuri** *Chair: Massimo Poletto*	
Topic	**TUSAIL Symposium**	**Mechanical behavior of bulk materials**
Chairs	*J. Ooi – V. Magnanimo*	*H. Zetzener – E. McGee*
09.30-09.50	**Introduction to TUSAIL Symposium** Jin Ooi University of Edinburg	**The Role of Archimedes Number in Particulate Bed Void-Fraction and Flowability** Haim Kalman Ben-Gurion University of the Negev, Israel
09.50-10.10	**Keynote Using a commercial rheometer to determine a particle-particle cohesion model** Christine M. Hrenya University of Colorado, United States	**Case Study: Silo and System Design for Fibrous Recycling Materials** Hans Schneider Zeppelin Systems GmbH, Germany
10.10-10.30		**A combined DEM and CNN model for characterizing and evaluating the performance of ball mills** Yaoyu Li University of New South Wales, Australia
10.30-11.00	Exhibition Hall	
Topic	**TUSAIL Symposium**	**Mechanical behavior of bulk materials**
11.00-11.20	**Keynote Benefits and open problems in coarse graining methods for DEM-based simulations of fluid-particle systems** Alberto di Renzo Università della Calabria, Italy	**Keynote Rheology of Cohesive Powder Mixtures** Mojtaba Ghadiri University of Leeds, United Kingdom
11.20-11.40		
11.40-12.00	**Comparison of CFD-DEM and TFM approaches for the simulation of the single- and multiple-spout fluidized beds** Behrad Esgandari Johannes Kepler University Linz, Austria	**Experimental study of granular heap flow under vertical vibrations** Ghita Marouazi TU Kaiserslautern, Germany
12.00-12.20	**Modelling fluidization by recurrence CFD (rCFD)** Varun Dongre Johannes Kepler University Linz, Austria	**How a Granular Pile becomes a Glass** Stefan Boettcher Emory University, USA
12.20-12.40	**Workshop Upscaling Particle Systems**	**Density Instabilities and Compaction Efficiency in a tapped granular pile.** Paula Alejandra Gago Imperial College London, United Kingdom
12.40-13.00		**Optimization of a Flighted Rotary Drum Cross-Sectional Characteristics** Dmitry Portnikov Ben-Gurion University of the Negev, Israel

Wednesday, 6 July 2022 - morning

Room Furore	Room Ischia/Capri	
Conference registration		8.00-8.30
New Opportunities for Granular Matter Research Heinrich Jaeger, University of Chicago, United States of America		08.30-09.30
Pneumatic and mechanical conveying	**Multiphase flow and fluidization**	Topic
D. Schott – A. Levy	*R. Ocone - R. Solimene*	*Chairs*
Analysing Impact Forces & Overcoming Speed, Heat and Pressure Issues in High Capacity Belt Support Applications Cameron Portelli Kinder Australia, Australia	**Confined-fluidization as a way of improving CO_2 capture by adsorption on solid sorbents** Maria Turano Università della Calabria, Italy	09.30-09.50
Motion Resistances in Trough Chain Conveyors Andre Katterfeld University of Magdeburg, Germany	**Hydrodynamics of Pulse-Assisted Fluidization of Cohesive Powder** Mohammad Asif King Saud University, Saudi Arabia	09.50-10.10
Understanding the Total Cost of Ownership of Bulk Solids Handling Systems: A New Paradigm to Reduce Risks in Procurement of Solids Handling Systems and Equipment Michael Bradley Wolfson Center, United Kingdom	**Fluidization and flow behavior of powder coatings when approaching their glass transition temperature** Helena Weingrill Anton Paar GmbH, Austria	10.10-10.30
Coffee break		10.30-11.00
Pneumatic and mechanical conveying	**Multiphase flow and fluidization**	Topic
Keynote Refill Strategy Optimization of a Twin-Screw Feeder with DEM Peter Toson Research Center Pharmaceutical Engineering, Austria	**Keynote Hydrodynamics of a novel directly irradiated fluidized bed autothermal reactor for thermochemical energy storage** Stefano Padula Università di Napoli Federico II, Italy	11.00-11.20
		11.20-11.40
Development of bulk material dosing equipment using DEM Jan Nečas University of Ostrava, Czech Republic	**The role of Temperature and Moisture on Polymer Materials for Additive Manufacturing, and their Implications for the Process** Denis Schuetz Anton Paar GmbH., Austria	11.40-12.00
Effect of Particle Size Distribution on Frictional Head Loss in Pipe Flow of Sand-Water Slurry Vaclav Matousek Czech Academy of Sciences, Czech Republic	**Classification of fine gas born particles in superposed electric and acoustic fields** Krischan Sandmann Leibniz Institute for Materials Engineering - IWT, Germany	12.00-12.20
Exploring "Big Data" on the Effect of Different Materials on Pressure Drops in Pneumatic Conveying, Identifying Bend and Straight Pipe Losses and Bend Equivalent Lengths Michael Bradley University of Greenwich, United Kingdom	**Investigation of the wet contact behavior of particles in CFD-DEM simulations of a rotor granulator** Philipp Grohn TU Kaiserslautern, Germany	12.20-12.40
Study on characteristics of flow rate regulation in the dense-phase pneumatic conveying of pulverized coal Lizhuo Zhu East China University of Science and Technology, China	**An experimental investigation on channelized granular flows** Luca Sarno Università di Salerno, Italy	12.40-13.00

Wednesday, 6 July 2022 - afternoon

13.00-14.30	Mezzanine	
14.30-15.30	**Plenary: Room Tafuri** *Chair: Diego Barletta*	
	Room Tafuri	**Room Vietri**
Topic	**Computational models**	**Mechanical behavior of bulk materials**
Chairs	*A. Benassi – S. Luding*	*H. Schneider – H. Wilms*
15.30-15.50 15.50-16.10	**Keynote** **DEM Calibration of Cohesive Bulk Materials** Corne Coetzee University of Stellenbosch, South Africa	**Keynote** **Comparison of different test methods for the flow property evaluation of fibrous materials** Steffen Beitz Zeppelin Systems GmbH, Germany
16.10-16.30	**DEM Model for the Quantitative Prediction of Cohesive Powder (ESKAL) Flowability.** Maheandar Manokaran Université de Technologie de Compiègne, France	**Reverse Janssen Effect in Narrow Granular Column** Massimo Pica Ciamarra Nanyang Technological University, Singapore
16.30-17.00	Exhibition Hall	
Topic	**Computational models**	**Silo design**
17.00-17.20	**DEM Simulation of Moist Sand over a Transfer Point** Otto Scheffler University of Stellenbosch, South Africa	**Proposal to Structure Silo Failure Analysis** Harald Wilms Wilms-ITC, Germany
17.20-17.40	**DEM Modelling of Elastic-Plastic Contact Behavior for Cohesive Powders** Robert Hesse TU Kaiserslautern, Germany	**Process intensification of hopper discharge of cohesive powders based on modulated pulsed airflow** Lizhuo Zhu East China University of Science and Technology, China
17.40-18.00	**An SPH study on the compaction of soft deformable grains** Francisco Goio Graz University of Technology, Austria	**Parametric study and flow regime map for planar silos and hoppers** Evgeny Rabinovich Ben-Gurion University of the Negev, Israel
18.00-19.00		

Wednesday, 6 July 2022 - afternoon

Lunch		13.00-14.30
DEM-based metamodeling - the booster for design of bulk solids handling equipment? Dingena Schott, Delft University of Technology, The Netherlands		14.30-15.30
Room Furore	**Room Ischia/Capri**	
Pneumatic and mechanical conveying	**Multiphase flow and fluidization**	Topic
F. Rizk – P. Toson	*S. Heinrich - M. Troiano*	*Chairs*
Keynote **Determining and Comparing Breakage Matrices to Predict Particle Attrition in Pneumatic Conveyors** Michael Bradley University of Greenwich, United Kingdom	**Keynote** **Neural network-based filtered drag model for cohesive gas-particle flows** Josef Tausendschön University of Graz, Austria	15.30-15.50 15.50-16.10
Pneumatic Conveying of Solids: Scale-Up and Design of Long Line Systems Farid Rizk R & D Solids Handling BASF Formerly, Germany	**Terminal Velocity and Drag Coefficient for Accelerating Spherical Particles** Haim Kalman Ben-Gurion University of the Negev, Israel	16.10-16.30
Coffee break		16.30-17.00
Pneumatic and mechanical conveying	**Multiphase flow and fluidization**	Topic
Workshop **Pneumatic conveying**	**Investigation of endogenous bubble-induced segregation of a single biomass particle in fluidized bed reactors** Stefano Iannello University College London, United Kingdom	17.00-17.20
	Solids mixing/segregation in high temperature dense gas-solid fluidized beds by capacitance and pressure measurements Laura Molignano Università di Napoli Federico II, Italy	17.20-17.40
	Efficiency of stand-alone filters: effects of filter aperture and meshing design Paula Alejandra Gago Imperial College London, United Kingdom	17.40-18.00
	CHoPS International Scientific Committee Meeting	18.00-19.00

Thursday, 7 July 2022 - morning

08.30-09.30	**Plenary: Room Tafuri** *Chair: Haim Kalman*	
	Room Tafuri	**Room Vietri**
Topic	**Computational models**	**MATHEGRAM Symposium**
Chairs	*M. Sousani – A. Katterfeld*	*C. Wu – A. Venkatesh*
09.30-09.50	**Simulation of hierarchical structure formation during spray drying using CFD-DEM coupling** Silas Wolf TU Braunschweig, Germany	**Heat generation by friction and deformation during an oblique impact** Francisco Kisuka University of Surrey, United Kingdom
09.50-10.10	**CFD-DEM simulations of strongly polydisperse particulate solids in thecyclonic flow of dry powder inhalers** Alberto Di Renzo Università della Calabria, Italy	**Calibration of CFD-DEM Heat Transfer Model using Packed Bed Experiment** Aman Rastogi Johnson Matthey, United Kingdom
10.10-10.30	**Using the Material Point Method (MPM) to Model Bulk Materials** Corne Coetzee University of Stellenbosch, South Africa	**DEM modelling of granular material swelling** Domenica Braile University of Surrey, United Kingdom
10.30-11.00	**Exhibition Hall**	
Topic	**Computational models**	**MATHEGRAM Symposium**
11.00-11.20	**Keynote** **Multiscale modelling of granular materials – Calibration of discrete particle models** Thomas Weinhart University of Twente, The Netherlands	**Modeling particle-scale deformation and heat conduction for a highly dense granular system with finite volume method** Ranjan Dhakal Graz University of Technology, Austria
11.20-11.40		**CFD-DEM Model for High-Temperature Processes** Jelena Macak DCS Computing GmbH, Austria
11.40-12.00	**An in-depth study of mixing and turning behavior of a compost pile using Discrete Element Method and Big-Data analysis** Mohsin Ajmal, O.v.Guericke U, Germany Max Cichocki, Graz UT, Austria	**Sources of error when measuring the hydraulic conductivity of a granular material at different temperatures** Marina Bortolotto Imperial College London, United Kingdom
12.00-12.20	**An optimal calibration procedure for the Discrete Element Method** Farheez Mohamed Université de Technologie de Compiègne, France	**Fundamental basis for a novel approach to indirectly measure the effective thermal conductivity of granular materials** Tokio Morimoto Imperial College London, United Kingdom
12.20-12.40	**Digital twins to improve the calibration of DEM simulation of powder processes** Aurélien Neveu Granutools, Belgium	**The effect of temperature on the spreading of powder layers in selective laser sintering** Sina Zinatlou Ajabshir Università di Salerno, Italy
12.40-13.00	**Robust Estimation and Validation of Contact Parameters of Iron Ore for Transfer Chute Simulation** Rodrigo Magalhães de Carvalho Universidade Federal do Rio de Janeiro, Brazil	**In-situ monitoring and modeling of single-layer selective laser sintering of polyamide powders** Balaji Soundararajan Università di Salerno, Italy

Thursday, 7 July 2022 - morning

Flow of bulk materials into small confined spaces: characterisation and modelling Chuan-Yu (Charley) Wu, University of Surrey. United Kingdom		08.30-09.30
Room Furore	**Room Ischia/Capri**	
Powder testing and characterization	**Particle design and manufacturing**	Topic
D. Schuetz – P. García-Triñanes	*A. Kwade – P.A. Gago*	*Chairs*
An X-ray micro tomography study of packing behaviour metal powders during filling, compaction and ball indentation process Mozhdeh Mehrabi University of Leeds, United Kingdom	**Keynote** **Production of Composite Materials from Spray Drying and Warm Compaction** Hannah Sophia Rothberg Hamburg University of Technology, Germany	09.30-09.50
Soft wheat flour quality parameters assessment by Near Infrared Spectroscopy (NIR): from laboratory to shelf Riccardo Gasbarrone Sapienza - Università di Roma, Italy		09.50-10.10
Bulk solids on the Moon - Characterization of the innovative Lunar Regolith Simulants TUBS-M, TUBS-T and TUBS-I Lisa Windisch TU Braunschweig, Germany	**The Virtual Formulation Laboratory: A Novel Means to Facilitate Smooth Transition of New Powder Formulations Across the Divide Between Formulation Development and Manufacturing** Michael Bradley Universities of Greenwich, United Kingdom	10.10-10.30
Exhibition Hall		10.10-10.30
Powder testing and characterization	10.30-11.00	Topic
Keynote **Effect of Moisture Content, Size Distributions and Particle Shape on Flowability: Angle of Repose, Tilting Angle, and Hausner Ratio** Haim Kalman Ben-Gurion University of the Negev, Israel	**Keynote** **Predicting Turbulent Shear Stress in Pharmaceutical Vessels** Roisin Hurley University of Limerick, Ireland	11.00-11.20
		11.20-11.40
An investigation into the effect of drying on the flowability of the bulk pulverised cassava grits Hamed Johnny Sarnavi University of Greenwich, United Kingdom	**A regime map for dry powder coating** Mary Khala University of Surrey, United Kingdom	11.40-12.00
Moisture Caking: Accelerated Caking Tests Jairo Paternina Jenike & Johanson Inc., United States	**Investigating particle properties and process parameters for generating efficient dry particle coated system** Vikram Karde University College of London, United Kingdom	12.00-12.20
A novel method developed to measure tensile strength of cohesive powders Vivek Garg University of Greenwich, United Kingdom	**Water Storing Bulk Granular Materials for Concrete 3D Printing** Leigh Duncan Hamilton TU Braunschweig, Germany	12.20-12.40
Influence of particle size and void fraction on evaluation of flowability and cohesiveness of a test of powder discharge by air pressure Koichiro Ogata National Institute of Technology, Japan	**Development of hyperspectral imaging classification model applied to the recognition and sorting of post-earthquake construction waste** Oriana Trotta Sapienza - Università di Roma, Italy	12.40-13.00

Thursday, 7 July 2022- afternoon

13.00-14.30	Mezzanine	
14.30-15.30	Plenary: Room Tafuri *Chair: Arno Kwade*	
	Room Tafuri	**Room Vietri**
Topic	**Computational models**	**MATHEGRAM Symposium**
Chairs	*T. Weinhart – C. Coetzee*	*C. Wu – J. Macak*
15.30-15.50	**Keynote** **Investigations of abrasive sliding and impact wear - a DEM calibration approach** Thomas Roessler University of Magdeburg, Germany	**A Numerical Study of Heat Transfer Mechanisms in Dense Particulate Systems Using DEM** Rafael Rangel Universitat Politècnica de Catalunya, Spain
15.50-16.10		**Analysis of sintering of ceramic powder systems by in-situ synchrotron nano-tomography** Aatreya Manjulagiri Venkatesh Université Grenoble Alpes - SIMAP, France
16.10-16.30	**DEM Simulations of Industrial Scale Granular Chute Flows** Satyabrata Patro Indian Institute of Technology Kanpur, India	**Modeling grain growth and arbitrarily shaped particles in sintering with the discrete element method** Brayan Paredes Goyes Université Grenoble Alpes - SIMAP, France
16.30-16.50	**Predicting Time Dependent Behavior of Surface Granular Flows** Anurag Tripathi Indian Institute of Technology Kanpur, India	
16.50-17.10	Exhibition Hall	
18.30-23.00	Arechi Castle	

Thursday, 7 July 2022- afternoon

Lunch		13.00-14.30
The Rheology of Granular Materials: from Fundamentals to Applications Raffaella Ocone, Heriot-Watt University, United Kingdom		14.30-15.30
Room Furore	**Room Ischia/Capri**	
Powder testing and characterization	**Miscellaneous**	Topic
K. Ogata – W.P. Goh	*R. Cenni- A. Neveu*	*Chairs*
Keynote **Comparison of low-stress flowability measurement techniques: ball indentation and shear cell** Colin Hare University of Surrey, United Kingdom	**Poster flash presentations**	15.30-15.50
		15.50-16.10
Measurement of Particle Contact Area Using a Mechanical Surface Energy Tester and Influences of Surface Texture of Powders on Particle Adhesion Vivek Garg The Wolfson Centre for Bulk Solids Handling Technology, United Kingdom		16.10-16.30
Flowability and granular compaction from industrial powders to frontier science seeking for the missing key Maria Graciela Cares Université de Lorraine, France		16.30-16.50
Coffee break		16.50-17.10
Social dinner		18.30-23.00

Friday, 8 July 2022 - morning

08.30-09.30		**Plenary - Room Tafuri** *Chair: Mojtaba Ghadiri*
	Room Tafuri	**Room Vietri**
Topic	**Computational models**	**Industrial case studies**
Chairs	*A. Di Renzo – J. Morrissey*	*K. Johanson - T. Destoop*
09.30-09.50	**Resolved simulation of particle collisions on wet microstructured surfaces** David Strohner TU Kaiserslautern, Germany	**Improving a Pneumatic Conveying System for Coffee Beans to Reduce Attrition** Harald Wilms Wilms-ITC, Germany
09.50-10.10	**Development and application of BPM-DEM to study mechanics of frozen granular materials** Tsz Tung Chan Hamburg University of Technology, Germany	**Leveraging Artificial Intelligence to speed up DEM simulations: A wheel loader case study** Marina Sousani Altair Engineering, United Kingdom
10.10-10.30	**Multi-Scale and Multi-Physics Modelling of Particle and Fluid-Particle Flow using DEM and CFD-DEM** Christoph Goniva DCS Computing GmbH, Austria	**Innovations in particle technology modelling to improve industrial product development** Stefan Bellinghausen Siemens, United Kingdom
10.30-11.00		**Exhibition Hall**
Topic	**Computational models**	**Industrial case studies**
11.00-11.20 11.00-11.40	**Keynote** **Tensor-based Coarse Graining Method** Zorica Ristic DCS Computing GmbH, Austria	**Keynote** **The Application of Multi Screw Feeders to Avoid Flow Problems** Eddie McGee Ajax Equipment Limited, United Kingdom
11.40-12.00	**On the use of coarse-graining to bridge the discrete and continuum descriptions of granular materials** Hongyang Cheng University of Twente, The Netherlands	**Improved processing in extrusion by BASF** Rou Hua Chua BASF SE, Germany
12.00-12.20	**Modelling hopper discharge of elongated particles with different shape representation methods** Marina Sousani Altair Engineering Ltd, United Kingdom	**Examples for Handling of Post-Consumer Plastic Waste** Harald Wilms Wilms-ITC, Germany
12.20-12.40	**Effect of coarse-grain scaling in Discrete Element Method (DEM-CFD) modelling of CFB riser reactors** Erasmo Salvatore Napolitano Università della Calabria, Italia	**Estimation of the temporal variations of the feed of a sinterization process aided by a voxelization-based numerical approach** Horacio Andrés Petit Universidade Federal do Rio de Janeiro, Brazil
12.40-13.00	**MercuryDPM: Fast, flexible, particle simulations** Anthony Thonrton University of Twente, The Netherlands	**Modeling of stockpile drainage and seepage in real applications** Jairo Paternina Jenike & Johanson, United States

Friday, 8 July 2022 - morning

Interaction between dry grains and liquids inspired by industrial processes Pierre Jop, Glass Surface and Interfaces, CNRS/Saint-Gobain, France		08.30-09.30
Room Furore	**Room Ischia/Capri**	
Compaction and tableting		Topic
M.G. Cares – A. Santomaso		*Chairs*
Modeling the shear sensitivity of lubricated powders in a paddle feeder Daniel Puckhaber TU Braunschweig, Germany	**MATHEGRAM Meeting**	09.30-09.50
Processing of Living Microorganisms: Fluidized-bed Granulation and Tableting Karl Vorländer TU Braunschweig, Germany		09.50-10.10
Material and Process Analyses for the Derivation of Process and Property Models in Food Compaction René Rösemeier-Scheumann TU Braunschweig, Germany		10.10-10.30
Coffee break		10.30-11.00
Compaction and tableting	**Thermomechanical behaviour of granular materials**	Topic
	C. Schilde – J. Necas:	*Chairs:*
Keynote **Modeling of High-Density Compaction of Pharmaceutical Tablets Using Multi-Contact Discrete Element Method** Kostas Giannis TU Braunschweig, Germany	**Keynote** **Powder Flow and Heat Transfer in a Rotary Kiln with Baffles** Benjamin Glasser Rutgers University, United States	11.00-11.20 11.00-11.40
Three-dimensional discrete element modelling of diametrical compression of annular tablet Chuan-yu Wu University of Surrey, United Kingdom	**Hot or Cool; Powder Characterization in non-ambient conditions – High- and Low-Temperature Ring Shear Testing** Denis Schuetz Anton Paar GmBh., Austria	11.40-12.00
Material-independent description of die filling in rotary tablet presses Ann Kathrin Schomberg TU Braunschweig, Germany	**Influence of temperature on the packing dynamics of powders** Aurélien Neveu Granutools, Belgium	12.00-12.20
The effect of particle adhesion on die filling performance in a gravity filling device Mohammadreza Alizadeh Behjani University of Surrey, United Kingdom	**The effect of temperature on the flow properties of SiC powders** Pablo García-Triñanes University of Greenwich, United Kingdom	12.20-12.40
The protective potential of cushioning coatings on enteric-coated pellets during tableting Jan Henrik Finke TU Braunschweig, Germany	**DEM simulation study: the effect of temperature on powder spreading in selective laser sintering** Sina Zinatlou Ajabshir Università di Salerno, Italy	12.40-13.00

Friday, 8 July 2022 - afternoon

13.00-14.30	Mezzanine	
14.30-15.30	**Plenary - Room Tafuri** *Chair: Christine Hrenya*	
	Room Tafuri	**Room Vietri**
Topic	**Computational models**	**Mixing and Segregation**
Chairs	*A. Thornton – C. Hare*	*M. Ghadiri – S. Kiesgen de Richter*
15.30-15.50	**Keynote** **Triaxial Testing for Granular Materials Using the Discrete Element Method** John Morrissey University of Edinburgh, United Kingdom	**Keynote** **Description of size segregation in multicomponent mixtures using a probabilistic continuum model** Andrea C. Santomaso Università di Padova, Italy
15.50-16.10		
16.10-16.30	**Coupling of DEM and Flowsheet Simulations for Screen Mills in Roller Compaction Process** Christian Eichler Hamburg University of Technology, Germany	**Solid state material driven turbine to reduce segregation effects in bunkers** Michael Denzel University of Leoben, Austria
16.30-17.00	Exhibition Hall	
Topic	**Computational models**	**Mixing and Segregation**
17.00-17.20	**Benchmark of different discrete particle models for the simulation of pneumatic conveying of additive manufacturing metallic powders** Lorenzo Pedrolli University of Deusto, Spain	**The development of new radial stress theory to predict segregation: The relationship between mass flow, segregation prevention, and stress and gas pressure gradients** Kerry Johanson Material Flow Solutions Inc., United States
17.20-17.40	**Analysis of micron-sized particle emission from the capsule of a DryPowder Inhaler through DEM simulations** Francesca Orsola Alfano Università della Calabria, Italy	**Batch versus Continuous Powder Mixing of Excipients and Active Pharmaceutical Ingredients** Maarten Jaspers DFE Pharma GmbH & Co, Germany
17.40-18.00	**Wear deformation prediction of convex pattern surface using DEM** Yunpeng Yan Delft University of Technology, The Netherlands	**Advantages of a continuous measurement of great mass flows in a mixing process for cement plant application using an electromagnetic + time of flight online massflow meter** Gilles Campagnola ENVEA SpA, Italy

Friday, 8 July 2022 - afternoon

Lunch		13.00-14.30
Potential and limitations of CFD and DEM simulation in the design of orally inhaled drug products Andrea Benassi, Chiesi Farmaceutici S.p.A, Italy		14.30-15.30
Room Furore	**Room Ischia/Capri**	
Agglomeration and Granulation	**Dust and aerosol emissions**	Topic
J. Paternina - J.H. Finke	*H. Kalman – R.H. Chua*	*Chairs*
Keynote **Novel Approach for the Characterization of Powder Caking** Alessandra Hausmann Imperial College London, United Kingdom Lukas Blesinger BASF SE, Germany	**Optimization of a sampling method of airborne metallic ultrafine particles by cascade impactors** Naïma GAUDEL INRS, France	15.30-15.50
	Novel technique for economic and continuous analysis of dust exposure levels in real-life production Michael Pilz BASF SE, Germany	15.50-16.10
Pellet Screenings Sintering Antonio Peres Federal University of Minas Gerais, Brazil	**Impact of powders flowability improvement on their dustiness generation** Maria Camila Jimenez Garavito Université de Lorraine, France	16.10-16.30
Coffee break		16.30-17.00
Agglomeration and Granulation		Topic
Parametric Study of Residence Time Distributions and Granulation Kinetics as a Basis for Process Modeling of Twin-Screw Wet Granulation Timo Plath University of Twente, The Netherlands		17.00-17.20
Influence of Spray Configuration and Material on Particle Formulation in Fluidized Beds with Liquid Injection Maike Orth Hamburg University of Technology, Germany		17.20-17.40
Structuration of plant-based milk powder for improved reconstitution Kathrin Kramm Hamburg University of Technology, Germany		17.40-18.00

Saturday, 9 July 2022

08.30-09.30	**Plenary - Room Tafuri** *Chair: Stefan Luding*	
	Room Tafuri	**Room Vietri**
Topic	**From particle contacts to bulk behavior**	**Additive manufacturing and powder sintering**
Chairs	*S. Luding - V. Garg*	*J. Schmidt – D. Barletta*
09.30-09.50	**Modeling Snow Deformation: From A Meso Grain to Bulk Behavior** Mohammed Hassan University of Twente, Netherlands Antilles	**Surface tailored metal particles for additive manufacturing** Arne Lüddecke TU Braunschweig, Germany
09.50-10.10	**A Study on the Charge Neutralising Effect of Aluminium Stearate in Triboelectrification** Jiachen Guo University of Leeds, United Kingdom	**Material properties and process parameter optimization in Selective Laser Sintering of polymers** Federico Lupone Polytechnic of Turin, Italy
10.10-10.30	**Adhesive particle-particle contact and how it affects ceramic's bulk flow behaviour** Zohreh Farmani Wageningen University & Research, The Netherlands	**Fluidized bed machining of AlSi10Mg samples produced by additive manufacturing** Maurizio Troiano Università di Napoli Federico II, Italy
10.30-11.00	**Exhibition Hall**	
Topic	**From particle contacts to bulk behavior**	**Additive manufacturing and powder sintering**
11.00-11.20 11.20-11.40	**Keynote** **From particles to continuum: Review of micro-macro approaches** Stefan Luding University of Twente, The Netherlands	**Keynote** **Quantitative analysis of the powder layer quality in the Selective Laser Sintering process: Experiments and DEM modelling** Marco Lupo Università di Salerno, Italy
11.40-12.00	**Implementation and Calibration of a Viscoelastic Bonded-Particle model:comparison of Burgers and Generalized Maxwell Relations and their flow prediction ability** Michael Mascara Graz University of Technology, Austria	**Spreadability versus Flowability: Transient Jamming Makes Them Different** Wei Pin Goh University of Leeds, United Kingdom
12.00-12.20	**Concrete parts from the powder bed – Material modification for selective cement activation** Niklas Meier TU Braunschweig, Germany	**Modelling of selective laser sintering of visco-elastic powders** Juan E. Alvarez University of Twente, The Netherlands
12.20-12.40	**Prediction of Bulk Flow Properties using Mechanical Surface Energy Tester** Vivek Garg University of Greenwich, United Kingdom	**A comparative study on polymeric materials for the selective laser sintering process** Daniele Sofia Università di Salerno, Italy
12.40-13.00		**A New Approach to Quantify Powder's Bed Surface Roughness in Additive Manufacturing** Hamid Salehi University of Leeds, United Kingdom
13.00-13.10	**Plenary - Room Tafuri - Conference Closure**	
13.10-14.30	**Mezzanine**	

Saturday, 9 July 2022

Characterization of feedstock materials for powder bed fusion Additive Manufacturing Jochen Schmidt, Friedrich Alexander University Erlangen, Germany		08.30-09.30
Room Furore		Topic
Particle deformation		Topic
K. Hanley – R. Tarodiya		*Chairs*
Particle-Wall Collision Characteristics for Non-Spherical Particles Under Normal Impact: Numerical Investigation Avi Levy Ben-Gurion University of the Negev, Israel		09.30-09.50
Discrete Element Modeling of Strongly Deformed Particles in Dense Shear Flows Nazanin Ghods Graz University of Technology, Austria		09.50-10.10
Water Content Related Changes on Wood Pellet Properties Abdullah Sadeq Hamburg University of Technology, Germany		10.10-10.30
Coffee break		10.30-11.00
Wear and attrition		Topic
Keynote **Understanding structured particle breakage using population balance modeling coupled with FEM calculation and phase-field model (PFM) prediction of crack propagation** Kerry Johanson Material Flow Solutions Inc., United States		11.00-11.20 11.20-11.40
Modelling of Surface Erosion for Polymers and Polymer Composites due to Solid Particle Impact Rahul Tarodiya Ben-Gurion University of The Negev, Israel		11.40-12.00
Modelling Particle Breakage Using a Bonded Particle Model John Morrissey University of Edinburgh, United Kingdom		12.00-12.20
Numerical Investigation of Hydro-abrasive Erosion of Pelton Turbine Injector Rahul Tarodiya Ben Gurion University of Negev, Israel		12.20-12.40
Simulation of surface abrasion in DEM Rosario Capozza University of Edinburgh, United Kingdom		12.40-13.00
Chairs: Massimo Poletto & Diego Barletta		13.00-13.10
Lunch		13.10-14.30

Posters, Room Atena

P1	**A numerical assessment of different bend geometries for reducing erosion during pneumatic conveying** Harald Kruggel-Emden TU Berlin, Germany
P2	**Pneumatic Handling of Bio and Recycled Solids (PHOBARS project)** Manuela Quezada Henry Université de Technologie de Compiègne, France
P3	**Impact of powder and tableting parameters on tablet properties** Amine Ait Ouazzou Hamburg University of Technology, Germany
P4	**Coating of the refractory materials by fine particles to increase the resistance against thermo-mechanical stresses** Olha Aleksieieva Donetsk National Technical University, Ukraine
P5	**Experimental investigation on the role of particle shape and cohesion in the bulk flow behaviour of glass particles in a rotating drum** Wei Pin Goh University of Leeds, United Kingdom
P6	**Preliminary investigation of fluidized bed reactors for carbon dioxide methanation by TPSIM Win software** Alessandro Guzzini Università di Bologna, Italy
P7	**Investigation of the Agglomeration of Particulate Matter in Chimneys Using Acoustic Flow** Kristina Kilikevičienė Vilnius Gediminas Technical University, Lithuania
P8	**Meso-scale DEM for flowability assessment of weakly consolidated fine powders in industry** Rahul Sharma Università di Salerno, Italy
P9	**DEM (meso-)particle property calibration with powder flow characterization techniques** Assem Zharbossyn Università di Salerno, Italy
P10	**Analysis of the interaction of a fine particle as a droplet on a specific surface** Rimantas Kačianauskas Vilnius Gediminas Technical University, Lithuania

LIST OF ABSTRACTS AND INDEX

ABSTRACTS

PLENARIES

6 July 2022 am

New opportunities for granular matter research

Heinrich Jaeger

University of Chicago - United States

The behavior of granular material is determined largely by the interfaces between constituent particles. These interfaces generate contact interactions that can be highly nonlinear and that depend on particle size and shape as well as surface properties. Together with the inherent disorder in the particles' configuration, this complexity poses challenges for predicting the behavior of particulate matter. However, in recent years there have been great strides in better understanding these interactions and controlling the interface properties, with major impact across many different areas where particle-particle contacts play a key role. At the same time, this has opened up new possibilities for designing granular material with novel, desired bulk properties. This talk will outline some of the emerging opportunities in areas ranging from collisional contact charging to dense suspension rheology and from jamming-based soft robotics to reconfigurable architectures.

6 July 2022 pm

DEM-based metamodeling - the booster for design of bulk solids handling equipment?

Dingena Schott

Delft University of Technology - The Netherlands

Developments in discrete element modelling (DEM) enable detailed modelling of granular flows in bulk handling equipment but due to the computational expense of DEM, however a wide use in analysing equipment performance or design optimisation procedures is not yet feasible. Metamodels, or a model of a DEM model in this context, are considered a viable option to effectively use DEM in analysing and improving equipment performance by exploring a wide range of design parameter values.

In this work we show ways of how to use DEM-based metamodeling to the benefit of designing bulk handling equipment. Firstly, we present a methodology to construct and validate DEM-based metamodels. Along with that we present a case study of a discharging hopper illustrating the use and benefits of metamodels in combination with DEM. Secondly, we demonstrate how metamodels can be applied on an industrial scale for complex operational conditions, such as varying bulk material states. The metamodel development in this case is based on a full-scale DEM-MBD co-simulation of a grab that has been used to generate the performance for various levels of bulk cohesion and compressibility (plasticity). By creating metamodels based on these results we could efficiently explore optimal design parameters using an optimization approach.

7 July 2022 am

Flow of bulk materials into small confined spaces: characterisation and modelling

Chuan-Yu (Charley) Wu

Department of Chemical and Process Engineering, University of Surrey, Guildford, GU2 7XH, UK

Many Powder handling and particulate product manufacturing processes involving deposition of bulk solids in confined spaces of a small volume, such as filling a die or a capsule with several hundred milligrams or a few grams of powder mixtures during manufacturing of pharmaceutical tablets/capsules, metallurgical and ceramic parts, as well as powder-based cosmetic products. It is crucial to consistently fill these spaces in order to achieve the desired product quality. However, it is an scientifically and technologically challenging task, requiring a thorough understanding of powder flow behaviours in these processes. This talk aims to discuss the challenges in depositing small quantities of powders into a confined space, to explore the complex powder behaviours in these processes and to evaluate how particle properties and their interactions will affect the bulk flow behaviour. Furthermore, how to effectively characterise powder flow properties for this application will be discussed. The impact of electrostatics and the presence of air on the flow behaviour will also be presented.

Keywords: Powder flow; flowability; die filling; segregation; electrostatics, DEM-CFD.

7 July 2022 pm

The Rheology of Granular Materials: from Fundamentals to Applications

Raffaella Ocone

Heriot-Watt University, United Kingdom

Granular materials exhibit a broad range of intricate dynamic behaviours. The study of their hydrodynamics is extremely relevant in the chemical and process industries, where those materials are widely produced and handled. Understanding how internal (e.g., particles size and shape) and external (e.g., applied stresses, moisture content) physical properties impact on the flow behaviour of solid particles helps industrial practitioners handle and produce particulates in an efficient and less costly way.

Powders can rearrange under stress and, as a result, granular flow is generally classified into three flow regimes, namely a quasi-static regime, dominated by frictional contacts, an inertial regime, dominated by collisional and kinematic stresses, and an intermediate regime where all three sources of stress are important to establish a stress-strain rate relationship. Characterisation of powder flowability is gener0ally restricted to the flow initiation in quasi-static regime, even if, transition into inertial conditions is very common and relevant in practical applications.

The talk will present a critical review of available techniques to characterise the departure from the quasi-static regime into an intermediate flow. We revise the application of shear cells and, in the effort to characterise the departure for the quasi-static regime, we explore the challenges associated with elucidating the rheological behaviour of aerated powders. A commercial instrument, namely the Freeman FT4 Powder Rheometer, is modified to generate Couette flow. The development of the modified instrument, called the “Aerated Bed Virtual Couette Rheometer” (AB-VCR), is presented. The AB-VCR is employed in both non-aerated and aerated modes to determine the rheology of monodispersed spherical glass beads with and without moisture. Systematic measurements of the stresses which develop within the granular medium are presented and a rheological law is proposed. The validity of such a constitutive law is tested and discussed.

8 July 2022 am

Interaction between dry grains and liquids inspired by industrial processes

Pierre Jop

Glass Surface and Interfaces, CNRS/Saint-Gobain, France

Blending grains with a liquid is often the first step in an industrial process, however it is difficult to give a global description due to the triphasic nature of the medium: Cohesion induced by capillary bridges and the progression of liquid in the system create boundaries between zones of different mechanical behavior. Such spatial heterogeneities need to be erase during mixing steps for example. While the static behavior of a homogeneous, partially saturated media is rather well understood, the time evolution of a heterogeneous system is less described. One key ingredient during this presentation is the capillary forces that constrain the movement of the grains. In this lecture, I will illustrate different situations inspired by industrial applications in which the behavior of a granular material evolves with the amount of liquid, relevant for mixing or aggregation topics. From very low liquid contents to dilute suspensions, I will focus on capillaries effect through model experiments that highlight the role of the liquid interfaces to describe the propagation of the fluid, the morphology of the interfaces and the mechanic of the media.

8 July 2022 pm

Potential and limitations of CFD and DEM simulation in the design of orally inhaled drug products

Andrea Benassi

Chiesi Farmaceutici Spa, Parma (Italy)

Orally inhaled drug products (OIDPs) are pharmaceutical forms involving the entrainment of powder particles or droplets by an air stream generate by patient breathing or by a single inspiratory act. Many aspects, in the design of these products, require an intimate understanding of fluid and powder behavior as well as their complex and non-linear interplay in determining the aerosol physics. Recently, simulation tools based on computational fluid dynamics (CFD) and discrete element modeling (DEM) have attracted a growing interest in the OIDPs community, thanks to their explanatory and predictive capabilities. Some recent and promising applications of CFD-DEM computational tools to problems of aerosol generation and deposition in human lungs will be reviewed. The characteristic numbers and orders of magnitude for the main physical quantities will be discussed along with the available experimental techniques we can use to characterize the phenomena and to generate data to validate the simulations. Achievements and current limitations of the computational models will be illustrated.

9 July 2022 am

Characterization of feedstock materials for powder bed fusion Additive Manufacturing

Jochen Schmidt[1,2]

[1]Institute of Particle Technology, Department of Chemical and Biological Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

[2]Colloborative Research Center 814 “Additive Manufacturing”, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Additive manufacturing (AM) processes allow for the production of individualized components of complex geometries without the need for tools or molds. If functional AM-built components of good mechanical properties are desired, typically powder bed fusion (PBF) AM processes are employed. In case of plastic components, PBF of polymers with laser beam (PBF/LB-P) also known as (selective) laser sintering, is an established AM method, while in case of additive manufacture of metal components, PBF of metals with laser beam (PBF-M/LB) and electron beam (PBF-M/EB) are frequently used.

In the aforementioned PBF-AM processes, a powder layer is spread onto the building platform within a heated build chamber and the contour of the part to be produced is selectively fused by the beam source. Then, the building platform is lowered, a new powder layer is spread and the next cross-section of the component is fused. The process sequence is repeated, until the build job is finished. The component quality is determined by the interaction of the AM machine with the feedstock powder. Moreover, the feedstock powders need to exhibit certain bulk solid characteristics, as well as appropriate thermal and rheological properties. Concerning bulk solid properties it becomes obvious from the sketched AM process sequence, that flowability and packing fraction, are the key towards successful powder spreading and preparation of a powder bed of homogeneous packing density and, thus, the reproducible manufacture of dense parts of sufficient mechanical properties and dimensional accuracy.

Within this contribution, powder requirements for PBF-AM processes will be addressed and established, state-of-the-art methods as well as novel approaches for characterization of bulk solid properties of AM feedstock powders under process conditions will be reviewed and assessed with respect to the method’s predictability of the feedstock’s AM processability. Moreover, some important plastic powder production and functionalization methods will be briefly sketched and the effect of particle (c.f. size distribution, shape) and bulk solid properties on part properties and processability, i.e. structure-property relationships along the AM process chain will be demonstrated for selected examples.

WEDNESDAY, 6 JULY 2022
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TUSAIL SYMPOSIUM

Using a commercial rheometer to determine a particle-particle cohesion model

Christine M. Hrenya
University of Colorado - United States

An accurate and robust particle-particle cohesion model, as is used in DEM, is notoriously challenging to obtain. For example, the AFM measurement of particle-particle cohesion is non-trivial at best for rough and/or non-spherical particle. In this work, we demonstrate how an Anton-Paar rheometer is used to obtain the cohesive force and energy for a given set of particles via bulk defluidization in the rheometer. The resulting simple, yet physically sufficient square-force model of cohesion is then applied to an experimental system for measuring the angle of repose. This (different) system is a robust validation test since it is shown to involve both force-dominated and energy-dominated contacts (enduring contacts and brief collisions, respectively). The DEM model predictions are in excellent agreement with the angle-of-repose measurements. The broader implications of these findings are discussed, namely (i) the ability to obtain an accurate DEM cohesion model from simple bulk experiments using a commercially available instrument, and (ii) the applicability of these findings to continuum models for cohesive particles in addition to DEM.

Benefits and open problems in coarse-graining methods for DEM-based simulations of fluid-particle systems

Erasmo S. Napolitano, Francesco P. Di Maio, Alberto Di Renzo

DIMES Department, University of Calabria, Via P. Bucci, Cubo 42C, 87036 Rende (CS), Italy

In the last decades, Discrete Element Method simulations proved to represent a significant leap forward in the capability to study and understand the complex hydrodynamics of fluid-solid systems. Yet, despite the progress in the computational power and parallel algorithms, their initial limitations on the number of particles still hinders widespread applications to scale of industrial, if not pilot or even laboratory relevance. Coarse-graining methods have been recently proposed to overcome these limits. They act at the physical level, representing sets of actual particles by larger, coarse-grained computational particles, or *parcels*, whose properties are derived in order to capture the physics of the original system. In the last years, coarse-grained simulations have been applied in very different fields, from dense, quasi-static systems to bubbling or fast fluidized riser reactors, and included thermal and reactive effects, as well as scaled properties for cohesive flow, showing orders of magnitude lower computational savings. In the face of an enormous potential, the ability of coarse-grained DEM to accurately represent the complexity of granular and multiphase flows has not been proved under all conditions and, especially, at all levels of coarse graining. This lecture summarises the approaches, the advantages and limitations of coarse graining strategies and levels, presenting applications of the method in riser flow and cyclones. Open problems are identified and discussed in detail along with directions for future developments.

Comparison of CFD-DEM and TFM approaches for the simulation of the single- and multiple-spout fluidized beds

Behrad Esgandari[1], Stefanie Rauchenzauner[2], Christoph Goniva[3], Rouven Weiler[4], Simon Schneiderbauer[1,2][1]

[1]Department of Particulate Flow Modelling, Johannes Kepler University Linz (JKU), Linz, Austria

[2]Christian Doppler Laboratory for Multi-Scale Modelling of Multiphase Processes, Johannes Kepler University Linz (JKU), Linz, Austria

[3]DCS Computing GmbH, Linz, Austria [4] BASF SE, Ludwigshafen, Germany

Keywords: Spout fluidized bed, KTGF, CFD-DEM, Experimental validation

Spout fluidized beds have been employed in various processes, including gasification, chemical looping combustion, and catalytic oxidation. Spout fluidized beds take advantage of both spouted and fluidized beds, enabling them to enhance particle circulation and mixing as well as action in wider operating ranges with less flow rate in comparison with other beds.

In the past decades, two main modelling approaches have been used to analyse spout fluidized beds. On the one hand, the Eulerian-Eulerian approach (e.g. two-fluid model, TFM), where both phases are treated as interpenetrating continua and the particle collisions are considered by the kinetic theory of granular flows (KTGF), is preferably used for larger scales. On the other hand, the Eulerian-Lagrangian approach (e.g. CFD-DEM), where the gas phase is considered as continuous phase and the particles are tracked individually, is commonly used for more detailed descriptions.

In the present study, we compare the predictions of TFM and CFD-DEM with experiments for multiple spout beds [1]. Thereby, we employ OpenFOAM in the case of TFM, where new boundary conditions (Schneiderbauer et al. [2]) and frictional models (Chialvo et al. [3]) have been implemented. In the case of CFD-DEM, the open source framework CFDEMcoupling is used. Computed time averaged velocities show fairly good agreement with PIV and PEPT measurements. Furthermore, bed expansion, time-averaged particle velocity and solids volume fraction profiles are compared in detail. In addition, granular temperature profiles and solids circulation rates were analysed.

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[1] Corresponding author, E-mail address: simon.schneiderbauer@jku.at

Modelling fluidization by recurrence CFD (rCFD)

Varun Dongre[1], Stefan Pirker[1]

[1]Department of Particulate Flow Modelling, Johannes Kepler University, Linz, Austria

Over the last decades, the numerical modelling of fluidized beds has become feasible even for industrial plant-scale. Commonly, continuous two-fluid models are applied to describe large-scale fluidization. In order to allow for coarse grids, novel two-fluid models account for unresolved sub-grid heterogeneities. However, computational efforts remain high – in the order of several hours of compute-time for a couple of seconds of real-time – thus preventing the representation of long-lasting heating or conversion processes.

In order to overcome this limitation, data-based recurrence CFD (rCFD) has been put forward in recent years (e.g. Lichtenegger & Pirker, 2016; Pirker & Lichtenegger, 2018). rCFD can be regarded as a data-based method, which relies on the numerical predictions of a conventional short-term simulation. This data is stored into a database and then used by rCFD to efficiently time-extrapolate the fluidization process in high spatial resolution. Previous studies report on computational speed-ups in the order of three to four orders of magnitude, eventually allowing for real-time simulations of fluidized beds (e.g. Dabbagh et al., 2020).

In this study, we apply rCFD to a set of fluidized beds of different sizes. In a series of short-term simulations, we will compare the numerical predictions of rCFD with corresponding full CFD reference simulations. For this comparison, we will focus on solid mixing, particle size segregation and heterogeneous gas-solid exchange rates. We further present a sensitivity study on how much rCFD predictions vary with modelling parameters and discuss on how rCFD could be calibrated in order to better agree with full CFD.

As a result, this study gives a clear indication on the applicability, predictive capabilities and existing limitations of rCFD in the realm of fluidization modelling.

References:

Lichtenegger & Pirker, Recurrence CFD – A novel approach to simulate multiphase flows with strongly separated time scales, ***CES*** (2016).

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WEDNESDAY, 6 JULY 2022

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COMPUTATIONAL MODELS

DEM calibration of cohesive bulk materials

Corné Coetzee, Otto Scheffler

Department of Mechanical & Mechatronic Engineering, University of Stellenbosch, Stellenbosch, South Africa

The Discrete Element Method (DEM) is a numerical modelling technique often used to analyse and predict the behaviour of bulk granular materials. One major drawback, however, is that it is not straight forward to determine the material micro-properties at contact level, which is required as input parameters. Accurate results can only be achieved if an appropriate parameter calibration process is first undertaken. During this process, simple laboratory experiments are performed to measure certain bulk properties, such as the angle of repose. The experiments are then numerically repeated, and the set of input parameters that produces the measured bulk properties the most accurately, is determined. This last step is either performed iteratively or using optimisation algorithms.

For non-cohesive materials, the calibration process has evolved over the last decade to a level where users can be confident in their results. Experiments such as the angle of repose (lifting cylinder) and the draw down test have shown to be efficient and suitable for the calibration of non-cohesive materials under low consolidation. However, when the material is cohesive (mostly due to moisture), additional contact parameters are required. The additional parameters add complexity to the calibration process. Firstly, the experiments used to calibrate non-cohesive materials are not necessarily appropriate, and the cohesive parameters do not act alone, but in combination with the non-cohesive parameters.

First, this paper reviews the contact models currently available to model cohesive materials, such as the Johson-Kendall-Roberts (JKR) model, the group of simplified-JKR models, a linearised adhesion model, and elasto-plastic-adhesion models. It also reviews the experiments used to calibrate cohesive materials.

Secondly, the paper compares the calibration of wet sand using various experiments, ranging from annular ring shear, angle of repose, draw down, cone penetration, rotating drum (dynamic angle of repose) and a new slope failure experiment in a centrifuge. The sensitivity of each experiment, and the corresponding DEM model, to the bulk cohesion (due to changes in the moisture content and the particle size distribution), is investigated. The aim of this exercise is to determine which experiment, or combination of experiments, is the most sensitive to cohesion and thus the best to use for calibrating the parameters of cohesive materials.

DEM model for the quantitative prediction of cohesive powder (ESKAL) flowability

Maheandar Manokaran[1], Martin Morgeneyer[2], Christophe Bressot[3]

[1]Génie de procédés Industriels, Université de Technologie de Compiègne (UTC), Compiègne, France

[2]Génie de procédés Industriels, Université de Technologie de Compiègne (UTC), Compiègne, France

[3]Direction des Risques Chroniques, Institut National de l'Environnement Industriel et des Risques (INERIS), Verneuil en Halatte, France

Many powders and particulate solids are stored and processed in large quantities in various industries. These solids often encounter handling and storage difficulties that are caused by the material cohesion. For example, high material cohesive strength as a result from high storage stresses in a silo can cause ratholing problems during discharge. Therefore, it is essential to consider the stress-history dependence when evaluating such handling behavior.

In recent years, the Discrete Element Method (DEM) has been widely used to study the complex behavior of granular materials. DEM models commonly used to model adhesions, such as JKR, DMT, and linear cohesion models, have shown that it is difficult to predict the stress-history dependent behavior. DEM modelling of cohesive solid at individual particle level is very challenging. To apply the model accurately at the individual particle level, it is necessary to determine the model parameters at the particle level and take into account the very complexities of interfacial interactions. In this work an adhesive elasto-plastic contact (DEM) model for the mesoscopic level with 3D non-spherical particles is proposed with the aim of achieving cohesive powder flowability. Simulations have been performed for uniaxial consolidation followed by unconfined compression to failure using this model.

The DEM model calibration was achieved by using an extended uniaxial tester to measure flowability of bulk solids. It produced highly repeatable flowability measurements and was shown to be a good candidate for DEM model calibration. The implemented contact model has been shown to be capable of predicting the experimental flow function (unconfined compressive strength versus the prior consolidation stress) for a limestone powder (ESKAL) which has been selected as a reference solid in the wide research network. It has been shown that the contact plasticity of the model has a significant effect on flowability and is thus essential for producing satisfactory computations of the behavior of a cohesive granular material. The results provide new insights and suggest a micromechanical based measure for characterizing the strength and flowability of cohesive granular materials.

DEM simulation of moist sand over a transfer point

Otto Scheffler, Corné Coetzee

Dept. of Mechanical and Mechatronic Engineering, University of Stellenbosch, Stellenbosch, South Africa

The accuracy of the Discrete Element Method (DEM) for replicating the behaviour of a cohesive material flowing over a transfer point is evaluated. The analysis serves as a validation procedure of a proposed method for calibrating the bulk response of a cohesive granular material. Three grades of silica sand serve as the bulk test material and cohesivity is controllably introduced to the material with the use of water.

Accordingly, four degrees of material saturation (or moisture content) are evaluated for each of the three test materials. A specific amount of material is loaded evenly onto a test conveyor before the conveyor delivers the test material to the transfer point. Subsequently, an impact plate is placed in the path of the flowing material. Additionally, fins are secured to the impact plate and the test material loaded onto the finned impact plate and scraped level before each test. The latter minimises the uncertainty of particle-wall effects when cohesive material buildup is assessed.

The aforementioned system is replicated numerically using DEM. A generic linearized liquidbridge contact model is employed for governing the particle interactions. The material input parameters and contact model parameters have been calibrated for each of the three test sands – at a range of particle scale ratios and moisture conditions. Agreement between the physical system and the numerical counterpart is assessed through two quantitative measures and two qualitative measures. The increase in residual weight, as material cohesion increases, is considered the most important quantitative measure. Hereafter, the peak force experienced by the plate is next evaluated. The main qualitative comparison between the physical system and numerical counterpart is the height of the residual material left on the plate. After this, the overall shape of the material build-up is simply visually assessed for agreement.

Quantitatively, a good agreement is achieved for smaller scaling factors. Nonetheless, the divergence between the physical system and numerical counterpart grows as the scaling factor is increased. The degree to which particles can be upscaled whilst still maintaining reasonable accuracy also appears to increase as the material cohesivity increases. Qualitatively, the residual material build-up height is also in good agreement for smaller scaling factors. However, the overall replication of the cohesive material shape build-up does not seem to mirror the physical system with only an approximation of the physical profile obtained. Although, in both the numerical and physical systems, a distinctive bulk cohesive system can be intuitively recognised.

DEM modelling of elastic-plastic contact behavior for cohesive powders

Robert Hesse, Sergiy Antonyuk

Institute of Particle Process Engineering, Technical University of Kaiserslautern, Kaiserslautern, Germany

Powder processing usually includes several production stages, whereby stresses on the powder can vary heavily. While storage and transport might enforce pressures of kilopascals, the final compaction step to a tablet or similar products will require orders of magnitude higher stresses to be used on the powder.

For low stresses, small powders can be assumed to be mostly elastic, whereby cohesion modeling is more forgiving and has already been accomplished in the past [1]. For elasticplastic contacts, we propose an extension of the model by Weis et al. [2] by including a pure elastic contact before the yield stress is reached. Due to the plastic flattening of the contact partners (Fig. 1), simple models like the Hamaker model for sphere-sphere or sphere-wall contacts [3] is no longer applicable. Therefore, an approximation of the Hamaker model is proposed for arbitrary plastic deformation, which allows usage of the data base that already is established for Hamaker constants of various materials. The model is converted for the opensource software LIGGGHTS® for Discrete Element Method (DEM) simulations.

For the validation of the model and simulations, a cohesive lactose powder (FlowLac 90, Meggle) was subjected to compaction tests of various normal pressures. The compaction cell (Fig. 2) consisted of a sliding outer shell that is suspended by a spring, which slides downwards during compaction. This reduced the wall influence, which allowed simplification of the simulation domain. Finally, the model accuracy and limitations are discussed.

An SPH study on the compaction of soft deformable grains

Francisco Goio, Stefan Radl

Institute of Process and Particle Engineering, Graz University of Technology, Graz, Austria

This contribution presents the results of a study on the compaction of soft deformable grains beyond the close packing limit. The newly developed numerical approach is based on Smooth Particle Hydrodynamics (SPH) and Discrete Element Method (DEM). The code is the result of the merging of a continuum mechanics oriented SPH formulation [1], and DEM [2]. The resulting software embodies the ability of simulating extreme particle deformations together with a wide variety of contact models that can include frictional or cohesive effects.

The compression is studied in different scenarios, considering both 2D and 3D simulations. In the 2D case, compressions are carried on a single grain as well as on an ensemble of grains. The stress strain data produced is interpreted using a micro mechanical model. The output is then compared to results obtained with state of the art methods in literature [3]. 3D compression simulations are carried on a sample of elastic spherical grains, and the results are discussed in light of available experimental data. Finally, an outlook on possible applications in the food and pharma sector is provided.

Keywords: soft grains, deformable grains, large deformations, compaction, granular materials, computational models, SPH, DEM.

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WEDNESDAY, 6 JULY 2022
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MECHANICAL BEHAVIOR OF BULK MATERIALS

The role of Archimedes number in particulate bed void-fraction and flowability

Haim Kalman[1,2] and Dmitry Portnikov[1]

[1] The Laboratory for Conveying and Handling of Particulate Solids, Department of Mechanical Engineering, Ben-Gurion University of the Negev, Beer Sheva 84105, Israel.

[2] Aaron Fish Chair in Mechanical Engineering – Fracture Mechanics, Israel.

All forces affecting the void fraction (VF) and density of a particulate bed are analysed. The bulk density of many materials, both spherical and non-spherical, with a variety of properties, including particle size and density, were measured in air and various liquids. The Archimedes number (Ar) was found to be an appropriate representation of the particle behavior that considered the van der Waals forces. The effects of buoyancy and viscous forces, as components of Ar, on the VF were shown by experiments in various liquids. Additional forces, such as friction, impact, and tapping were discussed quantitatively and qualitatively. Archimedes number was found to be an appropriate parameter to well describe also some flowability parameters, such as: Hausner ratio, angle of repose and angle of tilting. The many experiments presented clear trends enabled to develop accurate correlations for the various parameters revealing deep understanding of the behaviour.

Case Study: Silo and System Design for Fibrous Recycling Materials

Hans Schneider

Zeppelin Systems GmbH, Friedrichshafen, Germany

When processing powders to intermediate or final products in extrusion or calendaring it is inevitable to completely avoid reject or trim material. Therefore, it is very important for an efficient use of raw material to find a process to recover the reject and trim and reintegrate it into the process. The amount, composition, shape and size of reject and trim materials vary as much as industrial production processes vary, but most often these materials have completely different properties compared to their raw materials. The entire process is generally called inhouse recycling because the material does not leave the production site before it is reused.

In this case study the development of the material handling steps of an inhouse recycling process for a fibrous multi-component and multi-layer polymer material is presented.

The complete system consists of conveying, storage and compaction of the fibrous material and conveying and homogenizing of the compacted material. Prior to the system design the material had been characterized and tested to provide a reliable solution.

Product tests were executed in laboratory scale by means of shear tests for silo design as well as in pilot plant scale for pneumatic conveying, rotary feeder performance and silo discharge design. Based on these results the process was detailed and the respective plant was built and successfully commissioned.

Finally, it turns out that conventional methods for material characterization of fibrous bulk solids are reaching their limits and new methods need to be established. A new approach to characterize fibrous material in different ways is presented in the talk “Comparison of different test methods for the flow property evaluation of fibrous materials” by Beitz et. al. As a first approach these methods have been applied to the silo design of the present case study.

Keywords: Recycling, fibrous particles, elongated particles, silo design,

A combined DEM and CNN model for characterizing and evaluating the performance of ball mills

Yaoyu Li, Runyu Yan *

[1] School of Materials Science and Engineering, UNSW Sydney, NSW 2052, Australia

Ball milling is an important size-reduction operation in cement and mineral processing industries. It is a capital and energy intensive process with low efficiency. Therefore, it is necessary that ball milling circuits are properly designed and monitored. Predicting the performance of a full-scale mill, such as product size, grinding capacity and power requirement, based on the data from lab or pilot scale mills is a challenging task. Previously, various scaleup procedures have been proposed mainly based on Bond model and specific energy (input energy per unit mass of product). However, they are not effective because only a fraction of the input power is used for the actual grinding. Therefore, it is more intrinsic to link those useful energy, such as damping energy between grinding media, with grinding kinetics. This requires the knowledge of energy information at the particle scale. Discrete element method (DEM) can provide particle scale energy information as it treats the particle flow as an assembly of particles and computes the motion of each particle according to Newton's second law of motion.

In the work, we first develop a modified breakage selection function model to describe the relation between damping energy and particle breakage probability from DEM simulations. The damping energy for each contact is calculated by integrations of damping force and movements at each time step. The process grinding rate is then be calculated based on the model by adding up all broken mass divided by total particle mass. Fig. 1a shows an example of grinding rates of a small mill on different rotation speeds. We finally develop a new scale-up procedure to link the process grinding rate with the damping energy.

Development of models of the collective dynamics is the key to online process monitoring, which relate the key internal process variables to the external measurable variables. In industries, monitoring the operation of drums or mills often relies on acoustical signals. We develop a modelling framework based on multi-source information (AE signals, specific power draw and rotation speeds) from DEM simulations, combining the convolutional neural network (CNN) with transfer learning, to quickly predict particle size distributions and grinding rates of the ball mill system. The proposed model was separately trained at a single collision system (Pre-training), a small drum system (Fine-tunning) and validated by a lab-scale drum system (Validation). Fig. 1b shows predictions results in comparisons with simulated grinding rates.

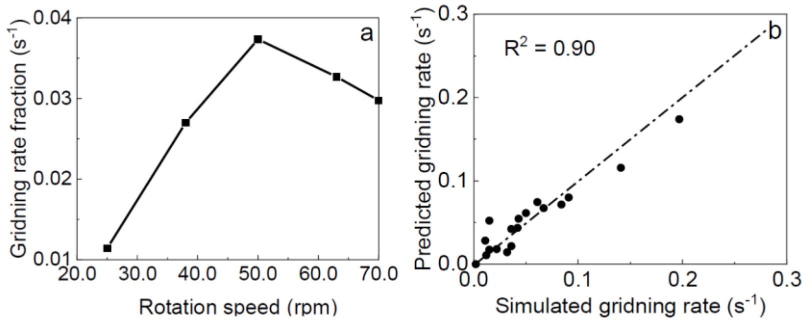

Fig. 1 Process grinding rates: (a) simulated examples of a small drum on rotation speeds when particle mill load is 3.63 kg; (b) comparisons between predicted and simulated ones.

Rheology of cohesive powder mixtures

Mehrdad Pasha[1,2], Wenguang Nan[1,3], Muzammil Ali[4], Xiaodong Jia[1], Mojtaba Ghadiri[1]

[1]School of Chemical and Process Engineering, University of Leeds, Leeds, UK

[2]UCB Pharma, Chemin du Foriest B-1420 Braine l'Alleud, Belgium

[3]School of Mechanical and Power Engineering, Nanjing Tech University, Nanjing 211816, China

[4]Fluid Comp, Leeds, UK

Flow behaviour of powder mixtures is of great industrial interest. Formulated powders have both free flowing and cohesive components, which can influence the powder flow depending on their constituent amount. A question which naturally arises in formulation science is whether this is predictable from the properties of the individual components. We present our work on flow characteristics of binary and ternary mixtures under dynamic conditions using Discrete Element Method. The expended mechanical work of a rotating impeller penetrating a packed bed is simulated and used as an indicator of the ease with which the powder mixture flows under dynamic conditions. The individual particle cohesiveness is expressed by the granular Bond number. Three averaging methods are examined to express the Bond number of the mixture, namely arithmetic, geometric and harmonic mean, for which a weighting factor based on the fractional surface area of each component of the mixture is used. Forty binary and ternary mixtures are simulated and the relationship between the expended work and the mixture Bond number is explored. The transient rheological response of both single component and powder mixtures is deduced from the blade torque and is related to the inertial number and granular temperature, for which a unified power law is obtained covering both quasi-static and intermediate flow regimes. The analysis provides a model of bulk friction and viscosity, which can be used for obtaining flow field in complex geometry and dynamics using continuum mechanics by Computational Fluid Dynamics. This provides a methodology for use as a design aide for powder formulation based on the constituents single particle properties.

Experimental study of granular heap flow under vertical vibrations

Ghita Marouazi[1], Mathieu Jenny[1], Arthur Pascot[1], Sergiy Antonyuk[2], Fabian Krull[2], Sébastien Kiesgen de Richter[1]

[1]LEMTA, Université de Lorraine, CNRS, F-54000 Nancy, France

[2]Institute of Particle Process Engineering, Technische Universität Kaiserslautern (TUK), Kaiserslautern, Germany

Granular materials are widely encountered in industries (cosmetics, pharmaceutics, food processing...) and in nature (avalanches, sand castles, lava flows...). These materials flow like non-Newtonian fluids. The complex rheological properties need to be understood and described with physical based models to predict and to optimize the end-use properties of these products in connection with their formulation. For instance, the flowability of powders can be improved by applying adapted mechanical vibrations. However, the physical mechanisms that account for the effect of vibrations on particle contact dynamics, and subsequently on the rheology of spreading, are still poorly understood.

To study the flowability of powders, the heap flow is a good reference configuration. The flow occurs when the slope exceeds a critical value of the angle of repose are generally not produced unless slopes exceed more or less the angle of repose. When a system is subjected to mechanical vibrations, the critical angle of repose decreases, and it can even vanish to zero. The vibrations cause failures of frictional contacts among grains, which changes dramatically the rheological properties of the granular system.

For this study, a conical pile of grains made of spherical glassbeads (d=400-500µm) is placed on a rough disk, which is horizontally mounted to a vibration device. The vertical sinusoidal vibrations are controlled by an accelerometer used to adjust the instruction sent to the vibrator. The time evolution of the angle of repose is studied for multiple amplitudes and frequencies. A CCD camera is used to measure the slope of the pile. Moreover, the influence of the bottom surface properties is studied by varying the rugosity and the material of the disk.

We demonstrate that vibrations highly influence the volume of the system while keeping a selfsimilar shape throughout time for multiple rugosities. The influence of humidity is also investigated to reveal the effect of vibrations on cohesive heap flow.

How a granular pile becomes a glass

Stefan Boettcher*[1], Paula A. Gago+[2]

[1]Department of Physics, Emory University, Atlanta, USA;

[2]Department of Earth Science and Engineering, Imperial College London

*** sboettc@emory.edu, + paulaalejandrayo@gmail.com**

We have explored the compaction dynamics of a tapped granular pile in microscopic detail using extensive molecular dynamics simulations [1,2]. We will show data for the density and density fluctuations of the ensemble of mechanically stable configurations reached after the energy induced by the perturbation has dissipated [2]. By gradually decreasing the tap intensity at various rates, we find that density becomes a function of the rate, not the intensity alone, a tell-tale sign of non-equilibrium ("glassy") behavior arising for low intensities, after passing through a so-called glass transition. More specifically, we will argue that different horizontal sub-regions (layers) along the height of the pile traverse a glass transition in a similar manner but at distinct tap intensities. Our data shows that in each layer its transition is further marked by a corresponding peak in the density fluctuations. From this we infer that, at a given tap intensity, certain regions of the same pile may respond glassy while others remain equilibrated. Looking beyond these static configurations at the grain-scale dynamics *during* each tap, we find that the effective energy that particles dissipate is a function of tap intensity as well as of the particles location in the pile. In turn, when plotted as a function of that effective energy, the transitions for those layers align and the data for their density fluctuations collapse. We conclude that this internal energy provides a "temperature-like" parameter characterizing a glass transition similar to those in thermally driven materials.

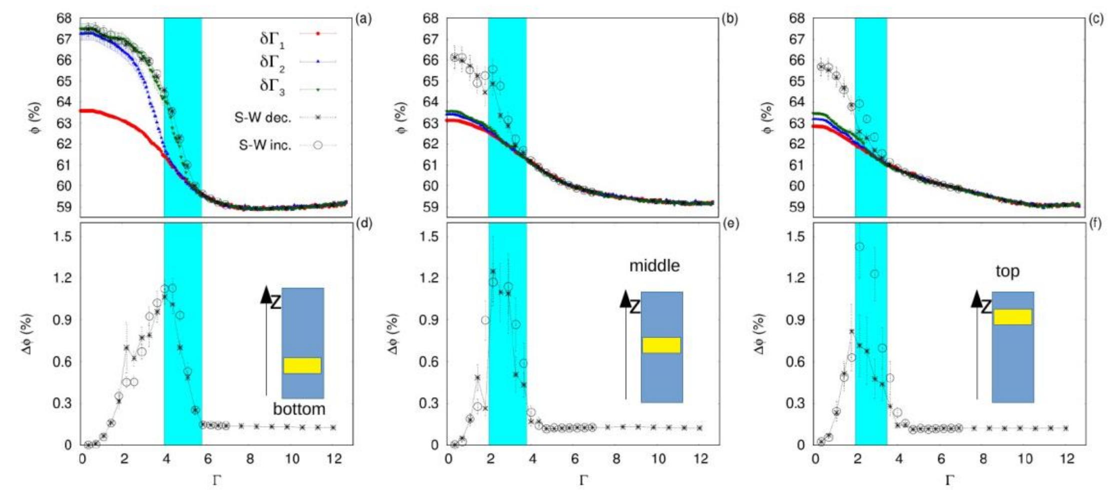

Figure: Packing fraction f in the granular pile measured over three different horizontal layers at the: bottom (a), middle (b) and top (d). For the continuous protocol it is dG_1 (red circles), dG_2=dG_1/4 (blue triangle-up) and dG_3=dG_1/8 (green triangles down). For the step-wise (S-W) protocol, crosses correspond to a decreasing protocol and open circles to its reverse, i.e., increasing protocol. Density fluctuations Df as a function of G for the same three layers displayed in (a)-(c), respectively, as obtained by the step-wise protocol. For each protocol, 16 independent realizations were performed, and error bars in all the figures correspond to the standard error of their mean. Shaded areas mark the G-range corresponding to the right slope of each peak in Df vs. G.

[1] Gago, P. A. and Boettcher, S. (2020). *PNAS*, *117*(52), 33072-33076.

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Density instabilities and compaction efficiency in a tapped granular pile.

Paula A. Gago*[1], Stefan Boettcher+[2]

[1]Department of Earth Science and Engineering, Imperial College London;

[2]Department of Physics, Emory University, Atlanta, USA

*** p aulaalejandrayo@gmail.com ; + sboettc@emory.edu**

The compaction of a granular pile subjected to a series of discrete tapping has been widely investigated due to its relevance in both, basic and applied science. The well know Chicago experiment [1] showed that, given a granular pile subjected to taps of controlled intensity, it is possible to define the density of the system as a *reversible* function of the tap intensity. Using a continuum annealing protocol, where the intensity (G) of the tap was reduced at different (constant) variation rates (dG) after each tap, we have showed [2,3] that although for high tap intensities, the density f of the system can indeed be defined solely by the tap intensity, for low tap intensities f will become *also* a function of the protocol followed to reach the given intensity. This behaviour, shown in the figure (a) below, is characteristic of non-equilibrium ("glassy") systems. The transition between these two regimes is accompanied by a region of high susceptibility, as shown in the figure (b) below, where a peak on the density fluctuations (Df) can be observed while the pile traverses the "glass" transition. In this presentation we will show how, by taking advantage of the high susceptibility of the density, it is possible to develop annealing protocols that allow to maximise compaction along the pile while expending minimal time and energy.

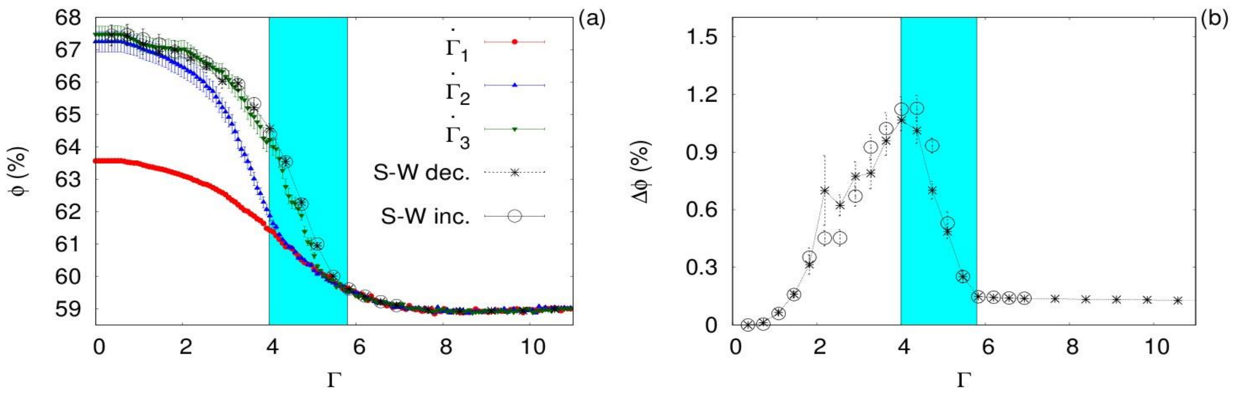

Figure: (a) Packing fraction f in the granular pile as a function of the tap intensity G. For the continuous protocol it is dG1 (red circles), dG2=dG1/4 (blue triangle-up) and dG3=dG1/8 (green triangles down). For the step-wise (S-W) protocol, crosses correspond to a decreasing protocol and open circles to its reverse, i.e., increasing protocol. (b) Density fluctuations Df as a function of G for the same system displayed in (a) as obtained by the step-wise protocol. For each protocol, 16 independent realizations were performed, and error bars in all the figures correspond to the standard error of their mean. Shaded areas mark the G-range corresponding to the right slope of each peak in Df vs. G.

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[2] Gago, P. A., & Boettcher, S. (2020). Universal features of annealing and aging in compaction of granular piles. *PNAS*, *117*(52), 33072-33076.

[3] Gago, P. A. and Boettcher, S. (2021). Density fluctuations in granular piles traversing the glass transition: A grain-scale characterization of the transition via the internal energy. (Sci. Adv. in press)(https://arxiv.org/abs/2107)

Optimization of a flighted rotary drum cross-sectional characteristics

Dmitry Portnikov[1], Gennady Ziskind[1,2] and Haim Kalman[1,3]

[1]The Laboratory for Conveying and Handling of Particulate Solids, Department of Mechanical Engineering, Ben-Gurion University of the Negev, Beer Sheva 84105, Israel.

[2]Anne Tanenbaum Chair in Engineering Thermodynamics, Israel.

[3]Aaron Fish Chair in Mechanical Engineering – Fracture Mechanics, Israel.

The current work involves experimental and computational study of rotary drum cross sectional characteristics such as: kinetic angle of repose (AoR), flight holdup, drum filling degree, drum discharge energy and drum discharge power. Experiments with two spherical and three non-spherical particulate materials with sizes between 70 µm and 2 mm were performed in a home-made rotary drum to measure the kinetic angle of repose and flight holdup as a function of flight angular position and drum rotational speed. As a result, an empirical model was proposed to predict the kinetic AoR as a function of the Archimedes number, Froude number, and flight angular position. In addition, a simple computational algorithm was introduced to predict the flight holdup as a function of flight angular position, which also considers the effect of drum filling degree. Validation with the experimental data showed a good agreement of the model. Furthermore, a discharge energy and discharge power characteristics were introduced, and a parametric study showed that these characteristics can be used as key parameters for optimization purposes.

Comparison of different test methods for the flow property evaluation of fibrous materials

Steffen Beitz[1,2], Harald Zetzener[1], Hans Schneider[2], Arno Kwade[1]

[1]Institute for Particle Technology, TU Braunschweig, Braunschweig, Germany

[2]Zeppelin Systems GmbH, Friedrichshafen, Germany

Nowadays, topics like recycling and handling of fibrous products from biomass sources lead to new challenges facing the processing of non-spherical elongated particles. Since conventional methods and measurement devices have not been proven suitable for reliably predicting flow of these bulk solids in silos and related plant equipment, alternative approaches have to be tested and evaluated. Therefore, experiments were carried out with modified and custom-made testers: horizontal tensile tester [1] and shear testers with horizontal or vertical shear zones (similar to [2]). As test materials dry wood chips of different sizes, monodisperse model fibers and actual industrial recycling fibres were used. Therefore, particle beds have been loaded vertically (at 1, 2 and 4 kPa) and their bed strengths have been determined in various directions to investigate the anisotropic flow behavior of elongated particles. Further data was gathered by measuring the wall friction against vertical and horizontal wall samples.

It can be concluded from the results that the flow behaviour of elongated particles differs strongly from spherical ones. The calculated strength values depend on the stressing direction and alignment of the particles as well as their single particle properties such as size and shape (e.g. convexity via dynamic image analysis). Additionally, the filling method and bed height have a significant impact on the obtained strengths. Shear tests with transparent cells revealed the limits of shear testing (no single horizontal shear band, elongated particles tend to pile up, etc.). In contrast, the determination of tensile strength seems to be much more repeatable in comparison even at low consolidation stresses. The strengths that are obtained from the vertical testers depend strongly on particle size, stiffness and the testers' geometries (position of the edges between the punch and the outlet where the material is pushed through). Nevertheless, the variation test geometry dimensions provided deep insight into the progression of transferred pressure between particles due to interlacing and interlocking. In addition, the wall friction tests show that there is an industrial relevance of the anisotropic measuring approach. Depending on the stressing direction, e.g. wall friction can be over- or underestimated. Further details involving those results are discussed in the talk by Zeppelin Systems ("Case study: silo and system design for fibrous recycling materials").

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[2] Van der Kraan, M.; Scarlett, B.: Development of a Tester for Measuring Caking Behaviour of Powders; PARTEC 95 Preprints, p. 57-68

Keywords: Biomass, elongated particles, method development, particle shape, anisotropy

Reverse Janssen effect in narrow granular column

Shivam Mahajan[1], Michael Tennenbaum[2], Sudhir N. Pathak[1], Devontae Baxter[2], Xiaochen Fan[2], Pablo Padilla[2], Caleb Anderson[2], Alberto Fernandez-Nieves,[2,3,4], Massimo Pica Ciamarra[1,5]

[1]Division of Physics and Applied Physics, Nanyang Technological University, Singapore

[2]School of Physics, Georgia Institute of Technology, Atlanta, Georgia, USA

[3]Department of Condensed Matter Physics, University of Barcelona, Barcelona, Spain

[4]ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain

[5]CNR–SPIN, Dipartimento di Scienze Fisiche, Università di Napoli Federico II, Napoli, Italy

In a celebrated experiment, Janssen found a mass m of grains in a silo to exert on the silo bottom a pressure corresponding to an apparent mass $m_{app} < m$, and that m_{app} saturates as m increases. This experiment demonstrates that, as more grains are added to a silo, the walls support an increasing fraction of their weight through frictional interactions. This experiment, which has engineering relevance in silo design, emerged as a testbench for stress propagation theories.

Here, we demonstrate via experiments and numerical simulations a reverse Janssen effect. If grains are gently poured into a narrow column, then the apparent mass overcomes the true one for some filling heigh. We show that this reverse Jannsen effect originates from the presence of frictional wall-particle interactions that compress the grains rather than sustain them and clarify the microscopic mechanism leading to the formation of these compressive frictional forces. Furthermore, we develop a continuum stress propagation model that quantitatively accounts for our observed findings.

Overall, our work uncovers a novel phenomenon and challenges accepted theories of granular elasticity by demonstrating that the preparation protocol, which is commonly neglected, qualitatively affects how stress propagates in a granular assembly.

WEDNESDAY, 6 JULY 2022
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SILO DESIGN

Proposal to structure silo failure analysis

Harald Wilms[1], Hans Schneider[2], Christian Dietsche[2]

[1]Wilms-ITC, Innovation-Technology-Consulting, Bremen, Germany

[2]Zeppelin Systems GmbH, Friedrichshafen, Germany

Silo malfunctions and failures, both operational and structural, cause plant downtime, significant implications on plant operation and immense cost for modification or repair. Thus, analysis of respective failures needs to be structured and as quick as possible. However, there are only very few failures with a clear single cause. Typically, only a combination of wrong design assumptions or operating conditions can explain a failure.

Numerous failures have been analyzed in the past and some cases with typical failure causes are presented. Experience from a variety of failures is used to establish a check list on potential failure causes. This check list can be used to investigate silo failures in the future more quickly.

The evaluation of failures by means of such a check list can also assist in attributing the responsibility for certain design or operational mistakes to the respective party and thus this proposal may serve as a tool to settle any economic dispute resulting from repair or modification cost.

Process intensification of hopper discharge of cohesive powders based on modulated pulsed airflow

Haifeng Liu*, Lizhuo Zhu, Haifeng Lu, Xiaolei Guo

Shanghai Engineering Research Center of Coal Gasification, East China University of Science and Technology, China

Cohesive powders are easy to agglomerate, have very poor fluidity, and cannot be discharged smoothly, which greatly restricts the large-scale industrial development of ultrafine particle technology. This research first proposed and developed a flow process intensification method based on modulated pulse airflow, and studied the mechanism of pulse parameters (frequency, amplitude, duty cycle) to enhance the pulse aerodynamic strength, provide high-frequency shear and short-term force. It reveals the evolution law of the rheological behavior of particulate matter under the control of an external field, that is, the pulse aerodynamic force exerts high-frequency oscillating shear on the particle system to soften the stiffness of the particle contact interface, thereby changing the contact mode between particles, reducing the interaction between particles and reduce the internal viscous resistance of particle flow. It is found that the disturbance is amplified by the instability of the particle oscillation, which leads to the microscopic deformation and collapse of the powder, which breaks the limitation of the cohesion and cannot flow and greatly improves the fluidity, realizing the breakthrough of cohesive powder from "non-flowing" to "free-flowing".

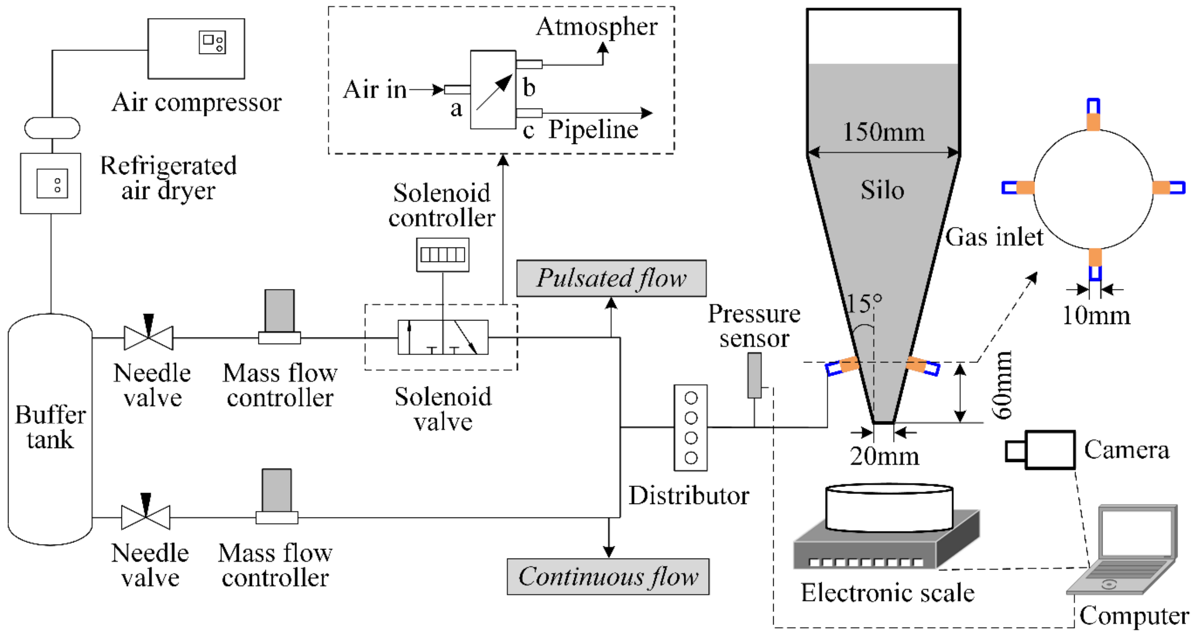

Figure 1. Sketch of experimental apparatus.

Parametric study and flow regime map for planar silos and hoppers

Evgeny Rabinovich[a,c*], Haim Kalman[b], Per F. Peterson[c]

[a] Nuclear Research Center Negev (NRCN), Beer Sheva, Israel

[b] Dept. of Mechanical Engineering, Ben-Gurion University of the Negev, Beer Sheva, Israel

[c] Department of Nuclear Engineering, University of California, Berkeley 94720-1730, US

[*]Corresponding author: erabinovich78@gmail.com

This study presents a new parametric study and flow regime map for wedge-shaped (planar) silos. The analytical part of this study is based on a previously reported theoretical model and includes new analyses regarding the influence of granular material properties, material height, bin and hopper geometrical dimensions, and the possible difference between the bin and hopper wall friction coefficients. It was found that the bin sidewall roughness, material height and bin width have a little influence on the transition from funnel flow (type B) to mass flow (type A) modes. In addition, the mass flow mode could be achieved even for very rough hopper walls, but in that case, a stagnant layer of material exists next to the hopper walls. The new flow regime map should help operators and designers of silos to increase the accuracy and flexibility in the assessment of granular flow regime, and therefore it might significantly improve the process efficiency.

WEDNESDAY, 6 JULY 2022
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PNEUMATIC AND MECHANICAL CONVEYING

Analysing impact forces & overcoming speed, heat and pressure issues in high capacity belt support applications

Cameron Thomas Portelli[1], Charles Camden Pratt[2]

[1]Engineering Department, Kinder Australia, Melbourne, Australia

[2]Operations & Sales Department, Kinder Australia, Melbourne, Australia

Belt conveyor transfers are the most likely location for high wear rates and failures. Belt transfers are necessary to change the direction of conveyed material and will remain a part of belt conveyor systems into the future.

Burden being accelerated due to fall and changes in direction from one system to the next, prevents steady state flow which introduces component fatigue. The conveyor belt is considered the greatest cost item over the life of a belt conveyor system and consumes considerable downtime to change out, therefore a financial incentive exists to preserve this high-cost item. Other issues created at the transfer include health risks of uncontained dust and product losses due to spillage.

Additional consideration to support the belt is one way to improve the life of components and contain dust within the transfer chute. The humble impact cradle/bed has changed little over the years whilst conveyor systems have achieved ever greater flow rates. Further development of the impact cradle is an opportunity to reduce maintenance costs and increase uptime.

The peak technology on the market for conventional impact belt support is the dynamic impact cradle, which ensures the belt support area under the chute allows for some dynamic travel, whilst also maintaining a consistent skirt board area. The impact energy at a transfer when installed with Kinder Australia's dynamic impact bed was measured to further understand the forces involved and how they compare with static belt support systems. Adding further dynamic capacity to the load zone has been shown to increase belt life by at least 30%. Other components also benefit from reducing impact energy in the transfer and the incorporation of polyurethane bushes at roller supports has been employed further increase roller and frame life.

Kinder Australia has developed a unique and innovative range of belt support technologies that further promote dynamic travel whilst maintaining a consistent skirt board area without a significant increase in belt-friction tension by combining slider rails with rollers that can absorb impact independently within the support system and/or utilising exotic slider materials to overcome high belt speeds and/or system capacities. Kinder Australia has a vast library of documented case studies and application data to ensure the future systems being offered will survive, provide better chute sealing and protect the conveyor belt.

Motion resistances in trough chain conveyors

Andre Katterfeld

Institute of Logistics and Material Handling Systems, Otto-von-Guericke University Magdeburg, Germany

Trough chain conveyors often also called En-Masse conveyors belong to the group of continuous material handling technology. This kind of conveyors is often used to transport medium quantities of bulk material. Especially for the transport of agricultural products these conveyors close the gap between screw conveyors and belt conveyors.

In opposition to screw or belt conveyors the calculation of the motion resistances of trough chain conveyors is not defined in ISO, DIN or CEMA standards. However, industrial guidelines like the German VDI 2320 do exist. For the revision of the VDI 2320, a new approach for the calculation of the motion resistances for horizontal, inclined and vertical was developed. This paper summarises the main ideas of the calculation approach and explains how the calculation of the motion resistances allows the calculation of the required drive power as well as the chain strength and the necessary pre-tension.

While the classical analytical calculation approach is useful for the definition of the general design of a trough chain conveyor, the paper will also give an outlook about how DEM simulations could help to overcome the problems and weaknesses of the classical calculation approach.

Understanding the total cost of ownership of bulk solids handling systems: a new paradigm to reduce risks in procurement of solids handling systems and equipment

Charles Williams, Michael Bradley

The Solids Handling And Processing Association, UK

It is very widely the case that industries that process bulk solids as feedstocks, intermediates or finished products, suffer with poor performance and excess operating costs of their handling processes. Unexpectedly low throughput, bulk solid quality problems, plant wear and high downtime hurt user companies, whilst extended commissioning and warranty claims for retrofit to correct problems often hurt system suppliers.

The reasons for this are mainly to do with over-emphasis on project capital price, insufficient attention to bulk solid behaviour, over-confidence in the sufficiency of under-engineered solutions and pressure on programme, without sufficient consideration of likely costs to the business due to unexpected down-time, energy consumption, quality and reliability effects.

This paper presents a novel paradigm for facilitating a more constructive relationship between buyer and supplier of solids handling equipment, which has been developed within SHAPA over the last three years based on the experience of vendors, users and consultants. The new paradigm centres on reviewing in the sales process between both sides, the likely full cost of ownership of the equipment and not just the capital price. This is presented in the form of a document that is designed to stimulate discussion between the two sides, of many factors that often do not make it onto the list of considerations in the usual process of procurement.

The fundamental problems, means for mitigating these and the structure of the new approach are discussed in some depth with the intention of persuading both vendors and purchasers of equipment to test it and provide feedback for its improvement.

Refill strategy optimization of a twin-screw feeder with DEM

Peter Toson[1], Johannes G. Khinast[1,2]

[1] Modeling and Prediction, Research Center Pharmaceutical Engineering, Graz, Austria

[2] Institute of Process and Particle Engineering, TU Graz, Graz, Austria

RTD (residence time distribution) has proven to be a valuable tool for material tracking in continuous pharmaceutical processes. Whereas the impact of feeder fluctuations and other disturbances after refilling has been thoroughly studied in the literature, the impact of feeders on material tracking is often overlooked. Since the experimental methods to measure the RTD feeder discharging processes feeder are complex and material intensive, there is are only limited experimental RTD data available in the literature.

A DEM (discrete element method) simulation of a discharge of a Coperion KT-20 feeder in volumetric mode is available in an open access repository [1]. The results show that the simplest of material tracking assumptions – first in, first out (FIFO) – does not hold in this feeder because of the large fraction of material that is moved by the agitator. The DEM simulation shows that it is a much better approximation to assume discharge of a perfectly mixed material. In addition, the simulations show that there is a tendency to discharge material located above the agitator early. In order to predict the behavior during multiple refill events, three models in order of increasing complexity are presented:

1. A simple reduced order model that assumes perfect intermixing of old and new material, leading to an exponential decay of the concentration of the old material in the hopper.
2. A RTD model based on the discharge of material layers. This model is able to capture the preferred discharge of the top material layers at high fill levels.
3. A DEM extrapolation method colloquially called "Relay Race" [2]. This model accurately describes the trajectories of individual particles over multiple refills.

Refilling at fill levels below 30%, which corresponds to the agitator axis, can be accurately described by any of these models. However, cohesive powders often require refilling at higher fill levels in order to ensure a stable mass flow rate. In this case, discharge of material above the agitator axis plays an important role and one of the more complex refill models is then required.

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Development of bulk material dosing equipment using DEM

Jan Nečas[1,2], Jakub Hlosta[1,2], David Žurovec[1], Jiří Rozbroj[1], Jiří Zegzulka[1,2]

[1]VSB-Technical University of Ostrava, Faculty of Mining and Geology,
17. listopadu 15/2172, 708 33 Ostrava, Czech Republic, EU

[2]VSB-Technical University of Ostrava, CEET, ENET Centre, Bulk Solid Centre,
17. listopadu 15/2172, 708 33 Ostrava, Czech Republic, EU

Research and development in the field of industrial automation has accelerated exponentially in the last decade. Efficiency, cost-effectiveness and reduction of production waste have forced the company to constantly innovate its technological methods and processes. Bulk materials processing is one of the more difficult areas for Industry 4.0 applications. The prediction of the behaviour of innovated but also existing granular material mixtures even with respect to low waste industrial activities is becoming a more relevant topic today. Based on current requirements, equipment for efficient and automated operation in the field of pipe or moulded parts production with the help of press technology has been developed for industrial areas such as ceramic, foundry and metallurgical industries, construction or also metal powder or plastic processing. The efficiency of the mould filling process is solved by the synchronous distribution of two granular materials. This process is fully controllable with possible extension applications to modify or evaluate the mechanical-physical properties of the materials when deployed in an automated or autonomous production process in the future. The mould distribution and filling methods have been developed, validated and tested based on long-term research in the field of mechanical-physical properties at the Bulk Solids Centre (BSC) using modern measuring equipment such as Schulze RST, Brookfield PFT, Freeman FT4 Powder Rheometer, Retsch Camsizer, LaVision PIV, EDEM and Rocky DEM. Shape optimization of controllable rotating elements for efficient non-contact (non-mixing) synchronized mass distribution process with the same or different mechanical and physical properties was solved using DEM. Besides the quality of the material distribution, the whole process was also influenced by technological parameters such as filling speed and geometrical properties of the moulds. The research of the device was supported by the PRE SEED Fund II project of the VŠB - Technical University of Ostrava funded by GAMA programme of the Technology Agency of the Czech Republic.

This innovative equipment meets all the requirements and demands for modern technology in the field of mould filling and other production processes, not only for multi-shell tubes. The equipment is fully capable of working in an automatic process and therefore able to work with specific settings for certain granular masses. This technology is designed for a wide range of bulk materials with different mechanical, granulometric, morphological and chemical properties. The aim is to replace part of the effective expensive component of the bulk material with a more affordable material within the production of a ceramic tubes. These bulk materials are conveyed to the mould separately by a single filling head which is partly inserted into the mould. The designed and field-proven technology has been patented by the Industrial Property Office of the Czech Republic and is registered under the name “Method of filling a mould when manufacturing multi-shell tubes and the apparatus for this” with a registration number 308289.

Effect of particle size distribution on frictional head loss in pipe flow of sand-water slurry

Václav Matoušek, Zdeněk Chára, Jiří Konfršt, Jakub Novotný

Czech Academy of Sciences, Institute of Hydrodynamics, Prague, Czech Republic

Grading of solids transported with carrying liquid (usually water) in the form of settling slurry through a pipeline has a profound effect on the behavior of slurry flow and particularly on the frictional head loss in the pipeline. Mutual interactions of particles of different sizes cause that friction mechanisms alter, and the overall effect is usually benign – the frictional head loss is less in the broadly-graded slurry than in the narrow-graded slurry of the same median size of particle (d_{50}) at the same flow velocity and the same concentration of transported solids. Although this trend is well known, mechanisms responsible for friction altering due to the presence of different solids fractions in the flowing slurry are not sufficiently understood. This limits an ability of existing predictive models to successfully estimate the frictional head loss and the energy consumption of pipeline transport of slurry. Although most industrial slurries transported hydraulically in pipelines tend to be broadly graded, until recently the information quantifying the effect of the particle size distribution on the frictional losses in pipes has remained confined to few laboratory experiments and was exploited in a very small number of models taking the solids grading into account.

In 2016-2021, a set of extensive experimental campaigns has been carried out in the Hydraulic Laboratory of GIW Industries Inc. in Grovetown, USA to test the effect of the particle size distribution on the pipeline friction loss in pipes of different sizes (from 103 mm to 489 mm) and for solids of different densities (from sand to iron ore). The main objective of the experiments was to supply experimental data for calibration and validation of the fourcomponent model (4CM) predicting the frictional head loss for settling slurries composed of components (fractions) from fine powders to coarse fractions of particles larger than 1.5 per cent of the pipe diameter. Careful measurements included information about integral flow parameters (flow rates of slurry and solids, pressure drop) and information about the particle size distribution instrumental for 4CM refinements. However, the measurements did not include information about the internal structure of the flow. That information is essential for identification of mechanisms through which different solids components affect flow friction.

Therefore, additional experiments have been carried out with pipe flow of multi-component slurries in the laboratory loop of Institute of Hydrodynamics of Czech Academy of Sciences. These included information on the distribution of solids in a pipe cross section and on the behavior of solids at and near the pipe wall at the bottom of the pipe. Bimodal-, threecomponent- and four-component slurries were tested and mutually compared to identity the role of individual components on slurry flow and pipe friction. The paper presents an analysis of the experimental results, identifies and quantifies a role of each individual component on the overall frictional head loss. Furthermore, it compares the observed losses with those by a predictive model for broadly-graded solids.

Exploring “Big Data” on the effect of different materials on pressure drops in pneumatic conveying, identifying bend and straight pipe losses and bend equivalent lengths

Michael Bradley, Tong Deng

The Wolfson Centre for Bulk Solids Handling Technology, University of Greenwich

The archives of The Wolfson Centre contain many years of data records on the pneumatic conveying properties of a huge range of different materials. These range across foodstuffs, fuels, minerals, chemicals and many more. This paper presents the results of a comparative review of a broad selection from amongst this data, where both the bend and straight pipe pressure drops have been determined, all measured on the same test rig and pipeline over the last 15 years. This is the first time on public record that such a wide data set of pneumatic conveying characteristics has been compared.

The results show a good representation of the range across which the pressure drop functions vary between materials. Certain interesting points emerge. First and perhaps most significantly, it is not uncommon for materials that are for all other purposes considered to be “the same”, i.e. the same name and made to the same agreed specification, even by the same company but at different sites, can display very significant differences in pressure drop, in spite of there being no measurable difference in particle properties or chemistry. Equally importantly, different methods of grouping the materials have been tested (for example by particle size, density, field of application or chemistry) and the lack of correlation of the pressure drops to any of these groups or variables is remarkable.

Equally, the relationship between bend and straight pipe pressure losses, expressed for example as “bend equivalent length”, is also strikingly variable, and absent of correlation against material type, particle characteristics or flow conditions.

This lack of any meaningful correlation of conveying properties against particle properties is counter-intuitive and at first frustrating. However it explains why many years of pneumatic conveying research and modelling amongst many institutions and experts has failed to produce any agreement on predicting pressure drop in pneumatic conveyors other than by undertaking trials. It also demonstrates the ongoing justification for such conveying trials with materials to be handled in new systems (or new materials to be handled in old systems) and shows that any hope of modelling pneumatic conveying behaviour based on particle properties that are commonly measured, is almost certainly forlorn.

Study on characteristics of flow rate regulation in the dense-phase pneumatic conveying of pulverized coal

Haifeng Lu*, Hu Ruan, Xiaolei Guo, Haifeng Liu

Shanghai Engineering Research Center of Coal Gasification, East China University of Science and Technology, China

Dense phase pneumatic conveying is one of the key technologies in the entrained-flow pulverized coal gasification process, where conveying pressure drop, regulation valve and nozzle all play important roles in regulating the flow rate of pulverized coal. In this paper, experiments were carried out in the dense-phase pneumatic conveying platform in the ECUST (East China University of Science and Technology) laboratory. The effects of conveying pressure drop, regulation valve and nozzle on system pressure distribution and solid flow rate regulation were investigated, to investigate the regulation mechanism on pulverized coal flow. The flow pattern of gas-solid two-phase inside the horizontal pipe were further studied and its evolution law were revealed based on the Electrical Capacitance Tomography (ECT) system. The study shows that the regulation valve and the nozzle are most important resistance components of the conveying system, which jointly bear more than 90% of the conveying pressure drop. The effective opening of the regulation valve is about 13%-40% within the experimental range, where the pulverized coal flow rate increases nearly linearly with the valve opening. The exit velocity of the nozzle can be up to hundreds of meters per second, which effectively realizes the gas-solid dispersion at the end of the conveying pipeline. Finally, a semi-theoretical and semi-empirical model for pulverized coal flow rate prediction was developed and related to characteristic pressure drop of the conveying pipeline, the regulation valve, or the nozzle, respectively. On this basis, the characteristics of flow rate regulation in the dense-phase pneumatic conveying of pulverized coal were revealed and, stable and controllable conveying was realized.

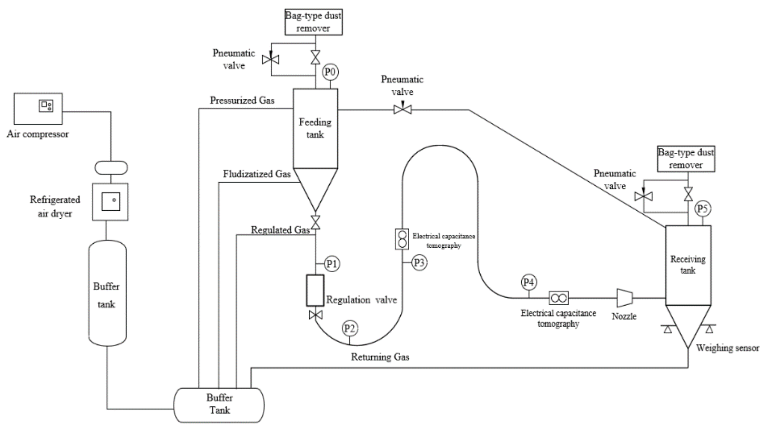

Fig.1. Schematic diagram of dense phase pneumatic conveying system.

Determining and comparing breakage matrices to predict particle attrition in pneumatic conveyors

Michael Bradley, Tong Deng

The Wolfson Centre for Bulk Solids Handling Technology, University of Greenwich

Breakage Matrices are a very useful means of representing the attrition properties of particles in impact processes, allowing data from one context (for example a test system) to be used to predict particle breakage in another context (eg a new plant system), provided that certain principles of similarity are maintained. However, determining breakage matrices in a rigorous experimental programme can be very challenging practically.

This paper introduces a novel means of short-cutting much of the experimental work needed to arrive at breakage matrices that can be used for practical prediction of particle attrition in a plant conveying system, based on a much more limited programme of pilot plant work and empirically-derived trends for the relationships between the elements in the matrices, which enables a breakage matrix to be fully characterised using only two numerical values. This is based on experimental measurements across a substantial number of materials of different types.

Pneumatic conveying of solids: scale-up and design of long line systems

Rizk Farid

R & D Solids Handling BASF Formerly, R & D Solids Handling BASF Formerly, Ludwigshafen, Germany

The publication of studies concerning failures in the design of pneumatic conveying systems is alarming. These studies have triggered the need for new methods for solving this problem. Although pneumatic conveying of solids in pipes is a wide spread technology, failures occur in their design. The investigation of these studies has been carried out for systems operating in Canada, USA, Europe and Asia. Although a large amount of information and documentations pertaining solid characterisation are published, failures occur in the design of new systems.

Due to the complex phenomena between solid particles and the transport media, an attempt was made based on the similarities of flow in both pilot- and commercial- plants in conjunction with the standard modified evaluation of the pressure drop. The expansion and interaction of the two-phase gas /solids when scaling-up were taken into consideration. Most important is the application of dimensionless numbers such as the mass loading, the FroudeNumber and the geometric ratio pipe length to pipe diameter. The adaptation of the pipe diameter and pipe material is in both systems vital.

A systematic evaluation and comparison of test results are encouraging and represent the basis for design, taking flow conditions and their similarities into account. A modification step is introduced, where deficits in the design are visualised and eliminated. This modification step is based on tests in a large scale system.

WEDNESDAY, 6 JULY 2022
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MULTIPHASE FLOW AND FLUIDIZATION

Confined-fluidization as a way of improving CO_2 capture by adsorption on solid sorbents

R. Girimonte, F. Testa and M. Turano

Department of Computer Engineering, Modeling, Electronics and Systems (DIMES), University of Calabria, I 87030 Arcavacata di Rende (Cosenza), Italy

Confined-Fluidized Beds (also called Packed-Fluidized Beds) constitute a non-conventional arrangement to carry out fluidization of relatively fine particles in the interstitial voids of a packing of coarse spheres. The presence of the these as a packed bed prevents the onset of the bubbling regime past the incipient fluidization point of fine solids. By this method, even solids that belong to Geldart's group B become capable of reacting to an increase of the gas velocity over u_{mf} by homogeneously expanding up to unusually high values of voidage.

Systems of this kind can be of interest for applications in which bubbly flow plays a detrimental role on process efficiency, such as adsorption of CO_2 from flue gas streams.

To check these potentialities, the paper presents the results of an investigation regarding CO_2 adsorption on a fluidized bed of pellets of several types of sorbent (zeolite, aminofunctionalized silica, activated carbon, etc). A comparison is made between the performance of a confined fluidized bed and that of a conventional system at the same conditions of inlet gas velocity and CO_2 concentration. The paper discusses how the effect of the confined fluidization velocity allows optimizing the overall performance of the adsorber: the operating velocity can be set at a value at which the thermal effects connected to the operation are kept under control.

Effectiveness of CO_2 adsorption is assessed in terms of moles of CO_2 adsorbed per unit mass of sorbent, breakthrough time and fraction of bed utilized at the breakpoint. The results obtained confirm that the confinement of the sorbent allows exploiting fluidization technology in CO_2 capture.

Keywords: Confined-fluidized bed; Packed-fluidized bed; CO_2 capture; Adsorption; zeolite; amino-functionalized sorbent; Activated carbon.

Hydrodynamics of pulse-assisted fluidization of cohesive powder

Ebrahim H. Al-Ghurabi, Mourad M. Boumaza, Mohammad Asif

Dept. of Chemical Engineering, King Saud University, Riyadh, Saudi Arabia

Fine and ultrafine powders find widespread application in the process industries owing to their high specific surface area that helps to enhance surface based catalytic and non-catalytic rate processes, thereby ensuring high process efficiency. However, the large scale processing and dispersion of such powders is often challenging due to their cohesive behavior as a result of strong interparticle forces. Classified as Group C powders, their fluidization is marked by severe bed homogeneities, which is evident from the development of rat-holes and channels through which the gas phase tends to bypass the solid phase, resulting in poor interphase mixing. To improve fluidization of such powders, the commonly used strategy is to input extra energy to the bed for counteracting the effect of interparticle forces. Often referred to as assisted fluidization techniques, such strategies, for example, involve mechanical vibration of the bed, utilization of acoustic vibrations, and modifying the force field with the help of electric and magnetic fields. The viability of any assisted fluidization technique nonetheless depends upon two main factors, namely cost-effectiveness and ease of implementation. To this end, the assisted fluidization technique of flow pulsations that consist of pulsating the inlet flow to the fluidized bed at regular time intervals stands out on both counts, especially because no extra energy input is required. The regular flow interruptions causes frequent collapse of the bed, introducing disturbances that help to eliminate the bed non-homogeneities and mitigate the effect of interparticle forces.

In the present study, we have investigated the effectiveness of assisted fluidization technique of pulsed flow. A bed of activated carbon with strong cohesive behavior was subjected to square-wave flow pulsations of different frequencies as well as magnitudes using an electronic mass flow controller operated using a data acquisition system (DAQ). The disturbances introduced in the bed due to frequent flow interruptions were carefully monitored at a sampling frequency of 100-Hz using sensitive pressure transducers. The experimental data were processed to obtain characteristic hydrodynamic parameters describing the fluidization behavior in the presence of flow pulsations. Another set of experiments were also carried out under conventional fluidization conditions for comparison to delineate the effect of flow pulsations on the bed hydrodynamics. In addition, the data were analyzed in the frequency domain to obtain an insight into occurrences of different time events taking place during the pulsed flow fluidization.

Fluidization and flow behavior of powder coatings when approaching their glass transition temperature

Helena Weingrill[1], Christina Reichart[1], Timothy Aschl[1], Denis Schuetz[2]

[1]Department of Rheometry, Anton Paar GmbH, Graz, Austria

[2]R & D Rheometry, Anton Paar GmbH, Graz, Austria

As powder coatings contain only small amounts of volatiles or are entirely volatile-free, they present a preeminent alternative to conventional paints and coatings reducing their impact on the environment [1]. Thus, their application is part of the current strive towards greener engineering. To guarantee powder coatings' flawless processing, flow additives are typically mixed into the base powder coating to adapt their process-relevant properties such as their air-retention capacity and fluidizability. However, the powder behavior of the resulting formulations is expected to be highly temperature-dependent, due to its polymeric nature. Processing involves a curing reaction or melting of the contained polymer, while the flow aid itself remains as a particulate elevating the viscosity of the melt and significantly altering the achieved surface. This results in a multifaceted issue which needs to be addressed in detail.

Therefore, this study focuses on the investigation at elevated temperatures of a polyester-based powder coating containing different amounts of pyrogenic alumina as flow additive up to 0.3 wt%. The formulations' fluidization behavior as well as their flow behavior and fluidized bed viscosity are examined at temperatures up to 50°C, thus approaching the polyester's glass transition temperature where a significant change in the polymer's mechanical behavior is expected to occur. Furthermore, the impact of the powder's history in terms of precedingly applied loads to imitate storage and transport is assessed likewise. Finally, the viscosity of the powder coating in the liquid state is examined.

Interestingly, an impact from temperature on the powder's fluidization behavior only occurs for formulations containing flow additive suggesting certain interactions between the alumina and polyester particles. As opposed to that, the air-retention capacity - as crucial property for the coating process - proves to be highly temperature-dependent for all formulations including the pure powder coating without any additional flow additives. Furthermore, a decrease in the temperature-dependence with increasing flow additive concentration is detected for the powders' air-retention capacity. As expected, the powder's flow properties change with increasing flow additive content. Moreover, the temperature dependence of the powder's flow properties is decreased by the addition of the alumina. Similar trends are detected for the fluidized bed viscosity. This clearly demonstrates that this coating technology is a highly complex process where many parameters have to be considered to achieve an impeccable coating.

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Hydrodynamics of a novel directly irradiated fluidized bed autothermal reactor for thermochemical energy storage

Stefano Padula[1], Maurizio Troiano[1,2], Claudio Tregambi[2,3], Roberto Solimene[2*], Piero Salatino[1]

[1]Dipartimento di Ingegneria Chimica dei Materiali e della Produzione Industriale, Università degli Studi di Napoli Federico II, Napoli, Italy

[2]Istituto di Scienze e Tecnologie per l'Energia e la Mobilità Sostenibili (STEMS), Consiglio Nazionale delle Ricerche, Napoli, Italy

[3]Dipartimento di Ingegneria, Università degli Studi del Sannio, Benevento, Italy

***Corresponding author: Roberto Solimene, roberto.solimene@cnr.it**

Keywords: solar particle receivers; concentrated solar power; interconnected fluidized beds

Energy transition is today universally acknowledged as a pressing priority for a fully carbonfree energy sector. Concentrated Solar Thermal (CST) energy coupled with Thermal Energy Storage (TES) systems is an appealing alternative to fossil sources for power production. CST technologies consist of a set of sun-tracking mirrors that concentrate solar radiation onto a receiver, where it is absorbed by an energy carrier. The energy carrier can be then stored and used to drive a power cycle. Granular solids offer several advantages as energy carriers and open the path to Thermochemical Energy Storage (TCES), which consists in exploiting solar energy to sustain a reversible and endothermic chemical reaction. The energy is stored in the reaction products, allowing larger densities and longer times of storage. The design of gas-solid reactors is crucial for the success of this technology.

A novel Directly Irradiated Fluidized Bed Autothermal Reactor (DIFBAR) is investigated. The key feature of the reactor is the autothermal operation: the sensible heat of the solid flowing out of the reaction zone is recovered to preheat the reactants, saving the energy needed to reach the high temperatures of TCES processes. This is obtained by means of a solid-solid heat exchanger composed of two vertical coaxial tubes connected at the bottom of a conical vessel, that serves as a receiver. The bed material is fed to the receiver through the inner tube (riser) by a fluidizing gas stream. There, the particles are exposed to a high flux of solar radiation and undergo a chemical reaction. Then they separate from the gas stream and fall into the outer tube (annulus). As particles descend through the annulus as a moving bed, they transfer their sensible heat to the counter-current gas-solid suspension in the riser. A lab-scale prototype was designed and built up, in which the material is taken from and re-injected in a same reservoir, in a closed loop circulating system.

In this study the hydrodynamics of DIFBAR is investigated with a Geldart B sand under various conditions. Eight pressure transducers are used to characterize the pressure loop and to control the sand level in the annulus. Solids circulation rates are determined through an optical access and time sampling tests. Moreover, gas flow patterns are studied by gas tracing technique.

The role of temperature and moisture on polymer materials for additive manufacturing, and their implications for the process

Denis Schütz[1], Helena Weingrill[1]

[1]R&D Rheology (Anton Paar Gmbh, Graz Austria)

Polymeric materials in additive manufacturing add a unique difficulty in characterization to a field that is used to deal with metal powders. Due to the molecular structure of these polymer powders, moisture and temperature change their behavior to a larger degree than is to be expected with the more common metal feedstock. Like in metals manufacturers have addressed this by bringing the temperature of the feedstock chambers to elevated levels, therefore reducing or eliminating the moisture effects. However, unlike metals, polymers show a substantial divergence from their room temperature This in turn creates the problem of reliably measuring the feedstock at these elevated temperatures to give an accurate picture of their properties during use. And in addition, the problem of moisture influence during storage prevails. In this work we will show measurements of polymeric feedstock under actual processing parameters and delve into the problems arising during drying and storage. It will consist of measurements with temperature and moisture-controlled ring shear cells as well as data from our novel temperature-controlled stirrer-based cell with fluidized methods.

Classification of fine gas born particles in superposed electric and acoustic fields

Krischan Sandmann[1], Udo Fritsching[1,2]

[1]Leibniz-Institut für Werkstofforientierte Technologien - IWT, Badgasteiner Straße 3, 28359 Bremen, Germany

[2]University of Bremen, Faculty of Production Engineering, Bibliothekstraße 1, 28359 Bremen, Germany

The growing demand for fine particle systems with tight specifications requires new approaches to solutions from mechanical process engineering. In particular, there are barely any technical scaled classification processes for finest particles (dp<10 µm). In the contribution, a modern approach for a separation process is presented, which acts on gas-borne particles with the superposition of acoustic and electric field and thus allows a particle size and materialdependent separation.

The following figı 1 sketches the process diagram

fraction	rel. particle size	chargeability	scheme
1	fine (f)	bad	
2	coarse (c)	bad	
3	fine (f)	medium	
4	coarse (c)	medium	
5	fine (f)	good	
6	coarse (c)	good	

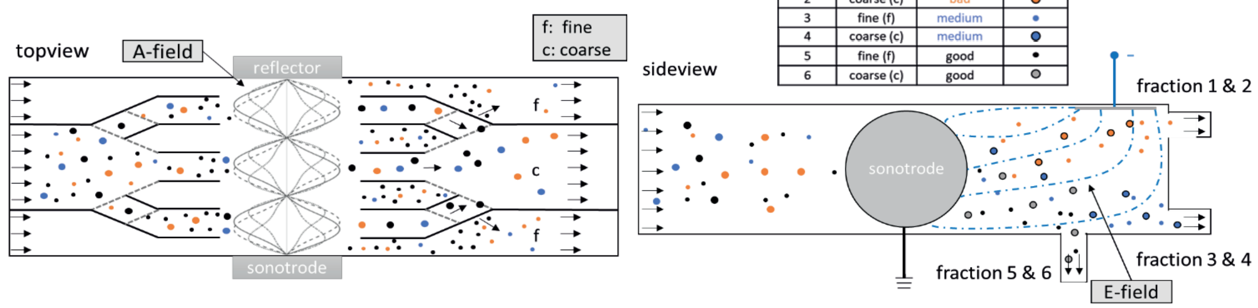

Figure 1: Process scheme of electrical assisted ultrasonic classification of fine particles

Several approaches were taken to describe and investigate the process presented. Mathematical models were set up and used as a basis for mapping the particle movement. Furthermore, numerical simulations of the flow conditions in the intensive standing ultrasonic field were carried out, which, in conjunction with experimental investigations, enable a more precise process analysis. The mathematical analysis of the process shows a high separation accuracy for the fractionation into coarse and fine material [1].

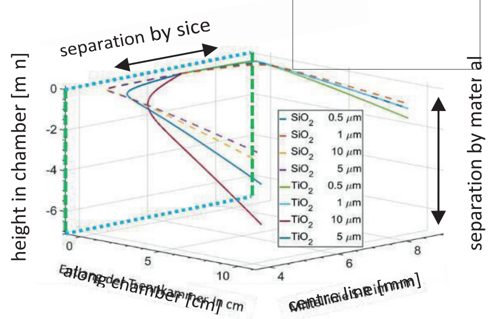

Figure 2: Mathematica modellinį of particle trajectories in process ce.ˡ

On the other hand, the simulations of the gas phase show pronounced non-linear behaviour under the intensive effects of the acoustic field, which can lead to backmixing. The current focus is on finding suitable process windows and minimising side effects for classification of particles with multivariate properties. This project is founded within SPP 2045 MehrDimPart by Deutsche Forschungsgemeinschaft (DFG)

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Investigation of the wet contact behavior of particles in CFD-DEM simulations of a rotor granulator

Philipp Grohn[1], Tobias Oesau[2], Stefan Heinrich[2], Sergiy Antonyuk[1]

[1]Institute of Particle Process Engineering, Technische Universität Kaiserslautern, Kaiserslautern, Germany

[2]Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology, Hamburg, Germany

Solids in particle form (powders, granulates or agglomerates) are widely used in the food, chemical and pharmaceutical industries, where they are further processed in various production steps, e.g. drying and coating in the fluidized bed [1]. To control and optimize these processes, it is essential to know and describe the particle kinematics and dynamics. An essential tool to obtain these data are numerical simulations of the multiphase flow with the computational fluid dynamics (CFD) coupled with the discrete element method (DEM). With CFD, the flow field of the gas in the process apparatus can be determined by the Eulerian-Lagrangian approach, which treats the fluid phase as a continuum. In DEM, the interactions are calculated for each single particle based on models describing physical properties of particles and their mechanical behavior stressing [2].

In this work, we studied first the wet particle contact by impact tests using a setup consisting of two high-speed cameras to record the pellet-wall collisions [3]. The influence of the impact velocity and liquid bridge volume on the length of the liquid bridge were determined by a MATLAB script using the Image Processing Toolbox. A model for a velocity-dependent maximum liquid bridge length was developed and used in an implemented liquid bridge contact model in DEM. The additional dissipative forces were modeled according to the fluid bridge model of Tsuazawa et al. and the viscous forces according to Adams and Perchard and Popov [4].

The simulation results were validated with experimental data obtained by magnetic-particle-tracking measurements of the particle movement in a rotor granulator. With the help of the simulations, the particle movement in this rotor granulator was analyzed in detail and used to determine the boundary conditions under which a successful fluidization in the rotor granulator can be realized.

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An experimental investigation on channelized granular flows

Luca Sarno[1], Maria Nicolina Papa[2], Paolo Villani[2]

[1]Institute of Fluid Dynamics, Dept. of Mechanical Engineering, TU Darmstadt, Darmstadt, Germany

[2] Department of Civil Engineering, University of Salerno, Salerno, Italy

Granular media are ubiquitously involved in many geophysical flows (like avalanches and debris flows) and in several industrial applications. Yet, the dynamics of granular materials is far from being completely understood and several aspects, such as the non-local rheological behaviour, the boundary effects, the grain segregation and the rheological hysteresis still represent extremely challenging open problems that can be hardly described by current mathematical models. Therefore, laboratory-scale experiments are irreplaceable tools for increasing the physical understanding of these still unclear aspects that cannot be easily isolated in field-scale investigations and are not yet properly described mathematically. Furthermore laboratory measurements are essential for the validation of models.

With the purpose of systematically investigating the steady state and the effects of the boundary conditions in the dense-collisional regime, here we report an experimental study on dry granular flows in a narrow laboratory flume, made of Plexiglas and having a rectangular cross-section of width 8cm. The investigated granular medium consists of small spheroidal beads ($d\approx3$mm), made of acetal resin (POM) and having grain density of 1410 kg/m^3. Different flume slopes were studied, together with various basal roughnesses, obtained by using different bed linings (sandpaper, smooth Bakelite, glued POM grains) that allowed the onset of different kinematic boundary conditions. Moreover, in order to study different flow regimes, various flow rates were imposed by modifying the opening of an upstream gate, separating the channel from an upper reservoir and located near the channel bed. The flume was equipped with a high-speed digital camera (AOS Technologies) and a no-flicker highbrightness LED lamp (Photo-Sonics), so that non-invasive optical measurements of both the velocity and the solid volume fraction (volume of solids ÷ total volume) could be obtained at the sidewall. For the velocity measurement we employed a multi-pass granular particle image velocimetry (g-PIV) [Sarno et al., *Adv. Powder Tech.*, 2018], while a stochastic-optical method (SOM) [Sarno et al., *Granul. Matter*, 2016] was employed for the volume fraction measurements. The advantage of the proposed integrated approach is to use the same digital pictures, obtained from the high-speed camera, to concurrently estimate both the velocity field and the more challenging solid volume fraction that is strongly coupled with the granular dynamics. The innovative SOM method is based on the direct measurement of a quantity, named *two-dimensional volume fraction*, which is easily measurable under controlled illumination conditions and was found to be highly correlated with the near-wall volume fraction thanks to a stochastic transfer function, previously determined from extensive Monte Carlo simulations of random distributions of perfect spheres.

The combined measurements of velocity and volume fraction allowed a better understanding of the flow dynamics and, specifically, revealed the coexistence of different flow regimes in the same cross-section. Different momentum exchange mechanisms of frictional and collisional-type were found to cause the rheological stratification of the granular flow.

Neural network-based filtered drag model for cohesive gas-particle flows

Josef Tausendschön[1], Stefan Radl[2], Sankaran Sundaresan[3]

[1]Institute of Process and Particle Engineering, Graz University of Technology, Graz, Austria

[2] Institute of Process and Particle Engineering, Graz University of Technology, Graz, Austria [3] Dept. of Chemical and Biological Engineering, Princeton University, Princeton, USA

Simulations of industrial-scale gas-particle flows based on the filtered Two-Fluid model (fTFM) approach, and therefore with coarse grids, depend critically on constitutive models that account for the effects of inhomogeneous structures at the subgrid level [1]. Around this issue, an artificial neural network-based drag correction model was developed by Jiang et al. [2,3] for non-cohesive gas-particle systems.

The complexity of accounting for inhomogeneous structures increases when considering cohesive gas-particle flows [4]. Therefore, we aim to analyze the influence of cohesion on the drag force closure and integrate it into a machine learning-based drag correction concept. Prior studies [5] identified the sub-grid drift velocity as the crucial quantity for modeling the filtered drag coefficient and the drag model as a whole. Unfortunately, the drift velocity is unavailable in filtered simulations. To correctly reproduce mesoscale structures, and since the drift velocity is also computable, we start with detailed CFD-DEM (Computational Fluid Dynamics-Discrete Element Method) simulations and filter them with different filter sizes to emulate an fTFM simulation.

Based on these simulations, we create a dataset by varying the cohesion level from cohesionless to highly cohesive and changing the size of the systems using coarse-graining. We then subject the markers available in a basic fTFM simulation to systematic analysis considering their correlation with the target value, namely the drift velocity. With the identified markers we then create, train, and test neural network-based drag correction models. Finally, we demonstrate the accuracy of the developed models for drag correction for a wide range of cohesion levels and system sizes.

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Terminal velocity and drag coefficient for accelerating spherical particles

Haim Kalman[1,2], Dmitry Portnikov[1] and Erez Matana[1]

[1] The Laboratory for Conveying and Handling of Particulate Solids, Department of Mechanical Engineering, Ben-Gurion University of the Negev, Beer Sheva 84105, Israel.

[2] Aaron Fish Chair in Mechanical Engineering – Fracture Mechanics, Israel.

Empirical correlations and experimental works relating the drag coefficient (C_D) of spheres to the Reynolds number (Re) and Re to the Archimedes number (Ar) were reviewed with a focus on the correlations applicable to the entire Re range. In addition, experiments with various spherical particles and fluids for the entire range of Re were conducted using high-speed video and added to the literature data. One of the correlations from the literature for Re–Ar and a modified correlation for C_D–Re were found to best fit the experimental results. The analysis also established new correlations for Re–Ha (a non-dimensional number for velocity not including particle size) and C_D–Ar. The latter is easier to use than the common C_D–Re curve. The research was then increased to test accelerating particles and testing the effects of the added mass and history term. It was found that the drag coefficient for accelerating particles is much larger than for that calculated by the steady-state drag using the instaneous velocity.

Investigation of endogenous bubble-induced segregation of a single biomass particle in fluidized bed reactors

Stefano Iannello[1], Massimiliano Materazzi[1]

[1]Department of Chemical Engineering, University College London, London WC1E 7JE, UK

Fluidised bed reactors are among the most promising technologies for the thermochemical treatment of solid feedstocks for sustainable applications, due to their enhanced heat and mass transfer, and operating flexibility. Nevertheless, there are still unsolved challenges when operating with highly volatile solid feedstocks, such as biomass or waste. Because of their relatively low density, these materials experience axial segregation, tending to segregate along the bed height causing complications in the hydrodynamics of the bed. Moreover, volatiles released within the bed evolve in form of endogenous bubbles, which further enhance segregation of the feedstock. As a consequence, both solid and gas phases do not take advantage of the bed-to-fuel transfer phenomena, which are essential for high product yields and quality. All these aspects are essential part of the design of industrial fluidized bed units and relevant to all thermochemical conversions, since the evolution of volatiles is the first and common stage in pyrolysis, gasification and combustion operations. The aim of this work is to provide a better understanding of the devolatilization behaviour and bed-feedstock interaction in fluidized bed reactors. This is done by investigating reacting wood biomass particles in a lab-scale fluidized bed reactor at high temperatures and different fluidization regimes relevant to industrial operations. A non-intrusive X-ray imaging technique, coupled with gas analysis measurements, has been used to investigate the thermal decomposition behaviour of a single particle after under-bed feeding. The experiments were conducted under either inert (pyrolysis) or semi-oxidizing (gasification/combustion) conditions. A comprehensive assessment at minimum fluidization condition provided deeper insight about the devolatilization behaviour within the bed, which is found to be independent of the oxidizing nature of the fluidization medium. Size and void fraction distribution of endogenous bubbles were measured via X-ray imaging. Results show that a fully developed endogenous bubble carries with it a volume of volatiles considerably larger that the volume predicted by a pseudo-first order rate law, which is usually used to describe the devolatilization behaviour of solid feedstocks. Gained knowledge provided by direct visualization from the collected X-ray images allows an estimation of the lift effect acting on the reacting particle, which can then be used to develop a one-dimensional model to validate experimental results. The model accurately predicts the behaviour of biomass particles at minimum fluidization, while showed inconsistencies in bubbling regime. This finding was attributed to endogenousfluidizing bubbles coalescence, which appeared to take place in an unpredictable fashion. Preliminary results obtained from this study highlighted the importance of developing systematic methodologies for the investigation of single particle devolatilization which, at present, appears to be the most effective approach to gain deeper insight on the interaction between feedstock and fluidized bed during thermochemical conversions.

Solids mixing/segregation in high temperature dense gas-solid fluidized beds by capacitance and pressure measurements

Laura Molignano[1], Maurizio Troiano[1], Roberto Solimene[2*], Sina Tebianian[3], Piero Salatino[1], Jean-François Joly[3]

[1]Dipartimento di Ingegneria Chimica, dei Materiali e della Produzione Industriale, Università degli Studi di Napoli Federico II, Napoli, Italy

[2]Istituto di Scienze e Tecnologie per l'Energia e la Mobilità Sostenibili, Consiglio Nazionale delle Ricerche, Napoli, Italy

[3]Direction Conception Modélisation Procédés, IFP Energies Nouvelles, Solaize, France

*Corresponding : roberto.solimene@cnr.it

Keywords: Fluidization, Solid mixing/segregation, Self/mutual dispersion

The performance of thermochemical processes achieved in gas-solid fluidized beds (FB) strongly depends on the level of mixing/segregation of solid fuel and bed material. In the vertical direction, effective solids mixing is typically beneficial to ensure sufficient contact time between fuel and fluidizing gas. On the other hand, for some applications, axial segregation is useful for separation of two solids with different physical properties. Efficient lateral fuel mixing avoids undesired transversal temperature profiles and, in turn, pollutant emissions and helps to minimize fuel feeding ports over the cross-section of industrial units. Conversely, in two interconnected FBs, where fuel losses in the second reactor are undesired, lateral mixing is to be discouraged. Thus, the proper extent of solid mixing depends on the specific process and solid fuel type.

Despite previous studies on solids mixing, very few works report data obtained from pilot-tolarge scale units at typical industrial conditions. Moreover, the variability in physical properties of different solid fuels, especially for biomass, is another aspect, which directly influences the mixing behavior. Therefore, further comprehension of solid mixing and segregation phenomenology, studied under operating conditions significant to industrial processes, is required for *ad hoc* design and optimization of each process.

In the present study, stimulus-response tracing experiments are performed in non-reactive bubbling fluidization conditions. As for the diagnostics, custom-made capacitance probes for high temperature environments are adopted in addition to pressure transducers placed along bed height. A distinction is made between self-dispersion experiments, where two solids are chosen with same particle density and diameter, and mutual-dispersion ones, where the solids are chosen on the basis of the inert bed and the fuel particles properties. For these tests, a calibration is needed to investigate dense phase voidage trend with volumetric composition of the binary mixture. Results about experiments at 600°C are presented for a medium-size laboratory scale unit at relevant operating conditions. Tracer feeding and mixing phenomena in the reactor are modeled in detail to estimate solids dispersion. To conclude, results are critically compared with the most notable ones from the scientific literature, especially those obtained in higher dimension reactor scales.

Efficiency of stand-alone filters: effects of filter aperture and meshing design

Paula A. Gago*[1], Raphael Blumenfeld[1,2], Sheik Rahman[3], Stephen Tyson[4], Peter King[1]

[1]Department of Earth Science and Engineering, Imperial College London;

[2]Cavendish Laboratory Cambridge, UK;

[3]School of Petroleum Engineering, University of New South Wales, Australia;

[4]Universiti Teknologi Brunei, Jalan Tungku Link, Gadong BE1410, Brunei Darussalam

* pgago@ic.ac.uk

Hydrocarbon extraction from unconsolidated sandstone reservoirs commonly produces sand, causing erosion of equipment, plugging, and flow reduction. These not only lead to losses of millions of dollars every year but also pose direct and indirect environmental risks. Standalone screens are normally used to reduce sand production, but they give rise to pressure loss along the “filter cake”, which the screens generate. The main approach in the industry involves a quest for an optimal design, which is unique to each specific well. This is a major challenge because it requires balancing the screening of particles against the permeability reduction owing to the build-up of the filter cake. While there have been significant advances in modelling the unconventional behaviour of granular materials in recent years, many open questions remain. In particular, the formation of the filter cake requires modelling of its jamming dynamics, the statistics and properties of its structure, its permeability, and how the stress is distributed in it, given that the incoming slurry consists of particles with broad size and shape distributions. We use discrete element method (DEM) numerical simulations to study at the grain-scale the dynamics of a slurry flowing downward under gravity through a pipe capped by a filter at the bottom. We measure the particle filtration rate through a screen as a filter cake builds up against it. We investigate several filter apertures and mesh weaving designs. We show that at least 80% of the total solid production occurs before the first layer of filter cake particles has formed, in agreement with previously reported results. Our findings provide evidence that the filtering of particles is in fact mainly done by the filter cake rather than the screen. We propose that a central line of investigation should be into the design of a screen that generates a predetermined optimal structure of the filter cake, which in turn, would optimise the flow rate against the volume of solid production.

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COMPUTATIONAL MODELS

Simulation of hierarchical structure formation during spray drying using CFD-DEM coupling

Silas Wolf, Nane Kühn, Carsten Schilde

Institute for Particle Technology, Technische Universität Braunschweig, Braunschweig, Germany

Nanoparticulate functional structures are becoming increasingly important, for example in pharmacy as carrier systems for poorly soluble drugs or in the form of porous catalysts. The properties of the subsequent products depend to a large extent on the microstructure of the particle systems. One possibility for producing defined structured aggregate structures is spray drying. By varying the process and formulation parameters, the structure formation can be specifically controlled during the process [1-3]. However, the exact processes that control the formation of the particle structure during the drying process have not yet been sufficiently explored. One possibility to elucidate the mechanisms of aggregate formation is provided by simulations. These allow process-structure-property relationships to be established without any experimental effort as well as the optimization of the production of such aggregates. One way to simulate the structure formation during the spray drying process is to couple computational fluid dynamics (CFD) with the discrete element method (DEM). This allows to consider influences of particle-particle as well as fluid-particle interactions. For the CFD simulation of multiple fluid phases, the volume-of-fluid method is used, which has been extended to include a source term to represent a constant evaporation rate along with coupling to DEM. This allows the processes involved in drying a single suspension droplet to be studied. By taking into account a capillary force, the effect of surface tension on the individual particles can be represented [4], by which the particles finally aggregate. The additionally acting collision and friction forces, cohesive forces, long-range interactions according to the DLVO theory and the Brownian motion of the particles can then additionally influence the structure formation. In the context of this study, these models will be used to investigate the effect of different process parameters, such as drying rate and temperature as well as suspension properties, e.g. solid content, particle size distribution, surface charges and particle material, on the structure formation. The main focus will lie on hierarchical structuring, where, for example, a gradient of particle size or pore size as a function of radius is present. The results will then be compared with findings from experimental investigations in order to evaluate the applicability of the simulation models used.

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CFD-DEM simulations of strongly polydisperse particulate solids in the cyclonic flow of dry powder inhalers

Francesca Orsola Alfano[1], Andrea Benassi[2,3], Roberto Gaspari[2], Alberto Di Renzo[1], Francesco Paolo Di Maio[1]

[1] DIMES Department, University of Calabria, Cosenza, Italy

[2] Chiesi Farmaceutici S.p.A., Parma, Italy

[3] International School for Advanced Studies (SISSA), Trieste, Italy

Fine particle lift and dispersion by gas flows is widely used as specialized technology in pharmaceutical, such as Dry Powder Inhalers (DPI), and dust handling devices. In DPIs for carrier-based formulations (i.e. drugs with two solid phases, the active pharmaceutical ingredient, API, and an excipient, carrier), the drag force exerted by the air flow and the impacts of the particles on the walls of the device promote the deaggregation of the agglomerates, in such a way that small, cohesive individual API particles can reach the lower lung airways. The two-phase flow structure and its interaction with the drug powder is generally complex due to the combination of the revolving gas flow field and its modifications induced by the presence of the particles. CFD-DEM simulations can be useful to get an accurate digital reproduction of such applications (digital twin). However, the presence of a strongly polydisperse system and very fine particles makes the simulation challenging, so the choice of appropriate models is essential. In the present work, unresolved 4-way coupled CFD-DEM simulations were performed on a representative swirl-based DPI geometry with 10 mg of 200 μm diameter carrier particles, one of which is coated with 5 μm diameter API particles (see Figure 1). The effect of different force contributions (i.e. Saffman and Magnus lift forces) and drag models on the deaggregation and consequent aerodispersion of the medication was assessed by analysing the detachment of the API from the carrier and the fragmentation of fine particle agglomerates.

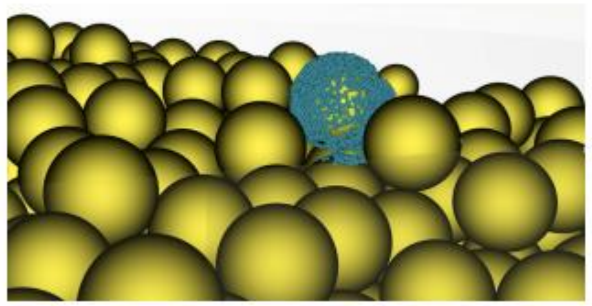

Figure 1. Bed of 200 μm diameter carrier particles, one of which covered with 5 μm diameter API particles.

Using the Material Point Method (MPM) to model bulk materials

Corné Coetzee

Department of Mechanical & Mechatronic Engineering, University of Stellenbosch, Stellenbosch, South Africa

The flow of bulk granular materials is usually associated with large deformation, such as the flow of grains from a silo. For this reason, the Discrete Element Method (DEM) has become the method of choice to model, analyse and design bulk handling systems. DEM models the material as discrete particles and can easily cope with the very large bulk deformation. On the other hand, continuum approaches, such as the Finite Element Method (FEM), have difficulty in modelling large deformation when the element distortion is too severe. The only remedy here, is to make use of re-meshing techniques which introduces mapping errors and can be time consuming and difficult to perform for complex 3D geometries.

However, there is a family of so-called “meshless” continuum methods, where the mesh (in FEM terms) is either absent or does not take part in the deformation. These methods can model large deformation and overcome some of the limitations associated with classic FEM. One such method is the Material Point Method where the material is discretised by a set of Lagrangian material points, and a fixed Eulerian background mesh is used to solve the momentum equation. The material points are allowed to move through the mesh, resulting in a combined Euler-Lagrange approach.

In terms of typical bulk handling, literature have demonstrated that MPM can be used to model silo discharge and excavator bucket filling. However, these demonstrations were limited to 2D and non-cohesive materials. Also, since those publications, new developments have rendered MPM more accurate and robust to model large deformation. In this study, a newly implemented 3D MPM code is used to model typical bulk handling processes, such as silo discharge, angle of repose (stock piling) and draw down. The aim of this study is to investigate the option and limitations of MPM in modelling bulk materials, both non-cohesive and cohesive. If successful, MPM can be considered as an alternative to DEM, in modelling the identified applications.

Multiscale modelling of granular materials – Calibration of discrete particle models

Thomas Weinhart[1,2], Mohammed Reza Vesal[2], Raquel Weinhart-Mejia[2], Donna Fitzsimmons[2], Anthony R. Thornton[1,2]

[1] Thermal and Fluid Engineering, ET, University of Twente, Enschede, The Netherlands

[2] MercuryLab, Enschede, The Netherlands

To develop trustworthy models for granular materials, one has to understand their behaviour on multiple scales: On the micro-scale, one needs the properties of single particles (their size, shape, density) and the contact behaviour of particle pairs (interparticle friction, cohesion, and elastoplasticity). These properties in turn influence the granular behaviour on the macro-scale.

We have developed a multiscale model for granular materials, combining the Discrete Particle Model (DPM, aka DEM) with an application-specific continuum model (CM). Starting from simplified particle and contact models, DPM captures the collective behaviour of a granular material by simulating the movement of the individual grains. Bulk properties are then extracted from the DPM simulations and coupled to the continuum model.

To calibrate a DPM model, developers often use analytic relations between the micro- and macro-parameters that are either phenomenological or derived from contact mechanics. Alternatively, they use numerical studies, where hundreds of simulations are run for different parameters to develop a mapping between the micro and macro parameters. However, both approaches are not feasible for complex industrial materials, where wide particle size distributions, agglomeration, inclusion of liquids, sintering, drying, and other phenomena require complicated contact models with many micro-parameters.

To deal with these issues, we have developed an automated calibration technique: First, we measure the basic material parameters (e.g., size distribution, material density) and apply them directly to the discrete particle simulation. Next, we select standard bulk experiments (heap test, rotating drum, shear cell) appropriate for the process we want to model. We simulate these processes in MercuryDPM [1] and measure the response of the simulated material. Then we apply numerical optimisation to find the micro-scale parameters for which the response of the experiments and simulations match. This optimization is done using a probabilistic optimization technique as implemented in the open-source code GrainLearning [2].

We have preliminary data suggesting that this technique and methodology works, in fact it has already been used in several projects, yielding good results. The technique can find local optima in only two to three iterations, even for complex contact models with many microscopic parameters. We present several case studies, discuss the strengths and weaknesses of the technique, when and why it fails and when it does succeed.

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An in-depth study of mixing and turning behavior of a compost pile using Discrete Element Method and Big-Data analysis

MSc. Mirkhagan Mustafazade[1], MSc. Mohsin Ajmal[1], Prof. Dr. Andre Katterfeld[1]

[1]Institute of Logistics and Material Handling Systems, OvGU Magdeburg, Magdeburg, Germany

Discrete element method is a useful tool in predicting bulk material behaviour which in real world scenarios is quite difficult to analyse with in-situ or ex-situ experimental techniques. During certain processes it is required to develop an in-depth understanding of dynamic bulk material properties distribution, therefore more sophisticated data analysis tools and techniques must be utilized. Here we report that a combination of simulation techniques and big data analysis tools gives a more detailed insight into bulk material behaviour. This combination will be applied to have a deep understanding of the mixing and turning behaviour of a compost pile. In the first place calibration of the compost is done by comparing the Angle of repose (AoR) in experiment and simulation. The friction parameters obtained will be used to simulate the pile formation of compost during the turning process. The simulation generates large amounts of data, which is comprehensive and contains valuable information which can be obtained by using big data analysis tools and to produce intelligible illustrations. Moreover, this data is used further to be displayed graphically on various correlations, which in the end gives some statistical indicators on which end user can derive data driven characteristics for bulk material.

Matrix analysis will be used to study the mixing behaviour of the compost in more detail. In the matrix analysis bulk material will be divided into small simulation boxes then compared with each other on a discrete particle level to understand the mixing efficiency more efficiently. A better understanding of the mixing efficiency gives a more accurate description of the temperature distribution inside the compost pile before and after the turning process which is a vital indicator of the quality and efficiency of the composting process.

An optimal calibration procedure for the Discrete Element Method

Farheez Mohamed[1], Elias Daouk[1], Mikel Leturia[1], Elodie Beaunac[1,2], Anne Charlotte Robisson[2], Carine Ablitzer[2], Khashayar Saleh[1]

[1]Université de Technologie de Compiègne, ESCOM, TIMR (Integrated Transformations of Renewable Matter), Centre de recherche de Royallieu, Compiègne, France

[2]CEA IRESNE/DEC/SA3E/LCU, Cadarache, France

Since its first appearance following the pioneering work of Cundall and Strack1 in 1979, the Discrete Element Method (DEM) has continued to gain in popularity for the simulation of granular media. The development of high-performance calculation algorithms as well as the increase in calculation capacities over the last decades have been the two incontestable pillars of the anguish that we know today for this method. However, the reliability of the results resulting from this method depends largely on the relevance of the numerical parameters used (Young's modulus, Poisson's ratio, coefficient of friction…) and a so-called calibration step is a preliminary step common to any DEM simulation. Trial-and-error is currently the most widely used calibration procedure, especially because of its simplicity. However, this method has several drawbacks: the number of simulations required for calibration is unknown and the adjustment of the parameters depends on individual experience. The objective of this study is to present an optimal calibration procedure comprising three major steps: Latin Hypercube Sampling (LHS), Kriging and Efficient Global Optimization (EGO). This procedure does not involve human interaction or excessive calibration time since it only requires a few DEM simulations. The angle of repose and Hausner's ratio were used for the calibration of spherical particles of 2 mm radius. The Young's modulus, the Poisson's ratio, the coefficient of interparticle friction and the coefficient of rolling friction of these particles were calibrated in only seven hours thanks to this procedure.

Keywords: Discrete Element Method, Simulation, Calibration, Optimization, Latin Hypercube Sampling, Kriging, Efficient Global Optimization

Digital twins to improve the calibration of DEM simulation of powder processes

Aurélien Neveu[1], Benjamin Jenkins[2], Dominik Werner[2], Andrei L. Nicusan[2], Christopher R.K. Windows-Yule[2], Geoffroy Lumay[3]

[1] Granutools SPRL, Awans, Belgium

[2] School of Chemical Engineering, the University of Birmingham, Birmingham, UK

[3] GRASP laboratory, CESAM research center, University of Liege, Liege, Belgium

DEM simulations are useful to predict the behaviour of powders and granular materials inside industrial processes. Conceptually, two methods can be used for the calibration of DEM simulation parameters. The first method is a bottom-up approach based on the direct measurement of the microscopic parameters at the scale of the contacts between the grains. Even if this bottom-up method makes sense conceptually, it is often practically impossible to use this approach based on complex measurement. The distribution of grain size and shape in real powders leads to strong fluctuations of the results. In addition, in many simulation models, the input parameters are not rigorously linked with these physical parameters. We propose an alternative top-bottom method based on a set of macroscopic measurements that can be used practically without difficulties to calibrate the simulation. The principle consists in measuring the powder properties in a laboratory and afterward to simulate the same process to tune the simulation parameters following an optimisation process. These measurements are performed in well-known geometries (tubes or rotating drum) and can be easily simulated. Finally, the best set of parameters will be used to simulate a complex industrial process for example. As for any powder characterisation task, the measurement geometry and the stress applied on the sample must be selected in accordance with the application. For a process involving high speed powder flow with a low confinement, the rotating drum methods (GranuDrum) will extract parameters that make sense for the application. On the other side, the flow through an aperture method (GranuFlow) provides a simple and quick classification of flowability. In between, the optimised GranuHeap angle of repose measurement is a good compromise. In this work, we demonstrate the potential applications of digital twins of these widely used powder characterization devices.

Robust estimation and validation of contact parameters of iron ore for transfer chute simulation

Guilherme P. De Oliveira, Rodrigo M. De Carvalho, Henrique A. Peixoto, Luís Marcelo Tavares

Dept. of Metallurgical and Materials Engineering, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil.

Transfer chutes are essential components during handling ores through conveyor belts. The flow of material through these devices is influenced by several variables. While traditionally designed using good practices based on experience, the increase in computational capacity has allowed the application of the Discrete Element Method in its simulation, from the modeling of the individual behavior of particles. Typically, the greatest challenge is the selection of contact model and parameters so that the material behavior can be described with high fidelity. The present work describes the approach used in calibration of these contact parameters of a sample of iron ore containing two moisture contents and two different contact surfaces. The approach starts with bench-scale tests, followed by experiments in a pilot-scale handling system, concluding with the verification in an industrial-scale chute. It was concluded that some of the tests respond more sensibly to certain material behaviors, so that their combined use demonstrated to allow realistic description of the material flow, even when simulating particles with simplified shapes and size distributions.

Investigations of abrasive sliding and impact wear – a DEM calibration approach

Thomas Roessler, Andre Katterfeld

Chair of Material Handling Systems, University of Magdeburg, Magdeburg, Germany

In the field of construction machinery and bulk material handling equipment, the main cause of equipment failure and downtime is the high level of wear caused by the handling of highly abrasive mineral bulk solids and powders. Due to the complex geometry of the conveyor systems and construction machinery and the interaction between the bulk material and the plant, conventional analytical and experimental methods for determining the type and location of wear images are of limited suitability. The existing approaches of wear prediction based on the Discrete Element Method (DEM) are mainly focused on the qualitative localization of wear phenomena and the quantitative description of effective forces. Therefore, only limited recommendations can be made where wear protection liners are necessary. Furthermore, predictions of the service lifetime and maintenance intervals are limited. This paper examines the possibility of a calibration of wear model parameters in the Discrete Element Method for the quantitative determination of abrasive sliding and impact wear. This includes a brief overview of the wear mechanisms mainly involved and the current status of research of wear measurement and prediction using Discrete Element Method including different wear model approaches. Based on this, the possibility of calibrating the discrete element method based on long-term experimental investigations is presented for selected wear models. For the experimental investigations, both impact wear tests and sliding wear tests are carried out, whereby an application-oriented investigation is ensured by a nearby free interaction between the liner samples and the bulk material. The experiments are based on the bulk materials granite and porphyry and the wall liner materials steel and alloy. The obtained macroscopic wear rates of the liner samples will be used to calibrate the wear coefficient of the single particle wall contact. The paper will also include the calibration of the bulk material parameters. After the presentation of the wear calibration approach the quality of this approach will be double checked by DEM validation simulations based on semi-industrial sized experiments of transfer chutes and impact plates.

DEM simulations of industrial scale granular chute flows

Satyabrata Patro, Nikhil Kumar Meena, Anurag Tripathi

Dept. of Chemical Engineering, Indian Institute of Technology, Kanpur, India

The flow of granular materials is seen in many solids processing industries as well as many geophysical situations. The understanding of the rheology of these bulk solids can improve the handling and processing on a large scale. Towards this goal, we perform large scale 3D discrete element method (DEM) simulation of inelastic and frictional spheres flowing on a chute with dimensions comparable to chutes used in some industrial applications. The mass flow rate over the chute is controlled by adjusting the orifice width of the storage hopper and the simulations are performed for different chute inclination angles. Various flow properties of interest are measured at different locations along the chute. The applicability of the inertial number based rheology at low chute inclinations (and hence inertial numbers) is typically assumed. However, most of the DEM studies used in literature use periodic boundaries in the flow direction, mimicking an infinite length of the chute. A detailed analysis of the flow properties measured in case of the finite length chute are performed to explore the applicability of the inertial number based μ-I rheology for flow over chutes of different inclinations. We observe that the flow does not achieve steady state for a large range of inclinations and deviations from the inertial number based rheology are noticeable. The results presented will be very useful for continuum simulations of industrial scale granular flows in large chutes.

Predicting time dependent behavior of surface granular flows

Anurag Tripathi[1], Satyabrata Patro[1], Sumit Kumar[2], Anubhav Majumdar[1]

[1]Dept. of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur, India

[2]Dr. Reddy's Laboratory, Hyderabad, India

Surface flow of granular materials occurs commonly in many industrial and geophysical situations. The flow behavior of such granular flows is studied using DEM simulations and compared with the predictions from a continuum model. In the DEM simulations, the particles are modeled as slightly polydisperse, inelastic, frictional disks. An assembly of disks flowing under the influence of gravity over a rough and bumpy surface is studied for a variety of surface inclinations. Evolution of various flow properties, such as the velocity profile, solids fraction, inertial number, shear stress, pressure etc. with time are presented.

The results obtained from DEM simulations are compared with the predictions of a continuum model utilizing the inertial number based rheology for dense granular flows. The continuum model solves the momentum balance equation along with the rheological model for time dependent flow using the pdepe solver in Matlab with appropriate boundary conditions. The continuum model predictions for the conventional inertial number based rheology fail to capture the flow properties evolution with time in case of high inclinations. A modified rheological model, proposed recently [Patro et.al., Phys. Fluids, 33, 113321 (2021)] to account for the presence of normal stress difference, is able to describe the evolution of the flow properties very well. These results show that accounting for the modified rheology in the continuum simulations is essential for accurate prediction of time dependent flow properties at high inclinations.

THURSDAY, 7 JULY 2022
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MATHEGRAM SYMPOSIUM

Heat generation by friction and deformation during an oblique impact

Francisco Kisuka[1], Colin Hare[1,2], Chuan-Yu Wu[1]

[1]Dept. of Chemical and Process engineering, University of Surrey, Guildford, United Kingdom

[2] School of Chemical Engineering, Newcastle university, Newcastle upon Tyne, United Kingdom

Particle transportation has a fundamental role in industrial applications including chemicals, pharmaceutical, agriculture and other manufacturing processes. Within such systems, particle impact characteristics govern the overall energy dissipation patterns particularly through plastic deformation, friction and/or viscosity. Therefore, as an effort to improving the design and efficiency of complex particulate systems, a good amount of effort has been invested in understanding the energy dissipation and conversion mechanisms at a particle level. Despite such effort, the scientific literature still lacks robust physical and mathematical models to bridge the impacting parameters (i.e., velocity and incidence angles) to the thermal-mechanical energy conversion phenomenon.The present work explores heat generation resulting from the plastic and friction dissipation when a spherical particle collides with a rigid surface at an oblique angle. This problem is implemented in finite element analysis model where the heat generation at different impacting angles and velocities is examined. Similarly, analytical solutions by Cross [1] and Carslaw & Jaeger [2] are used to calculate the heat generation and the rise in contact temperature respectively. The results, show that the plastic heating has a major contribution to the total heat for lower impacting angles while the frictional heating is important for the collisions at glancing angles. It is also observed that the analytical models and finite element analysis results are in good agreement (see Fig). The ability of the theoretical models to accurately predict the energy losses (i.e., heating) and rise in temperature implies that these models can be extended to other numerical tools like DEM to study the heat generation problems in bulk granular flows.

Keywords: Energy dissipation, Frictional heating, Plastic heating, contact temperature.

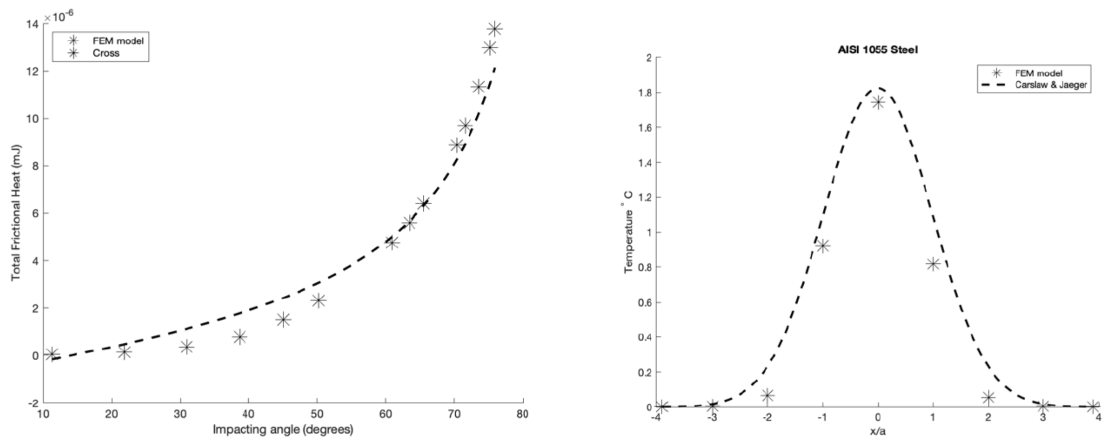

Fig. (left) heat generation due to impact (right) contact temperature distribution

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Calibration of CFD-DEM heat transfer model using packed bed experiment

Aman Rastogi[1], Colin Hare[2], Vincenzino Vivacqua[1]

[1]JMTC, Johnson Matthey, UK

[2]School of Engineering, Newcastle University, UK

*E-mail: aman.rastogi@matthey.com

Thermal processing is a necessary step in many granular materials manufacturing processes and may be used to affect a physical, chemical or phase transformation. The critical quality attributes for such processes depend strongly on the duration, intensity and uniformity of the heat received by the material. CFD-DEM method is now widely used to model heat transfer in multiphase systems, however their applicability to systems involving powders has been limited, due to rapid scaling of computational time with the number of particles. The aim of this research is to provide a reliable methodology for calibrating coarse-grained heat transfer models for powders. Transient heat transfer experiments are performed on packed powder beds with and without airflow, with three different materials. Unresolved CFD-DEM simulations are performed using LIGGGHTS-OpenFOAM coupling. The conductive and convective heat transfer to the powder bed, obtained through the simulations are then compared to the experimental and analytical results. The effect of coarse graining factor, the gas flow rate and the applied stress on the bed, on the heat transfer is also investigated.

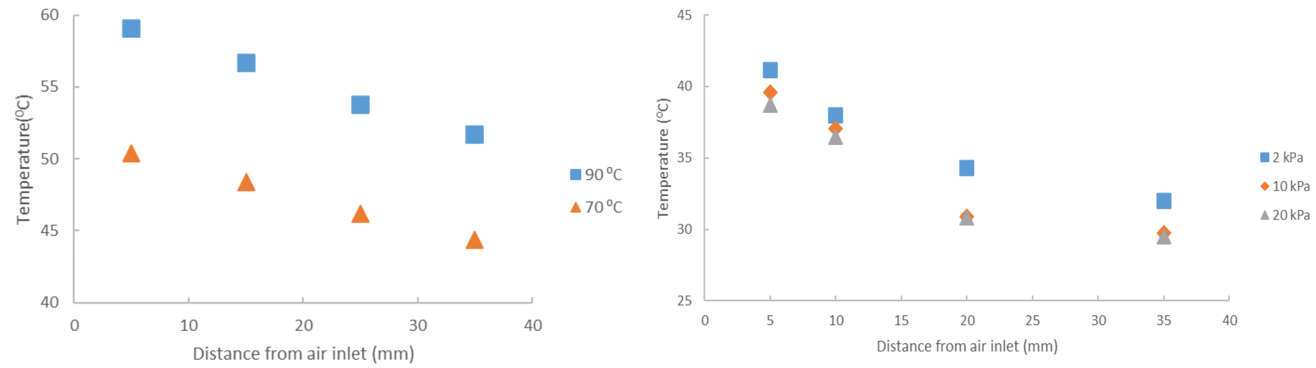

Figure. Experimental Results (a). Bed Temperature profile for MCC at 6 lpm gas flow rate and 90 ºC inlet temperature at different consolidation stresses, (b) Bed Temperature profile for glass beads (1 mm diameter) at gas inlet temperatures 90 ºC and 70 ºC at gas flow rate of 6 lpm

DEM modelling of granular material swelling

Domenica Braile[1], Colin Hare[1,2], Chuan-Yu Wu[1]

[1]Dept. of Chemical and Process Engineering, University of Surrey, Guildford, United Kingdom

[2]School of Chemical Engineering, Newcastle University, Newcastle upon Tyne, United Kingdom

The increase in volume of grains due to water absorption is common in many natural materials and industrial products. Hence, a thorough understanding of grain swelling is of great scientific importance. As the swelling phenomenon usually involves a large quantity of grains, a DEM model that can model the swelling of single grains and the deformation of the granular system is worth pursuing. In order to do this, rigorous numerical models for describing particle swelling are essential. In this work, a first order kinetic model is proposed and evaluated to predict the volume change of single particles. The model is then implemented into the DEM code LIGGGHTS and validated at the macroscale by comparing the time evolution of the expansion of a packed bed made of SAP particles obtained numerically and experimentally (Figure 1a). Furthermore, the validated DEM model was employed to simulate the swelling of three different materials, i.e. SAP, rice and microcrystalline cellulose (Avicel PH102). The swelling kinetics and capacity of a single grain of each material were obtained from published data and used to simulate the granular beds' expansion until the saturation state was reached. As expected, the swelling behaviour depends significantly on material properties; the fastest to reach its maximum expansion is the granular bed made of PH102, followed by SAP and rice (Figure 1b). However, as shown in the insertion in Figure 1b, the final bed expansion is greatest for SAP, followed by Avicel PH102 and rice. The developed model could be further advanced to study consequences of swelling phenomena in granular materials, such as segregation and heat generation.

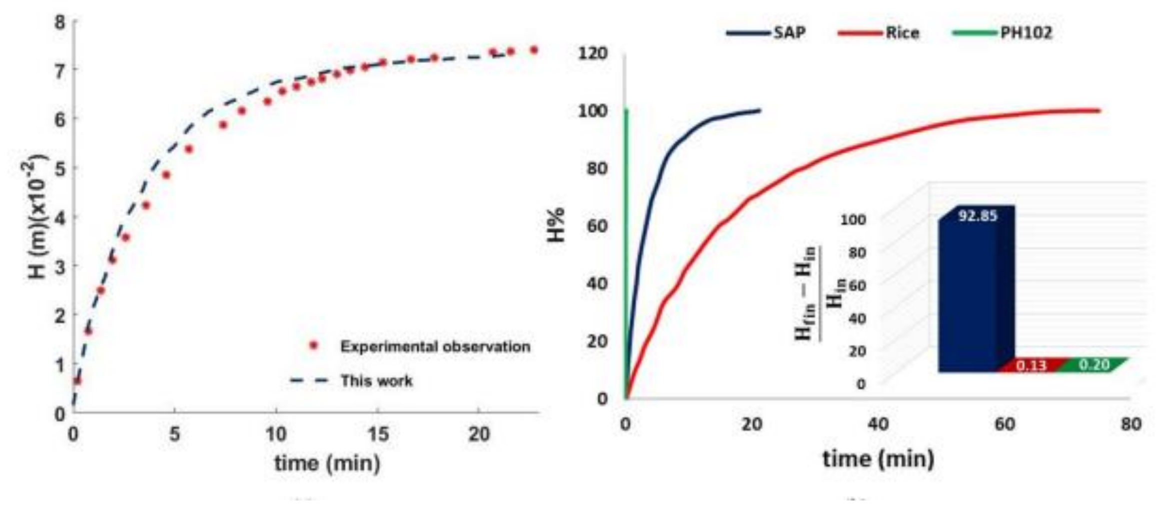

Figure 1(a) Comparison of the height (H) of the bed of SAP particles obtained numerically and experimentally, and (b) time evolution of the height (H%) of the granular beds made of SAP, rice and PH102. The insertion shows the swelling capacity of the granular beds.

Modeling particle-scale deformation and heat conduction for a highly dense granular system with finite volume method

Ranjan Dhakal[1], Philip Cardiff[2], Stefan Radl[1]

[1] Institute for Process and Particle Engineering, Graz University of Technology, Inffeldgasse 13/3, 8010 Graz, Austria

[2] School of Mechanical and Materials Engineering, University College Dublin, Belfield, D4, Dublin, Ireland

Analysis of powder compaction plays an important role in many applications, for example to guarantee the quality of metallurgical powders, pharmaceutical tablets production etc. Specifically, in many powder compaction process, temperature rise in the compressed powder can cause thermal degradation, which is critical to crystallinity and can affect, the physiochemical properties of the product. The reason for such rise in temperature is a consequence of stress and contact heterogeneities. Moreover, most of the modeling techniques utilizing finite element approaches treat the powder domain as a continuum with a uniform porosity. However, this simplified model limits the process understanding that can be gained. Therefore, it is of practical significance to understand the inhomogeneous distributions of density and residual stresses that occurs in the powder compaction process as a result of elasticity, plasticity, internal friction of porous medium and frictional effects at confining walls.

In order to investigate such processes, a detailed modeling of particle-scaled deformation due to contact has been investigated. This is based on a penalty method ([1], [2],) which has been implemented in the finite volume open-source software environment 'foam-extend-4.0'. As a step of verification, a contact stress distribution for 2 particles deforming within elastic limit was investigated and shows excellent agreement with an analytical solution. For the thermal contact boundary condition, a homogenized constitutive relation for a thermal contact resistance [3] has been utilized. This boundary condition was applied to study heat conduction in a thermo-elastic material during contact, specifically two particles with different temperatures. Also, the software tool was extended to ensure it is able to model multi-particle systems. Specifically, the computer code is now able to track multiple contact pairs, as a single interaction assuming anything can hit anything.

Acknowledgments

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CFD-DEM model for high-temperature processes

Jelena Mačak[1,2], Christoph Goniva[1], Stefan Radl[2]

[1] DCS Computing GmbH, Linz, Austria

[2] Institute of Process and Particle Engineering, Graz University of Technology, Graz, Austria

We present a numerical tool, based on coupled computational fluid dynamics and discrete element method (CFD-DEM), intended for high-temperature particle-fluid processes. Special attention is given to modeling of a compressible fluid and radiative heat transfer.

Neglecting compressibility of the fluid can lead to inaccurate conclusions. Using analytical and numerical tools, we demonstrate that systems with 25% change in fluid temperature along the streamline also necessarily feature a large change in fluid density. Isothermal systems, such as long pneumatic conveyors and low-pressure fluidized beds, can also exhibit large density gradients induced by gas-particle drag. Compressibility of such a system can be assessed using a simple relation of the Mach number.

At temperatures above 400°C, radiation becomes a significant mode of heat transfer. DEM-based radiation models are, due to complexity, often limited to systems with a small number of particles. To mitigate this limitation, we use the P1 radiation model. This model is well-suited for industrial-scale applications such as laser melting, solar particle receivers, and pebble bed reactors, since it can handle polydispersity and coarse graining with particles enlarged up to million times.

The CFD-DEM code is verified and validated using analytical and experimental data.

Sources of error when measuring the hydraulic conductivity of a granular material at different temperatures

Marina S. Bortolotto[1], David M. G. Taborda[1], Catherine O'Sullivan[1]

[1]Department of Civil and Environmental Engineering, Imperial College London, London, UK

Variations in temperature are a common issue for most engineers since such variations can be caused by both natural phenomena (changes in the weather) and human-made structures (e.g. nuclear waste repositories, buried pipelines and cables). Within a soil mass, these changes in temperature can potentially alter the arrangement of soil particles. This particle rearrangement might be difficult to desmonstrate unless indirect measurements that rely on the material's bulk response are used. Hydraulic conductivity is an appropriate alternative to investigate and characterise such rearrangement. However, its measurement has been shown to be challenging, even for isothermal tests due to the system's intrinsic head losses. These errors become increasingly significant when performing tests under non-isothermal conditions. This research describes the procedure adopted to identify and quantify errors associated with hydraulic conductivity tests performed in a bespoke temperature-controlled triaxial apparatus at different temperatures. Methodologies to mitigate such errors are also briefly described.

When testing granular materials in a triaxial cell, minimising and accounting for the system's intrinsic head losses are essential to obtain reliable results at different temperatures. This requires a thorough calibration procedure. Moreover, temperature changes affect the viscosity of the fluid, which has an impact not only on the hydraulic conductivity of the tested specimen, but also on the overal response of the system – which can be corrrected with calibration. Changes in water viscosity can be corrected by working in terms of intrinsic permeability. However, the sharp variation of this property with temperature can become a potential source of uncertainty if a reliable measurement of temperature is not available. To overcome this difficulty, an aditional temperature probe has been instaled inside the sample and drops in temperature have been observed due to the circulation of water imposed while performing hydraulic conductivity tests. Moreover, plastic deformation of the nylon drainage lines during thermal loading has also been identified as a possible source of error. Therefore, brass drainage lines have been installed to mitigate non-recoverable deformations with temperature.

Lastly, radiation and heat reaching instrumentation motivated investigations using an infrared camera. Images obtained from the camera have been crucial to understand the thermal performance of the equipment, with images revealing superficial temperatures of drainage lines close to the volume gauge as high as ~33℃ during tests at 60℃. Calibrating the volume gauge at different temperatures is technically difficult, so a heat exchanger was added to cool down the drainage line from ~33℃ to 22℃. Moreover, radiation reaching the instrumentation was observed while using a single layer of insulation (polyethylene closed cell foam) around the cell. Readings from pore water pressure transducers seem to be affected once their surface temperatures reach 4-5 ℃ higher than room temperature, prompting the use of additional insulation.

Fundamental basis for a novel approach to indirectly measure the effective thermal conductivity of granular materials

Tokio Morimoto[1], Catherine O'Sullivan[1], David M. G. Taborda[1]

[1]Dept. of Civil and Environmental Engineering, Imperial College London, London, UK

Estimating the effective thermal conductivity (ETC) of granular materials is of great importance for the effective operation of various engineering and industrial facilities (e.g. thermo-active piles, pebble-bed reactors, and packed-bed energy storages). The ETC of granular materials is affected by various packing characteristics of the granular materials such as the stress state, density, and anisotropy. Nonetheless, it is experimentally challenging to measure the ETC of granular materials with controlling the packing characteristics precisely. An indirect method to predict the ETC of granular materials would be beneficial.

This contribution combines analytical and Discrete Element Method (DEM) studies to provide the fundamental basis for a novel indirect ETC measurement only based on the density and elastic modulus of the granular materials. Both the analytical model and DEM model considered here use a thermal network model (TNM), where each particle is represented as a node and thermal pipes link pairs of nodes (particles) which are close to each other. The thermal conductance of heat pipes in the TNM is formulated using the model proposed Batchelor and O'Brien (1977) [1], which considers the conduction through pore fluid as well as the conduction through the contact area of the particles.

In the analytical study, the elastic modulus of the granular medium is determined using the packing density, the average contact radius and the average coordination number employing a uniform strain assumption. We show that the ETC of a granular medium can be formulated using the packing density, the average contact radius and the average coordination number employing a uniform temperature gradient assumption. Taking advantage of the similarity of elastic modulus and ETC formulations, we predict that the ETC of a granular medium can be estimated using the Young's modulus and the packing density of the medium.

The prediction in the analytical study was examined using a DEM coupled with a TNM. Virtual granular samples with a variety of packing densities, stress states, and levels of anisotropy were created. Small strain probes and heat transfer simulations were conducted to obtain the elastic moduli of samples and the ETCs of the samples. The data generated support the prediction made in the analytical study. (For full details, refer to [2])

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Keywords: effective thermal conductivity, stiffness, modulus

The effect of temperature on the spreading of powder layers in selective laser sintering

Sina Zinatlou Ajabshir *, Diego Barletta, Daniele Sofia, Massimo Poletto

Dipartimento di Ingegneria Industriale, Università degli Studi di Salerno, Fisciano SA, Italy

*sizinatlouajabshir@unisa.it

One of the Laser-based Additive Manufacturing (AM) is selective laser sintering (SLS). SLS allows manufacturing 3D products by adding powders layer by layer. In SLS, the powder feeding and spreading on the powder bed is an important step because, every layer plays a crucial role in the final product structure and properties. As a result, uniform powder layers are needed per each run. In other words, the proper spreadability of powders is necessary to make layers of good quality. Several parameters, as the particle size, the particle shape, the forces between the particles, the humidity, and the temperature, affect the powder spreadability. Temperature is an important process parameter because increasing the material temperature during sintering improves the quality of the sintered material by reducing the onset of residual stresses and the consequent formation of cracks. Temperature is also used to improve the final artifact density due to the improved wetting of the fused phase with the neighboring particles. Furthermore, the use of higher temperatures in the sintering chamber reduces the laser energy demand for sintering. On the other hand, powder pre-heating at high temperatures close to the melting point scan reduce the powder flowability and negatively affect the powder spreadability. In this work, the effect of temperature on the spreadability of polymeric powders was studied by the spreading apparatus developed at the Powder Technology laboratory of the University of Salerno. In particular, by means of a heating and temperature control system, this apparatus allows simulating the spreading step occurring in commercial machines at any fixed temperature. Furthermore, a method was proposed to evaluate powder layer quality from pictures taken after completing the spreading step at desired temperature in the presence of surface grazing light. The procedure is based on Wavelet Transform. This procedure allows identification of the characteristic size of surface roughness for comparison with the agglomerate size obtained by means of shear testing results' analysis.

In-situ monitoring and modeling of single-layer selective laser sintering of polyamide powders

Balaji Soundararajan[1], Daniele Sofia[1,2], Diego Barletta[1], Massimo Poletto[1]

[1]Dept. of Chemical Engineering, University of Salerno, Salerno, Italy

[2]Sense square Srl, Salerno, Italy

Selective Laser Sintering (SLS) is one of the most common types of layer-wise Additive Manufacturing (AM) process using granular materials which has the potential to revolutionize the manufacturing industry. One of the major sources of defects is the delamination of layers in the final specimen which is due to lack of fusion between layers. The temperature distribution along the depth of the powder bed, which is affected by the thermal conductivity of the powder bed is vital in calculating the optimum layer thickness. In this study, a stationary laser sintering experimental set-up equipped with two infrared cameras is built to measure the temperature distribution along the depth and the top surface. A thin layer of polymeric powder is spread on infrared-transparent Zinc Selenide (ZnSe) glass so one of the thermal camera can see the heat transfer along the depth from the bottom. The powders used in this study are carbon black treated polyamide 12 and polyamide 6.

The study also involves calibration of thermal cameras and calculation of powder surface emissivity at various temperatures. Using both the thermal cameras, the effective thermal conductivity of the powder bed is also calculated. The experiment is repeated for various layer thicknesses ranging from 200 microns to 1mm. A three-dimensional finite element model considering the powder bed conduction, convection, radiation and phase change of various layers is built and validated against the experiments. The thermophysical material properties are calculated experimentally, which in turn enhances the model. On the basis of the results from this study, it is possible to identify the optimum layer thickness needed for a good quality specimen.

Keywords : Laser Sintering, heat transfer, infrared thermography, finite element methods, layer thickness.

A numerical study of heat transfer mechanisms in dense particulate systems using DEM

Rafael Rangel[1], Alessandro Franci[1], Alejandro Cornejo[1], Francisco Zárate[1], Eugenio Oñate[1]

[1] International Center for Numerical Methods in Engineering (CIMNE), Universitat Politècnica de Catalunya (UPC), Barcelona, Spain

In this work, the Discrete Element Method (DEM) is used to explore different aspects of heat transfer in granular materials. In order to do this, a computational tool was developed to consider thermal effects in the classical soft-sphere approach of DEM[1] . This tool is able to simulate different mechanisms of heat transfer, through conduction, convection, and radiation, in addition to heat generated by friction. Although not coupled to a Computational Fluid Dynamics (CFD) solver, a 1-way thermal coupling between the particles and the surrounding fluid is possible. For each type of heat transfer mechanism, several numerical models were implemented to account for the respective effect. All these implementations were carried out within the open-source framework Kratos Multiphysics[2][3] . The focus of this study is on dense particulate systems with static or dynamic behavior, such as packed beds and granular flows. For the former, Representative Volume Elements (RVEs) are employed for simulating the static behavior. For the latter, a model of a rotating drum is taken as reference for performing the investigations. The results provided by all the numerical models are compared, at the same time that the contribution of each mechanism to the total rate of heat transfer is analyzed. Conclusions and discussions based on the obtained results will be drawn in order to achieve a better understanding on the thermal behavior of granular materials.

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Analysis of sintering of ceramic powder systems by in-situ synchrotron nano-tomography

Aatreya Manjulagiri Venkatesh[1], Didier Bouvard[1], Pierre Lhuissier[1], Julie Villanova[2]

[1]Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMAP, 38000 Grenoble, France

[2]ESRF - The European Synchrotron, 71 Avenue des Martyrs, 38000 Grenoble, France

Investigating sintering phenomena is challenging as it involves the collective behaviour of particles, whose accurate observation requires 3D imaging. For ceramics, owing to the complex and fine architecture of the individual grains, a significantly higher resolution is necessary. To this end, ultra-high-resolution capabilities at the nano-tomography beamline of the upgraded ESRF synchrotron facility have been taken advantage of to investigate ceramic powder sintering at the individual particle length-scale. A micron-sized alumina powder with fairly regular and non-agglomerated individual particles were chosen for the initial set of investigation. Nano-tomography experiments at the synchrotron employed a phase contrast X-ray holotomography technique which facilitated the inclusion of large volumes of interests and investigate subsequent stages of sintering. Complete 3D images were acquired with an interruptive in-situ mechanism at 1500°C with a voxel size as low as 25nm to depict particles and pores with enough details. Detailed morphological features were revealed due to the high resolution and the large field of view stemming from the multiple distance phase retrieval. Data resulting from subsequent quantitative image analyses were used to explore both densification and grain growth phenomena of sintering throughout the cycle.

Furthermore, extending the scope of the work to increasingly used set of agglomerated ceramic powders, zinc oxide particles with a size of few hundreds of nanometers were subjected to the tomography analyses. The inter-agglomerate pores present in the powder owing to its nano-size hinder complete densification during sintering of the compact, thus forming defects in the final material. Nano-tomography analyses were utilized to focus on better understanding the changes of these pores during the course of sintering. Further quantitative analyses of the images acquired provided the kinetics of the size and shape changes of inter-agglomerate pores and a means to track the resulting flaws induced in the compact.

The information obtained from the tomography experiments were subjected to classical sintering theories and models for further validation. The experimental results were also subjected to a DEM simulation to further compare key sintering parameters.

Modeling grain growth and arbitrarily shaped particles in sintering with the discrete element method

Brayan Paredes-Goyes[1], David Jauffres[1], Christophe L. Martin[1]

[1]Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP, Grenoble, France

Sintering is a well-known process for the consolidation of powders. Parallel to densification, grain growth appears during sintering, as it also decreases the interfacial energy. The discrete element method has been used for simulating densification during sintering. Here, we propose a realistic grain growth model coupled with the densification process. The model includes grain growth mechanisms valid for a widely variety of ceramics and metals: surface diffusion and grain-boundary migration. The model is in good agreement with alumina experimental data both for the mean grain size and for the grain size deviation. Using realistic initial size distributions, we verify wider distributions result in earlier grain growth. The influence of the heating rate ramp on the grain growth kinetics is analyzed.

In the above simulations, the particles are spherical in shape, which is a valid approximation for some sintering powders and sintering stages. As the driving force for shrinkage and grain growth is the curvature gradient, an accurate representation of the shape will add valuable information to the analysis. We choose the level set discrete element method (LS-DEM), that uses the classical dynamic description of DEM and the level set for representing any arbitrary shape. We implemented a contact detection algorithm based on an optimization scheme in order to decrease the computational cost of the original LS-DEM. The developed sintering LS-DEM model allows computing sintering and grain growth kinetics for different realistic powders and conditions.

THURSDAY, 7 JULY 2022
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POWDER TESTING AND CHARACTERIZATION

An X-ray microtomography study of packing behaviour metal powders during filling, compaction and ball indentation process

Mozhdeh Mehrabi[1], Ali Hassanpour[1], Andrew Bayly[1]

[1]Dept. of Chemical and Process Engineering, University of Leeds, Leeds, UK

A reliable quantification of bulk flow behaviour of particles is of paramount importance in powder processing. A good example is the use of appropriate metal powders and consistency of particles flow in high value additive manufacturing process which leads to significant effects on the quality of the final products. Identification of the most reliable method to characterise powder flowability in correlation to the conditions of powder spreading is still challenging. For instance, the low consolidation state of the powders within the process requires a characterisation technique which is capable of measurement for such conditions. The ball indentation method could be the trustworthy method for measuring flow behaviour of loosely compacted powders however, despite a number of reported papers, there is a lack of understanding of the powder packing behaviour during the indentation process. In this research the time lapse X-ray microtomography has been used to characterise the ball indentation of two different types of Ti6Al4V powders used in AM, namely the spherical gas atomized (GA) and irregular hydride-dehydride (HDH) particles. The packing behaviour of powders during the process of filling (loose), consolidation (compacted) and ball indentation (indented) have been studied. The results reveal there are differences in the packing behaviour of the two powders during the consolidation stage.

The study has led to deeper understanding of ball indentation method and therefore could be useful in further developing the technique.

Soft wheat flour quality parameters assessment by Near Infrared Spectroscopy: from laboratory to shelf

Giuseppe Bonifazi[1,2]*, Riccardo Gasbarrone[1], Silvia Serranti[1,2]

[1]Department of Chemical Engineering, Materials & Environment, Sapienza University of Rome, Rome, Italy.

[2]Research Center for Biophotonics, Sapienza University of Rome, Latina, Italy.

Near InfraRed Spectroscopy (NIRS) is a powerful tool for research and industrial applications. This technique, suitable for both qualitative and quantitative analysis, is arising in agri-food applications, because of its property of being non-invasive, not destructive and fast.

In this study, the possibilities of NIRS utilization for wheat flour quality evaluation are explored. In more detail, the utilization of a portable spectroradiometer working in Visible – Short Wave InfraRed (Vis-SWIR: 350 – 2500 nm) spectral range, coupled with chemometric techniques are investigated. NIR-based techniques offer the possibility not only to rapidly classify wheat grain on the basis of its variety or geographical origin (given a strong calibration set) but also to quantitatively predict quality parameters. The potential of this method for predicting protein content, starch content, wheat gluten content, ash content, water absorption and wheat flour strength (W) is discussed. Present findings show the reliability of using NIRS as a quality control tool not only at laboratory scale (i.e. by acquiring reflectance spectra on wheat flour arranged in Petri dish), but even in on-line industrial application and shelf storage control evaluation (i.e. by acquiring reflectance spectra on wheat flour sack).

Bulk solids on the Moon - Characterization of the innovative Lunar Regolith Simulants TUBS-M, TUBS-T and TUBS-I

Lisa Windisch[1], Stefan Linke[2], Arno Kwade[3], Enrico Stoll[4], Carsten Schilde[5]

[1,3,5]Institute for Particle Technology, TU Braunschweig, Braunschweig, Germany

[2,4]Chair of Space Technology, TU Berlin, Berlin, Germany

Growing international interest in scientific and commercial lunar exploration programs requires cost-effective, logistical solutions for raw and construction materials to enable medium- and long-term stays on the Moon. Lunar regolith covers the entire lunar surface, and is a fine, cohesive powder and the most abundant resource; its engineering usage through In-Situ Resource Utilization (ISRU) would greatly advance infrastructure construction to full habitats on the Moon. Before doing so, however, it is essential to develop and test the technologies (e.g., rovers or scientific equipment) needed for such endeavors on Earth. In order to be able to design such equipment accurately, analogous terrestrial materials (simulants) have to be developed and used, which come as close as possible to the properties of real lunar regolith.

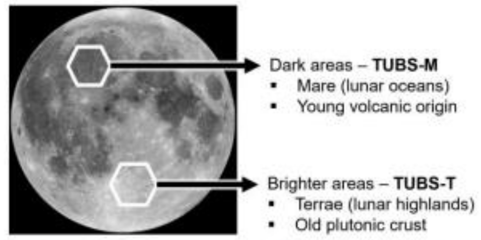

Fig. 1: Allocation of the regolith simulants to the lunar regions

In this context, the main objective of this study is the development and characterization of three lunar regolith simulants at the Institute for Particle Technology: the basaltic TUBS-M, the anorthositic TUBS-T (see Fig. 1) as well as the blended form TUBS-I.

The simulants will be adapted to the properties of real lunar regolith.

Mission risks can be drastically reduced by the systematic adaptation to the lunar terrains relevant for each specific mission. In the course of this, it is of high importance to thoroughly characterize and understand the properties of the lunar regolith simulants. Therefore, the simulants are analyzed with established and novel characterization methods from the field of particle and bulk solids engineering (e.g. flow and densification behavior; see Fig. 2) and compared with real lunar regolith and other reference materials.

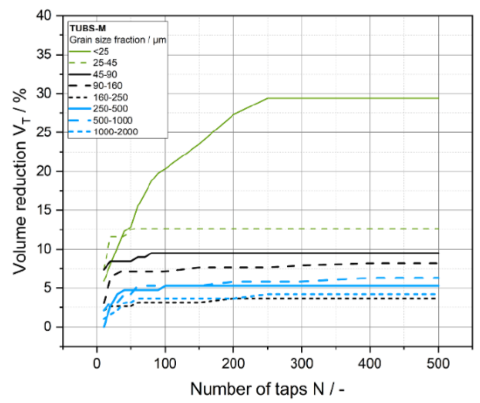

Fig. 2: Densification behavior of different particle size fractions of TUBS-M

It will be shown that promising regolith simulants can be obtained from terrestrial soils. In addition, the presentation will highlight the often-underestimated significance of bulk materials engineering in extraterrestrial applications, such as scientific spaceflight.

Effect of moisture content, size distributions and particle shape on flowability: angle of repose, tilting angle, and Hausner ratio

Haim Kalman

Aaron Fish Chair in Mechanical Engineering – Fracture Mechanics, The Laboratory for Conveying and Handling of Particulate Solids, Department of Mechanical Engineering, Ben-Gurion University of the Negev, Beer Sheva 84105, Israel.

The angle of repose, angle of tilting, and Hausner ratio are frequently used to estimate the flowability of a particulate material. In this study, these factors were determined for the effects of particle shapoe, moisture content and size distributions. In order to that many materials, some having a number of size fractions were tested. In respect to the effect of the moisture content, the flowability results clearly showed three types of materials according to their response to moisture content: solid particles, porous particles, and size-changing particles. A thorough analysis of various sizes of spherical solid particles enabled the identification of five zones from dry to fully immersed in water, and a zone map could be obtained. In addition, a model predicting flowability as a function of moisture content and Archimedes number could then be developed. The testing of various mixtures, either bi-modal or having a wide size distribution revealed very interesting behaviours. In any case, it was shown the the measured value of a mixture normalized by the mono-sized value of the median size of the mixture is a clear function of the distribution parameter. The same behaviour was found for spherical and non-spherical particles in all cases, but the tapped bulk density. More than 50 materials having different shapes (spheres, cylinders, flakes, irregular, etc.) were tested to found the effect of the sphericity. As a result of all the above, reliable and general correlations could be developed.

An investigation into the effect of drying on the flowability of the bulk pulverised cassava grits

Hamed J. Sarnavi[1], Marcelo Precoppe[1], Hamid Salehi[2,3], Michael S.A. Bradley[3], Pablo García-Triñanes[2]

[1] Natural Resources Institute, University of Greenwich, Chatham Maritime, UK

[2] Materials and Chemical Engineering Group, University of Greenwich, Chatham Maritime, UK

[3] Wolfson Centre for Bulk Solids Handling Technology, University of Greenwich, Chatham Maritime, UK

* Corresponding author email: **h.j.sarnavi@gre.ac.uk**

The effect of drying to promote the flowability of wet cohesive cassava (*Manihot esculenta* Crantz) grits has been studied in view of observation that the grits become easier to handle as they dry. Samples were prepared in two different ways using a grater and a food blender. Low strain measurements were conducted using a shear tester. Shear to failure data, obtained under four levels of consolidation (0.418 kPa to 4.892 kPa), was analysed to construct the nonlinear yield envelopes. The Warren-Spring model remarkably enhanced the quality of yield loci construction in comparison to the Mohr-Coulomb model for the studied samples. The failure envelops shrunk as the drying process progressed and the observed shrinkages were translated into quantitative flow property indexes. Furthermore, the bulk density was expressed as a function of moisture content and the applied consolidation stress, reflecting their combinational effect. The dependency of cohesion, tensile strength, and the internal friction angles on moisture content was explained over their variation with the consolidation history and the bulk density, according to the measured physical properties of the prepared samples. The morphology of the granules and their clusters which constitute the agglomerates was captured using scanning electron microscopy. Further information was collected using mechanical sieving and particle laser diffraction analysis. Based on the flow function classification, it was concluded that the very cohesive wet sample at 46 % wet basis (1/ffc equals 0.71 for blended and 0.66 for grated) evolved to a cohesive partially dried sample at 31 % wet basis (1/ffc equals 0.40 for blended and 0.38 for grated), and eventually approached to free-flowing state at the end of the drying process, reaching 14 % wet basis (1/ffc equals 0.08 for blended and 0.11 for grated). The findings of this research lay the foundation of the necessary understanding of the bulk flow properties of pulverised cassava grits for designing handling and processing facilities at processing centres.

Keywords:

Drying, flow properties, Warren-Spring, tensile strength, cohesion, internal friction

Moisture caking: Accelerated caking tests

Jairo Paternina, David Craig, Mason Parker

Jenike & Joahnson, Inc. (Tyngsboro, Massachusetts, USA)

Caking results when particles agglomerate and form solid lumps or masses. Caking is undesirable and can lead to several problems, including customer complaints and rejected product. The most common cause of caking is the presence of sufficiently high moisture, which can result in interparticle liquid bridges that subsequently solidify under dry conditions. In many industrial applications, caking occurs over a period of time. Laboratory tests can be conducted to identify conditions that can cause and/or prevent caking. However, duplicating the time for caking in the lab can be impractical, especially if many iterations are necessary. Therefore, it is desirable to find methods to accelerate these tests. Most stored or shipped bulk material units (FIBC's, 25kg bags, etc.) experience a range of temperature fluctuations. In order to conduct accelerated caking tests, a thorough understanding of the changes inside the unit packages is critical. This paper will highlight an approach to investigate the conditions materials can experience while in prolonged storage or shipment, and will characterize the effects of those conditions on caking. Real examples of the application and usefulness of this approach, including experimental results, will be presented.

A novel method developed to measure tensile strength of cohesive powders

Vivek Garg, Tong Deng, Richard Farnish, Michael Bradley

The Wolfson Centre for Bulk Solids Handling Technology, School of Engineering, Faculty of Engineering & Science, University of Greenwich, Central Avenue, Chatham, Kent, ME4 4TB, UK

The tensile strength of a cohesive powder is defined as the minimum pull-off stress required to separate a powder bed, normal to the plane of failure, when stresses in the orthogonal directions are zero. It varies with the compaction level preceding failure. In principle, tensile strength should be one of the most sensitive means for comparing the flow behaviour of cohesive powders. However, direct measurement of the tensile strength of a powder is challenging to adequately accomplish. A new technique has been developed to measure the tensile strength of cohesive powders. Approaches for determining the value of tensile strength include extrapolation of the yield locus obtained from an annular shear tester, measuring the pull-off forces from a Wolfson Tester and measurements using Sevilla Powder Tester.

An investigation has been undertaken using eight different powders possessing disparate particle properties. The tensile strength measured was correlated with the particle adhesion forces measured using the Mechanical Surface Energy Tester. The comparison revealed that the tensile strength values indicated from the Powder Flow Tester measurements were an overestimation as compared to the direct measurements using the Wolfson Annular Sear Cell Tester and novel tensile strength tester. It is concluded that there is a strong correlation between the measured tensile strength and the adhesion forces measured using Mechanical Surface Energy Tester (whichalso shows a good agreement with conventional models based on the use of the Warren Spring tester).

Influence of particle size and void fraction on evaluation of flowability and cohesiveness of a test of powder discharge by air pressure

Koichiro Ogata[1], Daigo Ariga[2], Shunta Tsukuma[2], Yuuma Hirose[2]

[1]Dept. of Mechanical Engineering, National Institute of Technology, Oita College, Oita, Japan

[2] Dept. of Mechanical and Environmental System Engineering, National Institute of Technology, Oita College, Oita, Japan

Particulate materials are used in various industrial processes because they have the advantage of superior reactivity, having a large specific surface area. However, fine powder handling is complicated due to the influence of cohesiveness. Therefore, evaluating flowability and cohesiveness is essential to the better operation of powder handling processes.

This study has experimentally investigated the powder's flowability and cohesiveness by using a test of the powder discharge from an orifice by air pressure. The material used was the silica particles of 5 μm and 16 μm, which are called SI-5 and SI-16 in this study. The powder discharge was induced by the air pressure supplied from the top and the bottom of the powder bed. Flowability was evaluated from the mass flow rate and the square root of the average air pressure during the powder discharge. Cohesiveness was also characterized by the Bond number, which is the ratio of separation force to gravity. In addition, the powder discharge test results were compared with a powder tester and a powder rheometer.

It was found that higher pressure was required to discharge the silica with smaller particle size and lower initial void fraction. The trend of mass flow rate of the powder against the square root of the average air pressure was the same when the initial void fraction became small. Therefore, it was concluded with the results of a test of the powder discharge by air pressure that the flowability of SI-5 was lower than SI-16. It was confirmed that the Bond number of the small particle size was higher than that of the large particle. Also, the Bond number was increased by decreasing the initial void fraction. The obtained result indicated that the cohesiveness of SI-5 was higher than SI-16. These results revealed that the particle of small particle size and low initial void fraction exhibited lower flowability.

The correlation between our test result and the existing evaluation tests, such as the Powder Tester and the FT4 was also confirmed. The same evaluation result of cohesiveness and flowability was obtained from all the tests. This means the powder discharge test using air pressure can evaluate flowability and cohesiveness.

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Comparison of low-stress flowability measurement techniques: ball indentation and shear cell

Azza Aly-Mahmoud[1,2], Colin Hare[1,3], Chuan-Yu Wu[1], Ali Hassanpour[4]

[1] Chemical and Process Engineering, University of Surrey, Guildford, UK

[2] Physics department, Alexandria University, Alexandria, Egypt

[3] School of Engineering, Newcastle University, Newcastle upon Tyne, UK

[4] School of Chemical and Process Engineering, University of Leeds, Leeds, UK

Powder flowability plays a crucial role in achieving a reliable manufacturing process in several industries. Several commercially available techniques are well-known for assessing powder flow behaviour at moderate to high consolidation stresses, however low stress powder flow measurement, which is important for industrial processing such as die filling, is more challenging. Therefore there is still a need to reliably measure and understand powder flow behaviour at low stresses (< 1kPa). Shear cell and ball indentation flowability measurement techniques were chosen for this study. This work further develops and optimises the ball indentation technique for low-stress flowability assessment. The two measurement techniques were then compared in terms of the reproducibility and accuracy of the obtained results. For the ball indentation technique, different bed preparation methods, namely, wireconditioning, blade-conditioning, pre-shearing, and sieve-filling methods, were investigated and compared. Employing the more reproducible sieve-filling preparation method, unconfined yield stress results were determined at consolidation stresses between 0 and 2 kPa for Gypsum powder. In addition, the Schulze low-stress shear cell, RST-XS.s, was used for determining the material flow function at a similar stress range. Using the material flow functions obtained from both measurement techniques, in addition to other required bulk flow properties, two mass-flow hoppers were designed and fabricated to compare the accuracy of the two techniques at low stresses. From the obtained unconfined yield stress results, the shear cell based design resulted in a larger hopper outlet size compared to the ball indentation based design. Flow tests were carried out for Gypsum powder using both hoppers, using two different filling approaches: scooping and sieving filling. Interestingly, both hoppers resulted in a mass-flow with sieve-filling technique, while only the larger hopper allowed a mass-flow for non-sieved powder sample.

Measurement of particle contact area using a mechanical surface energy tester and influences of surface texture of powders on particle adhesion

Vivek Garg, Tong Deng, Richard Farnish, Michael Bradley

The Wolfson Centre for Bulk Solids Handling Technology, School of Engineering, Faculty of Engineering & Science, University of Greenwich, Central Avenue, Chatham, Kent, ME4 4TB, UK

Particle adhesion is an important influence in powder flow behaviour; however, usefully quantifying this contribution is difficult. The Wolfson Centre has developed a new method for assessing particle adhesion using a mechanical surface energy tester. The Bond number is used as an indicator of powder cohesiveness by detecting particle adhesion at the median particle size. Particle adhesion measurements are combined with particle physical properties such as particle size, shape, and density in this method. This measurement enables the development of a correlation between particle adhesion, powder cohesiveness, and bulk powder flow behaviour.

The current study focuses on particle adhesion measurement and the effect of particle surface texture on particle contact area and particle adhesion forces between particles. The investigation has been undertaken on 15 different materials with varying particle properties. The particle adhesion forces are correlated against the particle contact areas calculated using the common adhesion theory and measured using Inverse Gas Chromatography. The comparison reveals a strong correlation, which contradicts the accepted theory. The reason for this is that particle surface texture is thought to be important for apparent particle adhesion. SEM image analysis was used to examine particle surface texture, and a Malvern Morphology G3 has been used to measure particle size and shape.

It is concluded that the effect of surface texture needs to be considered while estimating the particle contact area. If particle surface energy is assumed to be constant, particle contact areas for adhesion measurements must be determined experimentally using methods such as the mechanical energy tester.

Flowability and granular compaction from industrial powders to frontier science seeking for the missing key

Maria-Graciela Cares[1], Maria-Camila Jimenez[1,2], Andrea Suaza Montalvo[1], Véronique Falk[1]

[1] LRGP-CNRS, Université de Lorraine, Nancy, France

[2] Dep. of Process Engineering, INRS, Vandœuvre-lès-Nancy, France)

After water, granular media is the most handled industrial material. Those who may work with granular media, fine or coarse, such as powders, know that powder flow is complex. From a technological point of view, granular flow is essential to processing efficiency as it affects many aspects of manufacturing, including flow-through hoppers, sieving, pouring, blending, milling, filling, compaction, tableting, transport, and even storage. Nonetheless, unlike elastic solids or fluids when referring to granular materials flow, many crucial, open questions arise as lack of a unifying definition and a well-understood theoretical basis. Powder's flow behavior is complex in nature because it is not an inherent property of the material. It depends on: the intrinsic and extrinsic properties of the grains such as size and shape distribution, stiffness, inelasticity, the equipment design, the processing conditions such as stress levels, the processing environment such as temperature and humidity. The multiple flow testers available in the market help compare powders' macroscopic properties but do not provide any flow dynamics information. The word "flowability" is usually misinterpreted as describing grains flow behavior, or it is device-dependent as it represents the ability to flow in the desired manner in a specific piece of equipment under specific mechanical conditions. Each device "estimates/quantifies" flowability through different parameters or indexes; although necessary in industrial development, the compilation of these measurements lacks a clear physical foundation. Several industrial and fundamental studies focus on the densification of granular systems as it covers many technological fields. We have recently shown that flowability assessment from volume fraction is exceptionally pertinent when studied using a global net force (or energy) approach by implementing innovative tools and methods. Force/Energy approaches are of great interest for understanding grains interactions and are suitable for powders modeling. From cement to flour, our group gathers robust scientific data evidencing that the nature of the flow seems to be extremely sensitive to the stiffness and inelasticity of the grains, and it's a kinetic problem. Under this basis, we will describe granular flow using packing densification under vibration and compression, highlighting common trends with well-known physical empirical laws while seeking the missing key between frontier science and industrial development.

Production of composite materials from spray drying and warm compaction

Sophia Rothberg, Swantje Pietsch-Braune, Stefan Heinrich

Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology, Hamburg, Germany

Bio composites as nacre or bone show outstanding mechanical properties which surpass those of their single components. This is due to their complex structure, in which the building blocks of the hard component are embedded in a soft matrix, thus combining strength and toughness. The combination of both properties makes such materials particularly interesting for various applications, e.g. for tooth or bone replacement materials. Therefore, there is great interest to develop scalable processes for the production of artificial composites with strong mechanical properties. In this work, metal oxide-polymer composites are produced by a spray drying process and a subsequent warm compaction. In the first step, sub-micron particles are encapsulated with polymer in the spray dryer (see Fig. 1). Through warm compaction of the encapsulated particles, a polymer matrix is formed where the hard metal oxide particles are embedded, thus mimicking the structure of bio-composites such as nacre. The main reasons for the outstanding mechanical properties in natural composites are the low organic content and the size of their single units. Therefore, it is of great importance to keep the product size as small as possible. This is realized by using the Nano Spray Dryer B-90 by Büchi where droplets are generated with a spraying membrane with a mesh size of only 7 µm. Furthermore, previous studies have already shown that the product size and the composition can be easily adjusted by varying the suspension formulation. A higher polymer content within the composite leads to weaker mechanical properties. For the production of tailor-made composites, different materials are used in order to determine the composite with the best mechanical properties. Therefore, different metal oxides as magnetite or alumina are used and both commercial polymers as poly vinyl butyral and more complex ones as vitrimers are tested. The mechanical properties are determined by three- and four-point bending tests.

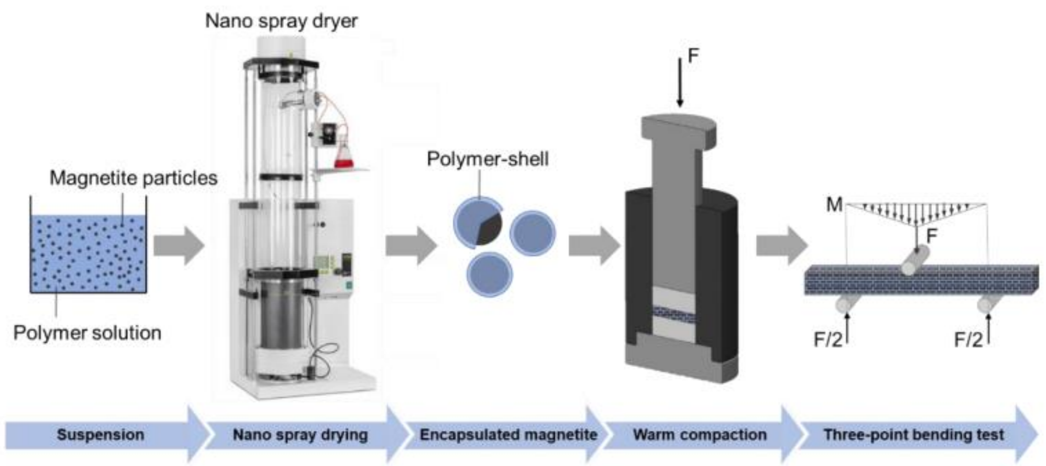

Fig. 1: Process route for the production and testing of composite pellets including spray drying, warm compaction and mechanical testing. We gratefully acknowledge financial support from the German Research Foundation (DFG) via the collaborative research center SFB986 (project number 192346071).

The Virtual Formulation Laboratory: a novel means to facilitate smooth transition of new powder formulations across the divide between formulation development and manufacturing

M. Bradley, C. Sinka, M. Ghadiri, J. Heng

Universities of Greenwich, Leicester, Leeds and Imperial

Resulting from a collaboration of three UK universities and a number of industry partners, the Virtual Formulation Laboratory is a suite of characterisation techniques and software models that together can predict the manufacturability of new powder formulations at an early stage. This can reduce the risk of costly and time consuming troubleshooting of powder processing problems arising when the new formulation is passed from development into manufacturing, by identifying, at the earliest stages of formulation, the need for either optimisation of the formulation design to reduce potential problems, or preparation of manufacturing lines that can cope with predicted challenging behaviour of the powder formulation.

Specifically , it deals with the most common difficulties that are encountered in the processing of powders, which are poor or inconsistent flow, segregation (de-mixing of blends) and compaction troubles. These problems are frequently found to be the cause of substantial financial losses when bringing a new or revised product to market, as they usually arise unexpectedly and can take a lot of time to solve, losing valuable time to reap the profit from a new product before patents expire and generic manufacturers move in to copy the product.

This paper will give an overview of the Virtual Formulation Laboratory, the development process behind it including some ground breaking science in powder behaviour and novel techniques for characterisation, and show some case studies of its use.

Predicting turbulent shear stress in pharmaceutical vessels

Róisín Hurley[1], Patrick Frawley[2]

[1]Dept. of Mechanical Engineering, University of Limerick, Limerick, Ireland

[2]Dept. of Aeronautical Engineering, University of Limerick, Limerick, Ireland

Crystallisation is a key unit operation for the separation and purification of pharmaceuticals. Batch crystallisation is typically carried out using seed crystals in mechanically agitated vessels. The crystal size distribution is recognised as an important indicator of crystal product quality [1]. Several mechanisms of secondary nucleation including breakage, attrition, contact nucleation and nuclei breeding may occur in a crystallisation vessel and contribute to the crystal size distribution. A narrow unimodal distribution increases the efficiency of downstream processing and smaller crystals are preferable for better dissolution properties and bioavailability [1] [2]. Crystallisation processes are difficult to scale up [3]. Mixing is an important mechanism to consider when designing a batch process for scale up. The growth and nucleation of individual crystals is dependent on the solution properties in the crystal microenvironment [3]. Mixing characteristics dictate the turbulent statistics in a crystallisation vessel as well as the environment for crystallization. A model of crystal nuclei breeding was proposed which describes clusters of solute molecules forming in solution that nucleate upon contact with the surface of seed crystals [4]. The nucleated solute molecules are weakly bound to the crystal surface and can be easily removed by fluid shear. In a mechanically agitated vessel within the turbulent mixing regime the turbulent shear stress is an important source of shear. The probability of crystal breakage is also influenced by the vessel hydrodynamics. Particle image velocimetry was used to accurately measure the hydrodynamics for several crystallisation vessels, impeller types and agitation speeds. The maximum turbulent shear stress (TSS) was related to the measured process input parameters. Knowledge of the distribuion of TSS combined with a mechanistic model [6, 7], would allow for the design and scale-up of a crystallisation process that controls and optimises secondary nucleation. Thus, a desired product could be achieved, reducing the need for downstream processing, and increasing process efficiency.

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A regime map for dry powder coating

Marv Khala[1], Colin Hare[2], Vikram Karde[3] and Jerry Heng[3]

[1]Dept. of Chemical & Process Engineering, University of Surrey, Guildford, UK

[2]School of Engineering, Newcastle University, Newcastle upon Tyne, UK

[3]Dept. of Chemical Engineering, Imperial College London, London, UK

Coatings are widely used in industry as a surface modification technique to improve flowability or manufacturability of powders. Dry powder coating is often preferred over the conventional solvent-based coating due to improved process safety and environmental friendliness (zero emission of volatile organic solvents), lower energy consumption (solvent evaporation not required), suitability for moisture sensitive materials and overall lower manufacturing costs. However, the dry powder coating process is often wasteful as an excessive amount of coating powder and energy input are typically required to ensure sufficient coating is achieved. In this study, the Discrete Element Method (DEM) is used to simulate the dry powder coating process in an impeller-agitated system. The effects of mixer operational conditions (blade design, blade rotational speed and fill ratio) and material properties (size, density and surface energy) on coating performance are investigated. A regime map for dry powder coating is developed to define the operational window for uniformly distributed coatings. The regime map gives useful understanding and knowledge of optimal combination of key parameters for good coating performance, thus providing precise control of the quantity of coating material and the energy input required.

Investigating particle properties and process parameters for generating efficient dry particle coated system

Vikram Karde[1], Marv J. Khala[2,3], Colin Hare[3], Jerry Y. Y. Heng[1,4]

[1]Department of Chemical Engineering, Imperial College London, London, U.K.

[2]Department of Chemical and Process Engineering, University of Surrey, Guildford, U.K.
[3]School of Engineering, Newcastle University, Newcastle, U.K.

[4]Institute of Molecular Science and Engineering, Imperial College London, London, U.K.

Particle properties and powder mixing conditions are critical to achieving efficient dry powder coating. The present work investigates different particle properties (size, morphology and surface energy) and operation parameters (mixing speed and time) which are critical to the dry coating process. This was achieved by employing four different guest-host combinations comprising lactose monohydrate and paracetamol as host particles and nanosilica and magnesium stearate as guest particles. These uncoated and coated particles were characterised for a range of properties like size using particle size analyser, morphology using scanning electron microscopy (SEM), surface chemistry using X-ray photoelectron spectroscopy (XPS) and surface energy using finite dilution inverse gas chromatography (FD-IGC). The efficiency of the dry particle coating process was also examined from the percent surface area coverage (%SAC) estimation through image processing. In addition, dynamic (flow energy test) and quasi-static (shear test) flow measurements were done on the uncoated and surface modified powders using an FT4 powder rheometer. The results show that the nanosize guest particle (nanosilica) was more effective in coating the host surfaces accompanied by an overall improvement in powder flow. Moreover, experiments were also conducted using iron oxide guest particles as a coloured tracer to validate the efficiency of the mixing set-up and operation parameters employed for dry coating. Furthermore, in a series of order of mixing studies with ternary powder systems, the importance of the order of addition of individual powder components during mixing was highlighted through imaging and colorimetry measurements.

Water storing bulk granular materials for concrete 3D printing

Leigh Duncan Hamilton[1], Sandra Breitung-Faes[2], Arno Kwade[3]

[1,2,3]Institute for Particle Technology, TU Braunschweig, Braunschweig, Germany

Key words: Additive manufacturing, water storage, dry water, granular material, flowability

The ever-growing demand for sustainable development within the construction sector has led to several innovative approaches. One such approach includes additive manufacturing (AM), whereby economical as well as ecological benefits are procured. AM in construction has the potential for higher efficiency in material usage. Furthermore, the capability of producing free-form structures without special moulds or tools leads to near independency of production cost and complexity of components. The project at hand is part of the collaborative research centre "TRR 277 Additive Manufacturing in Construction (AMC)" and involves a combination of two AM processes in order to create reinforced concrete. Firstly, Selective Paste Intrusion (SPI) is a particle-bed based AM technology, which constructs components by spreading an aggregate layer of coarse sand on a surface. Subsequently, the cement paste is extruded locally at the appointed areas. These steps are repeated until the desired element is completed. In order to qualify SPI for structural concrete, steel reinforcement must be integrated. Hence, Wire Arc Additive Manufacturing (WAAM) is combined with SPI. WAAM can create steel reinforcement by using arc welding. However, high temperatures during WAAM generate heat transfer into the particle-bed, consequently reducing water in the cement and decreasing concrete strength. For that reason, the present research intends to develop tailored aggregate sand particles that store water, and thus, compensate for water loss as well as promote cooling. It is hereby of utmost importance to maintain sufficient bulk properties for SPI in order to create consistent components regarding strength and shape accuracy. One possible solution arose with dry water, which is classed as a free-flowing, water-rich powder, storing up to 98 wt.% of water. Essentially, dry water consists of water droplets that are encapsulated with hydrophobic silica nanoparticles. Dry water is implemented into the bulk material by mixing, thereby storing water in the bulk with the potential of sustaining the initial flow and bulk properties. The integral part of this study is to investigate the influence of different mass-related variants of dry water as well as varying the water contents within the aggregate bulk material. For process related reasons, the main methods of analysis are the dynamic and static angle of repose as a measure of flowability. Additional analysis is conducted by drying the bulk material and investigating its behaviour towards agitation. This is executed by tapped and bulk density measurements. A critical question regarding the encapsulated water and its progression during the complete mixing process does occur. As a result, micro-computed tomography (µCT) and scanning electron microscope (SEM) are applied for image analysis.

Development of hyperspectral imaging classification model applied to the recognition and sorting of post-earthquakeconstruction waste

G. Bonifazi[1], O. Trotta[1], G. Capobianco[1], S. Serranti[1]

[1]Department of Chemical Engineering, Materials & Environment, Sapienza – University of Rome, Via Eudossiana, 18, 00184 Roma, Italy

[2]Research Center for Biophotonics, Sapienza University of Rome, Latina, Italy.

One of the major resource-consuming, and waste-producing sectors, in our modern society is the construction sector. More than 40% of the total raw materials extracted from the earth around the world, generate more than one-third of the world's solid waste by weight (up to more than 75% when excavated soil is accounted for, and are also responsible of approximately one-third of the total CO_2 and greenhouse gas emissions. Moreover, natural disasters, such as earthquakes, create significant volumes of rubbles and waste, strongly impacting the environment and posing health risks.

In recent years earthquakes have been among the most recurrent natural disasters in Italy. In particular, three seismic events hit four Italian regions from August 2016 to January 2017, including 8.000 sq km of territory and involving 140 municipalities, and produced 2.720.000 tons of waste. Such a material can be considered as Construction and Demolition Wastes (CDWs), composed by about 60-70% by weight an inert fraction, presenting a high potential for recycling and reuses since some of its components can represent, if properly separated, recovered and recycled, an important resource, thus avoiding non-renewable raw materials exploitation and favoring the circular economy. In this prospective, new technologies are needed for the characterization, sorting and quality control of CDWs derived products.

In this paper, the possibility to implement fast, low cost and reliable strategies addressed to classify different CDWs as resulting from the collapse of buildings due to an earthquake was investigated. The use of innovative sensing techniques, combined with classical mechanic processing, could represent an important step forward to prevent landfilling and to improve recycling.

A method based on hyperspectral imaging (HSI) to classify different types of CDWs coming from buildings damaged by an earthquake, is presented. Hyperspectral imaging (HSI) was applied based on the utilization of a platform working in the SWIR range (1000-2500 nm). The acquired hyperspectral images were analyzed by applying different chemometric methods: principal component analysis for data exploration and partial least-square-discriminant analysis to build classification models. Results showed that the proposed approach is particularly suitable to perform "complex" CDWs classification as produced by earthquakes, allowing to recognize and classify not only the different inert fractions (i.e. concrete, brick, aggregates and ceramic materials) from contaminants (i.e. wood, plastics and glass) but also to characterize the different inert fractions according to their chemical composition. The obtained results can represent an important starting point for further development of fully optical HSI based recognition CDWs procedures to be utilized both off-line (i.e. the analytical level at laboratory scale) and on-line (i.e. sorting level at industrial scale).

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COMPUTATIONAL MODELS

Resolved simulation of particle collisions on wet microstructured surfaces

David Strohner[1], Sergiy Antonyuk[1]

[1]Technische Universität Kaiserslautern, Institute of Particle Process Engineering, Kaiserslautern, Germany

During particulate processes collisions have a big influence on the overall particle dynamics resulting in energy dissipation or even sticking. In many processes like for example coating or agglomeration, a liquid is used which will cover the component or particle surfaces with a liquid layer causing additional energy dissipation. This dissipation is described by the coefficient of restitution which is an important input parameter for the simulation of particle processes. It can be determined by single particle collision experiments using high speed cameras to observe the particle dynamics [1]. The coefficient of restitution will decrease with higher liquid layers or higher viscosity due to viscous forces acting on the particle inside the layer during approach and rebound [2]. For the investigation of micro mechanisms during the particle collision, resolved simulations can be performed. Therefore, CFD simulations are suitable which can be either coupled to DEM or rigid body methods to resolve the particle [3]. An influencing factor that also needs to be considered is the morphology of the interacting surface. Micro structured surfaces can be used, to affect the particle rebound behavior. As the shape of these surfaces can be determined by the manufacturing method, regular surfaces can be generated. This enables to generate specific contact situations during the particle impact depending on the surface structure. In this study a regular topography is used to investigate its effects on wet particle collisions. CFD simulations are performed (figure1) resolving the particle as a rigid body using an overset mesh method recreating different contact situations during the particle impact. This data is then compared to experiments to determine the effects of the surface morphology on fine microparticles during impacts on thin liquid layers.

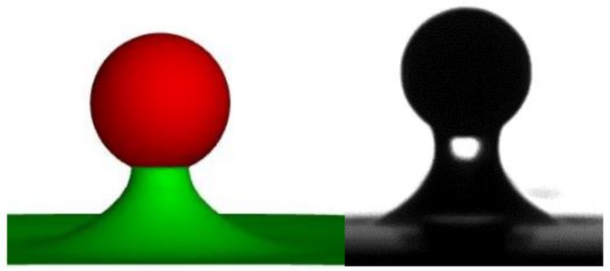

Figure 1: Simulation and experiment of particle collisions on a liquid layer

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Development and application of BPM-DEM to study mechanics of frozen granular materials

Tsz Tung Chan[1], Jürgen Grabe[2], Stefan Heinrich[1], Maksym Dosta[1]

[1] Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology (TUHH), Hamburg, Germany

[2] Institute of Geotechnical Engineering and Construction Management, Hamburg University of Technology (TUHH), Hamburg, Germany

Frozen Particle Fluid System (PFS) plays an important role in both natural and technical systems. Under freezing conditions, solid bonds (ice bridges) formed between particles, which alternate the mechanical properties (such as breakage stress, strain and stiffness) of the fluid saturated or moisturized PFS. In this project, the behaviour of the bridge area (single bond) and capillary area (multi-bonds) have been investigated. Bonded particle method (BPM) which is an extension of discrete element method (DEM) and which was widely used for modelling of various materials, has been used to describe the mechanical behaviour of the frozen PFS. In the experimental part, a climate chamber has been created for maintaining ambient temperature and coupled with TA.XT plus Texture Analyzer (Stable Micro Systems, Great Britain). Ice mechanical properties are greatly influenced by temperature, strain rate and grain size. Such effect also dominates the mechanical behaviour of frozen PFS, which alternation in temperature, volumetric content and strain rate lead to ductile, brittle or dilatant behaviour. These major factors have been covered by our experimental studies. In experiments, spherical particles (glass, alpha alumina, polymer), as well as non-spherical particles (quartz sand, I-SSO-sand) have been used. From the experiments, different material response were reviewed under varied strain rates, temperatures and saturation levels. The open-source DEM simulation framework MUSEN has been used for numerical investigation of PFS behaviour. To describe visco-plastic sample behaviour, a new rheological model of solids bond has been formulated. The new solid bond model combines the strain-dependent and time-dependent material behaviour for describing the complex rheological behaviour. The calculations in MUSEN are parallelized for graphic processing units that has allowed to perform simulation of large samples in a relatively short period of time. Obtained simulation results such as breakage strain or breakage stress are in good agreement with the experimental data. Moreover, experimental and numerical samples reveal similar breakage behaviour in 100% saturation level of frozen PFS. However, more significant deviations were observed from the modelling of PFS in lower degree of striation level.

ACKNOWLEDGEMENTS

The funding of the presented research in the framework of research training group GRK 2462 by German Research Foundation (Deutsche Forschungsgemeinschaft, DFG) is gratefully acknowledged.

Multi-Scale and Multi-Physics Modelling of particle and fluid-particle flow using DEM and CFD-DEM

Christoph Goniva, Riccardo Togni, Marcel Kwakkel and Christoph Kloss

DCS Computing GmbH, Linz, Austria

Discrete Element Method (DEM) and DEM coupled to Computational Fluid Dynamics (CFD-DEM) are established techniques for optimization and design of particle processes. Granular particles, the flow involving fluids and granular particles are everywhere - in industry, environment and everyday life. Sugar, sand, ores, tablets, chemicals, biomass, detergents, plastics, crops, fruits need to be harvested, produced, processed, transported and stored. While in the past, DEM and CFD-DEM software were tailored to a narrow field of application, modern software implementations allow for real multi-scale and multi-physics application. We give an overview of recent developments in the frame of the DEM and CFD-DEM software ASPHERIX®.

Processes that are driven by physics spanning a wide range of time and length scales are very challenging when it comes to numerical modelling as they require very detailed temporal and/or spatial resolution leading to enormous computational costs. We present different solution strategies allowing to bridge time or length scale and thus successfully model these processes. We give examples for successful application of integrated 3D-1D CFD-DEM modelling to model a plant scale chemical reactor. Further we highlight an integrated numerical approach combining particle-resolved and unresolved approach to capture soil erosion process. In particular, we summarize recent implementations and validation efforts regarding non-spherical shape representation in granular and fluid-granular systems, modelling and handling of soil, multi-scale modelling of chemical reactors and multi-scale modelling spray-drying process.

Tensor-based coarse graining method

Zorica Ristic[1, 2], Arno Mayrhofer[2], Stefan Radl[1]

[1] Institute of Process and Particle Engineering, Graz University of Technology, Graz, Austria

[2] DCS Computing GmbH, Linz, Austria

The Discrete Element Method (DEM) is extensively used both in academic research of granular systems as well as in industrial applications. As most real-world systems are comprised of several billion particles, direct simulation tends to be challenging. Thus, many DEM applications use different coarse graining approaches where groups of finely-grained, Original Particles (OPs) are represented by simulated particle representatives – Coarse-Grained Particles (CGPs). However, most such approaches are based on assumptions about material properties of CGPs including the matter-void distribution within them, as well as their contact model. Often both material properties and contact model of CGPs are simply transcribed from OPs with an addition of scaling laws for contact parameters. The latter in turn impose restrictions regarding analytical upscaling. The present contribution presents an approach to coarse graining based on various tensor variables representing the systems state and is therefore called the Tensor-based Coarse Graining Method (TCGM). It stipulates that the movement of the systems bulk comprised of CGPs mimics the movement of the same bulk when comprised of OPs. Moreover, TCGM is agnostic of the underlying contact model and makes no assumptions about the CGPs' material properties, all to ensure applicability to a wide range of granular flows. In order to recover the contact force network, a connection between tensor variables, such as contact fabric, stress and strain tensors, is used. This connection allows the recovery of the per particle and per interaction stress tensors which, when combined with strain tensor information, yield contact forces. The reconstructed contact force network preserves the form of key physical laws. From the reconstruction it is deduced that, for every CGP, an additional external force term arises due to the change of particle representation from original to coarse-grained one. Statistics regarding these additional force terms for different coarse graining ratios in oedometric compression tests are displayed in our present contribution.

Keywords: Discrete Element Method, coarse graining, contact force network, fabric tensor, oedometric compression

On the use of coarse-graining to bridge the discrete and continuum descriptions of granular materials

Hongyang Cheng[1], Stefan Luding[2], Thomas Weinhart[2]

[1]Department of Civil Engineering, Faculty of Engineering Technology, MESA+, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

[2]Multi-Scale Mechanics (MSM), Faculty of Engineering Technology, MESA+, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

Surface and volume coupling methods are reformulated for concurrent multi-scale modeling of granular materials. Based on a micro-macro transition technique called ``coarse-graining'' [1], we derive homogenization operators in more generalized forms than those reported in the literature. For surface coupling [2], coarse graining allows distributing the coupling forces beyond the finite elements that the particles are locally coupled with, namely, from contact points to their neighboring integration points. For volume coupling [3], coarse-graining is applied to enrich the homogenization/localization operations on particle-scale quantities, thereby offering a non-local coupling approach. The generalized coupling terms contain one user-defined parameter, namely, the coarse-graining width, setting a length scale for the "coarse-grained" fields.

The benefits of coarse-graining in surface and volume coupling are exemplified by modeling particle-cantilever interaction and wave propagation between discrete particles and continuum bodies. We show that the CG-enriched new formulation removes high-frequency/short-wavelength numerical oscillations and gives more physical predictions in the example of particle-cantilever interaction, compared with the conventional formulation using finite element basis functions. In the wave propagation example, the numerical dissipation, which is a known artifact of the volume coupling method, is reduced with an optimal coarse-graining width. In particular, the benefit of coarse-graining appears to be significant when the waveforms become increasingly complex and contain high frequency contents.

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Modelling hopper discharge of elongated particles with different shape representation methods

Marina Sousani[1], Stefanos-Aldo Papanicolopulos[2], Andreas Piskopakis[1], Timothy Heelis[1]

[1]EDEM, Altair Engineering Ltd, Edinburgh, United Kingdom

[2]School of Engineering, Institute for Infrastructure and Environment, The University of Edinburgh, Edinburgh, United Kingdom

The design of bulk material handling equipment in many industrial and process engineering applications is directly linked to the understanding of the material's behaviour. Hoppers are an important part of the chain since their smooth usage dictates whether the downstream process of the final product will be successful or not. Therefore, investigating the flow and the parameters that affect the discharge rate of the material play a crucial role in the design process. Over the years many researchers have looked at the material flow in hoppers by using spherical particles in the Discrete Element Method (DEM) [1-7]. However, fewer have focused on the behaviour of non-spherical elongated particles. Since most of bulk materials have complex shapes, it is important to understand the flow, interaction and kinematics of particles other than spheres. The proposed work uses DEM and replicates real-life elongated materials by using sherocylindrical particles that flow through a wedge-shaped hopper. Different aspect ratios have been employed in this work and the results have been compared against experimental studies as well as correlations reported in literature [8]. Furthermore, the DEM simulations have been repeated with equivalent multi-sphere and polyhedral particles, investigating the effect of different shape representation methods on the overall flow and discharge rate of the material.
Acknowledgement: This research has received support from the Industrial Fellowship scheme of the Royal Academy of Engineering.

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Effect of coarse-grain scaling in Discrete Element Method (DEM-CFD) modelling of CFB riser reactors

Erasmo S. Napolitano[1], Alberto Di Renzo[1], Francesco P. Di Maio[1]

[1] DIMES Department, Università della Calabria, Rende (CS), Italy

In the last two decades, the circulating fluidized beds (CFB) have seen their field of application expanded with the possibility to be used as gas-solid polymerization reactors. One of the engineering challenges concerns the hydrodynamics in the riser section: the fast fluidization regime is typically adopted to achieve the required contact of the monomeric gas phase with the solid particles on which the polymerization reactions occur. At the same time, the gaseous phase acts as heat dissipation carrier for the exothermic reaction. With insufficient contact (e.g. clustering) or stagnant areas, local temperature hotspots may form that involve melting and agglomeration of the particles, which can lead to the shutdown of the entire plant. In medium to large systems, as in case of industrial applications, accurate numerical models based on the DEM-CFD approach remain prohibitive due to the high number of particles involved and the corresponding computational cost. In recent years, methods have been proposed to reduce the number of particles by grouping them into representative particles, called parcels, to increase the size and reduce the number of elements and the corresponding computational burden. Despite the success of early attempts, much remains to be understood and characterized, such as the extent to which the predictive capability of the model is preserved also in complex flows and geometries. In the present work, coarse-graining methods and degree for solids in DEM-CFD simulations are investigated to model the two-phase hydrodynamics in a CFB riser with a lateral inlet at different solid and gas loads. The computational savings is examined first. Then, as far as accuracy is concerned, the effect of scaling of particle parameters, such as contact (elasticity, damping, sliding / rolling friction) and drag, is analyzed separately. The influence of the scaling strategy has been verified on the replicability of the results with respect to the pure DEM-CFD simulations. Macroscopic performance indicators, such as pressure drop and solids loading, and local distribution of gas and solid flows within the riser are examined and compared. The computational savings are eventually discussed in the light of the acceptable level of predictive ability of the computational model.

MercuryDPM: Fast, flexible, particle simulations

Anthony R. Thornton[1,2], Thomas Weinhart[1,2], et al.[3]

[1]Thermal and Fluid Engineering (ET), University of Twente, Drienerlolaan 5, 7500 AE Enschede, The Netherlands,

[2]MercuryLab, Mekkelholtsweg 10, 7523 DE Enschede, The Netherlands.

[3]A full list of contributors can be found here: https://www.mercurydpm.org/about-this-code/team

We introduce the open-source package MercuryDPM, a code for discrete particle simulations, that we are developing [1]. It simulates the motion of particles, by applying forces and torques that stem either from external body forces, (e.g. gravity, magnetic fields, etc...) or from particle interaction laws. For granular particles, these are typically contact forces (elastic, plastic, viscous, frictional). MercuryDPM is an object-oriented C++ algorithm with an easy-to-use user interface and a flexible core, allowing developers to quickly add new features. It is parallelised using both MPI and OpenMP and released open-source under the BSD 3-clause licence. Its developers' community has developed many features, including moving (wearable) curved walls (polygons, cone sections, helices, screw threads, level-sets, nurbs, triangulated, etc); state-of-the-art granular contact models (wet, charged, sintered, melting, cohesive, etc); specialised classes for common geometries (inclined planes/chutes, hoppers, etc); non-spherical particles (multisphere, superquadric, bonded particles, deformable clusters); general interfaces (particles/walls/boundaries can all be changed with the same set of commands); liquid droplet/spray models; STL readers for industrial geometries; restarting; visualisation (xBalls and Paraview); a large self-test suite; extensive Doxygen documentation; and numerous tutorials and demos. For efficiency, it uses an advanced contact detection method, the hierarchical grid. This algorithm has a lower complexity than the traditional linked list algorithm for polydispersed flows, which allows large simulations with wide size distributions. It also contains a coarse-graining tool: MercuryCG, which is both integrated and usable as a stand-alone tool. Coarse-graining is a novel way to extract continuum fields from discrete particle systems. It ensures by definition that the resulting continuum fields conserve mass, momentum and energy, a crucial requirement for accurate coupling with continuum models. The approach is flexible and the latest version can be applied to both bulk and mixtures; boundaries and interfaces; time-dependent, steady and static situations; and, even experimental data. It is available in MercuryDPM either as a post-processing tool, or it can be run in real-time, e.g. to define pressure-controlled walls. Finally, MercuryDPM is coupled with the open-source FEM solver oomph-lib via the integrated coarse-graining tool. There are many uses of this coupling (in development), including interaction with elastic bodies, both fully and unresolved fluids, and heterogeneous multiscale coupling. We will demonstrate the features of the code via several examples including: (wet) highly-polydisperse mixing in a rotating drum, wear on vibrating sieves, and sack filling.

Visit https://mercurydpm.org for more information about MercuryDPM. Training and

consultancy is available via our spin-off company MercuryLab (https://mercurylab.org).

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Triaxial testing for granular materials using the Discrete Element Method

John P. Morrissey[1], Stefan Pantaleev[1,2], Jin Y. Ooi[1]

[1] School of Engineering, University of Edinburgh, Edinburgh, UK.

[2] Altair EDEM, Edinburgh, UK

Granular materials are extremely common with approximately 80% of all industrial material feedstock being granular in nature. Triaxial tests are commonly used to evaluate the mechanical response of geomaterials under loading and can be applied to all granular materials providing valuable information on the materials behaviour. Discrete Element Method simulations of such tests have been carried out with the aim of gaining insight into the micro and macro- mechanical responses of the material under the triaxial stress application. In this paper, the DEM simulations of monotonic triaxial tests including the membrane boundary condition are presented. The simulations attempt to model railway ballast with and without geogrid reinforcement and these are compared with experiments for validation. A common approach in modelling is to apply loading to a representative volume of a material with periodic boundaries instead of modelling the physical boundaries. In this case the effects of the rigid piston and flexible membrane in a triaxial test are ignored. If the physical test is modelled, the boundary conditions are sometimes imposed by using rigid geometric assemblies to compress the sample or by applying forces directly to the sample. Both approaches ignore the presence of the flexible elastic membrane and the associated boundary condition effects which can lead to a poor representation of the physical test. In this study the membrane boundary of the triaxial test is modelled using a bonded assembly of particles to model the flexible membrane and investigate the effect of the membrane stiffness on the bulk stress-strain response. The confining pressure to the sample is achieved by applying individual forces to the bonded membrane particles to simulate a uniform radially inward equivalent stress. A coarse-graining analysis is performed to study the evolution of the internal stress field in the sample during loading. The influence of geogrid reinforcement in the ballast is also studied by comparing the results with and without the geogrid. The geogrid is modelled as a bonded assembly of particles that is calibrated against experimental measurements. The modelling approach leads to a close agreement with published experimental data on the railway ballast. The DEM model is also able to determine the stiffening effect of the rubber membrane used in the experiments, allowing for an improved interpretation of the test results. The computed internal stress field reveals significant stress non-homogeneity which provides useful insights of the evolving state of stress in the ballasts during its loading to failure.

Coupling of DEM and flowsheet simulations for screen mills in roller compaction process

Christian Eichler, Maksym Dosta, Stefan Heinrich

Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology, Hamburg, Germany

Dry granulation is an economical process to improve the flowability of heat and moisture sensitive powders. Roller compaction enables a continuous process to compact powder between two counterrotation rollers into ribbons. Afterward, these ribbons are comminuted by rotating or oscillating screen mills into any desired granule size. Flowsheet simulations offer an essential opportunity towards high Quality by Design products. However, the simulational comminution part bases commonly on empirical testing, which deterministic Discrete Element Method (DEM) simulations can supersede since the DEM allows mapping the ribbon's breakage behavior. Therefore, this study targets the complementation of comminution units of flowsheet simulations by coupling with DEM. The DEM simulations were performed in the open-source GPU-accelerated simulation Framework MUSEN, and flowsheet simulations utilized a python framework.

The DEM simulations used a bonded particle model to reproduce the breakage behavior of ribbons. During milling, the ribbon's main loads are caused by bending and compression. Therefore, three-point bending and compression tests of lactose tablets were performed experimentally and compared to simulations to calibrate DEM parameters. The focus of the calibration lay on the dependencies of tablet porosity on Young's modulus and breakage strain, respectively.

The milling process was implemented in DEM, as seen in Figure 1, and the particle size distribution passing the sieve was analyzed. Ribbons of different geometries and porosities were implemented, and machinery parameters like screen size and rotor velocity were variated. The results feed a database directly coupled to the flowsheet framework.

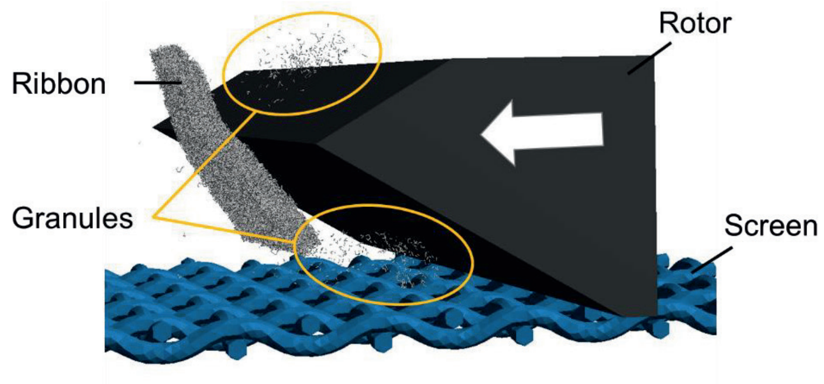

Figure 1: Simulation of ribbon breakage in abstracted rotating screen mill.

Benchmark of different discrete particle models for the simulation of pneumatic conveying of additive manufacturing metallic powders

Lorenzo Pedrolli[1*], Alejandro López[1], Inger Martinez de Arenaza[1], Beatriz Achiaga Menor[1]

[1]Dept. of Mechanics, Design and Industrial Organization, University of Deusto, Bilbao, Spain * corresponding author: l.pedrolli@deusto.es

Direct Metal Additive Manufacturing (DMAM) is becoming increasingly important in industrial manufacturing. Of the many technologies, this study is aimed to Laser Metal Deposition (LMD): in this process, a laser melts a stream of powder metal on a substrate to build solid objects layer by layer. The delivery of such powder is critical to the final quality of the parts produced. A good understanding of the flow characteristic in the pneumatic conveying is imperative to operate and design LMD systems, and the ability to analyze the process in detail is key to the increase of its capabilities and sustainability. This study presents a benchmark of current simulation models based on different Euler-Lagrange approaches for multiphase gassolid flows, such as CFD-DEM, MP-PIC, Lattice Boltzmann, both from commercial and opensource codes. An exploration of the parameters in the characteristic range of the pneumatic conveying of metal powders in the LMD process serves as a standardized benchmark for the comparison between the models, identifying the appropriate setup for each model, to obtain physically significant results. Special attention is posed to the particles' interaction models, using the material properties of the stainless steel 316L powder, with a Rosin-Ramler size distribution of the grains between $45\mu m$ and $150\mu m$.

Analysis of micron-sized particle emission from the capsule of a Dry Powder Inhaler through DEM simulations

Francesca Orsola Alfano[1], Alberto Di Renzo[1], Francesco Paolo Di Maio[1], Martin Sommerfeld[2]

[1] DIMES Department, University of Calabria, Cosenza, Italy

[2] Fakultät für Verfahrens- und Systemtechnik, Otto von Guericke University, Magdeburg, Germany

Pharmaceutical devices based on powdered formulations are relatively common. In Dry Powder Inhalers (DPI), particulate materials formed by excipients and active pharmaceutical ingredients (API) are delivered to the body using the respiratory system. In some devices formulations are prepared using directly fine powders. In others, larger size carrier particles coated with API powder are utilized to improve the flowability during both manufacturing, processing and aero-dispersion during inhalation. The performance of capsule-based DPI is highly influenced by the discharge process from the capsule itself. However, due to the unrealistically large computational cost associated to the entrainment of a considerable number of particles, the process is often overlooked in modelling studies. In the present contribution, the powder de-aggregation and discharge from a hard-shell capsule-based Dry Powder Inhaler has been analyzed through DEM simulations (Figure 1). The accelerated rotational motion of the capsule was simulated considering the point of view of a non-inertial internal observer by rotating the force of gravity and appropriately considering the contributions of fictitious forces. This approach allowed for a punctual mapping of the particle-wall collisions within the capsule. Finally, simulations were carried out on drug-carrier blends, considering adhesive interactions and evaluating the early-stage dynamics of the detachment process that occurs inside the capsule due to the interactions among the particles and with the walls.

a) b)

Fig. 1. Position of the powder in the inhaler hard shell capsule a) before dispersion, b) during dispersion.

Wear deformation prediction of convex pattern surface using DEM

Yunpeng Yan[1], Rudy Helmons[1,2], Craig Wheeler[3], Michael Carr[3], Dingena Schott[1]

[1] Department of Maritime and Transport Technology, Delft University of Technology, 2628 CD Delft, The Netherlands

[2] Department of Mineral Processing and HSE, Norwegian University of Science and Technology, 7031 Trondheim, Norway

[3] School of Engineering, The University of Newcastle, Callaghan 2308, Australia

A convex pattern surface has been proposed [1] and optimized [2] to reduce the sliding wear of bulk handling equipment, by adjusting the flow behaviour of the bulk material. Laboratory tests by a circular wear tester indicate that such a convex pattern sample reduces wear by 57% compared to a flat sample, after running for 40 hours. In this study, a short timescale numerical model is developed to compare with a laboratory test results on longer timescale. We combine the discrete element method (DEM) with an Archard wear model and a deformable geometry technique to capture the sample deformation. With this model, we investigate how the short term numerical result should be scaled to be applicable for long term wear tests. The results include stability analysis of the simulation setup, numerical wear coefficient selection and wear result comparisons. Stability of the simulation setup is analysed by evaluating the flow behaviour of the bulk material and the wear rate of the sample. The wear coefficient will be obtained by comparing the wear volume and wear profile with the experimental results. The wear distribution and the deformation of the sample will be reconstructed to analyse the effect of the convex pattern sample on wear reduction. We will evaluate to what extent the wear on long timescales can be predicted by means of a short timescale numerical model.

Keywords: wear; convex pattern surface; scaling factor; deformation; DEM

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FRIDAY, 8 JULY 2022
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INDUSTRIAL CASE STUDIES

Improving a pneumatic conveying system for coffee beans to reduce attrition

Harald Wilms[1], Sebastian Husheer[2]

[1]Wilms-ITC, Innovation-Technology-Consulting, Bremen, Germany

[2]Jacobs Douwe Egberts DE GmbH, Bremen, Germany

The required change of a compressor for an existing pneumatic dense-phase conveying system for roasted coffee beans offered the opportunity to re-check the existing system with respect to design parameters and to look for potential improvements regarding the reduction of particle attrition. The pneumatic calculations were revisited to check the possibility to reduce the conveying velocity – one major factor in breakage of the coffee beans. Additionally, the internal surface of the existing carbon steel conveying line was optically checked by a video camera to reveal potential wear, corrosion, or surface degradation. The conveying system was improved regarding air flow rate and routing of the terminal section. Due to available pressure reserves from the compressor, an upstream conveying system was integrated into the conveying system in question, reducing handling and dosing operations. The revamping resulted in a considerable reduction of fines and simultaneously in a significant reduction in energy consumption with associated CO_2-reduction. The reduced attrition resulted in a considerable operating cost reduction and thus yielded a short pay-back period of the upgrading. This study and revamping demonstrates the benefit of revisiting and improving older conveying system design with respect to performance and efficiency.

Leveraging Artificial Intelligence to speed up DEM simulations: A wheel loader case study

Spyridon Mallios, Marina Sousani, Livio Mariano

Altair Engineering, Troy, Michigan, United States

The vast majority of industrial engineering applications can be formulated as a multiphysics problem. Such applications can be tackled by engineers through high fidelity co-simulations. Though, these co-simulations, while accurate, might be complex to set up and are computationally expensive, making them not suitable in the design stage or in an optimization framework. Moreover, when DEM solvers are included in the co-simulations, these get even slower.

This paper shows a new methodology, based on artificial intelligence (AI), to replace the computational expensive DEM portion with a fast and accurate dynamical reduced order model. This methodology is carried over through a wheel loader example.

The wheel loader has been originally modeled and simulated through a co-simulation between hydraulics, controls, multibody, structural and DEM solvers. This model has been used as reference for the next steps. From this model, the DEM portion, which rules the interaction between the wheel loader bucket and a pile of bulk material, has been extracted. Then, some DEM transient simulations have been run, slightly varying the kinematics imposed to the wheel loader bucket. These DEM simulation results have consequently be leveraged to train an AI-driven dynamic reduced order model, capable of representing the interaction between the bulk material and the wheel loader bucket. Finally, the dynamic reduced-order model (ROM) has been inserted back in the original model, replacing the DEM portion.

At the end, in order to assess the accuracy of the new wheel loader model including the ROM a validation simulation has been run and its results have been compared with the one obtained from the reference model. In particular, the maximum Von Mises stresses on the boom and the maximum actuator forces have been compared. The difference has shown to be less than 1.3% for the stresses and 1.4% for the actuator forces. But the model including the ROM runs 30 time faster than the reference one, making it suitable for design studies and optimizations, such as of the hydraulic circuit.

Keywords : co-simulations, Reduced-Order Model, AI, DEM, system simulation

Innovations in particle technology modelling to improve industrial product development

Stefan Bellinghausen[1], Dana Barrasso[2], Sean K. Bermingham[1]

[1] Siemens Process Systems Enterprise Ltd., London, UK

[2] Siemens Process Systems Enterprise Inc., Parsippany, NJ, USA

In recent years, mechanistic models have been applied to a broad range of applications in pharmaceutical R&D and engineering, improving efficiency through reduced data requirements, facilitating scale-up and tech transfer, and enabling virtual design space exploration. Many pharmaceutical applications of mechanistic models focus on a single unit operation, using a component model for activities such as scale-up. However, an efficient workflow is required to apply these mechanistic models within the industrial product development cycle. An efficient workflow allows for a holistic assessment of the effects of operating conditions on product attributes and allow a combination of process parameters to be explored without increasing the experimental effort. In this talk, recent innovations in applying particle technology modelling approaches to support the industrial product development process. Within the workflows, efficient model calibration and validation are applied to generate a digital twin for the industrial process. The subsequent process design is based on process understanding and a model-driven sensitivity analysis approach. The benefits of the improved product development workflow are demonstrated in the context of industrial case studies of particulate processes including particle drying and compaction.

The application of multi screw feeders to avoid flow problems: Sometimes one screw is not enough!

Eddie McGee

Managing Director, Ajax Equipment Ltd, Milton Works, Mule Street, Bolton BL2 2AR, UK

Solids handling is one of the largest and most common processes across almost every industrial activity around the world, however, effective performance can be impeded by problems that arise in storage and handling.

From fine cohesive powders to shredded wastes, bulk solids can exhibit varied and awkward flow behaviour which present significant challenges for discharging from hoppers, bunkers and silos and providing stable, consistent feed to subsequent processes. Large hopper outlets can be needed to avoid stable arches and rat holes obstructing flow but the mass flow condition is only realised if the feeder can extract from the full area of the hopper outlet; if this is not achieved then flow reliability from the hopper is jeopardised and in fact mass flow cannot be realised. Consideration in type and design of the feeder to serve large outlets is an essential element in achieving reliable flow and proper feed control. This requires suitably interfacing and matching the needs of feed rate with constructional and geometrical aspects of the feeder which accommodate the material’s properties, for ensuring flow along the full width and length of the hopper outlet.

This paper will use shear cell tests and other techniques more appropriate for biomass and shredded waste applications to identify the important aspects of feeder selection for interfacing and for positive feed transfer capability. The paper will include industrial case studies ranging from fertiliser production to waste-to-energy processes, illustrating the approach used to solve plant operating problems with fine powders, shredded wastes and very low-density materials using twin, quadruple and even sextuple screw feeders (Figure 1) respectively.

Key words: Screw Feeders, Mass Flow, Powders, Biomass

Figure 1 : A sextuple screw feeder for feeding carbon fibre

Improved processing in extrusion by BASF

Rou Hua Chua[1*], Edward Bohres[1], Xue Liu[2], Alexej Michailovski[1], Maik Nowak[1], Frank Runge[1], Martin Kraus[1], Frank Kleine Jäger[1]

[1]BASF SE, Ludwigshafen, Germany

[2]BASF Corporation, Beachwood, United States

In the research area of paste extrusion, BASF is investigating process-structure-performance of pastes to increase extrusion processing stability and output, to improve the efficiency of new formulation development, and to achieve faster and more reliable scale-up. Efforts to elaborate the fundamental know-how on the relationship between the process of extrusion and the extrudate structure and its performance have become necessary, (i) to increase predictive reliability of pastes suitable for extrusion, and (ii) to decrease time-tomarket for newly developed products. The talk will discuss the main influencing factors impacting extrudate quality in production (i.e. porosity, strength), and show how upstream processing (e.g. mixing) impact paste properties.

Examples for handling of post-consumer plastic waste

Harald Wilms

Wilms-ITC, Innovation-Technology-Consulting. Bremen, Germany

Plastic scrap from post-consumer waste (PCW) collection systems has to be recycled. Lately, increasing recycling rates for PCW from packaging have been imposed by European regulations in order to increase circularity of polymers and to reduce incineration and landfill disposal. This calls for massive investment in new recycling facilities for mechanical and chemical recycling involving substantial handling of plastic PCW. This is the second phase of respective activities after an initial plastic recycling boom some 25 years ago. Thus, it is time to look into successful handling operations for waste plastic that was already developed at that time. The paper focusses on conveying system design and operation experience, silo discharge systems for plastic PCW and simultaneous feeding of a from a single source into a numerous pneumatic conveying systems. Process technologies are being defined, equipment design is presented and performance is being described.

Estimation of the temporal variations of the feed of a sinterization process aided by a voxelization-based numerical approach

Horacio Andrés Petit[1], Luis Marcelo Tavares[1]

[1]Department of Metallurgical and Materials Engineering, Universidade Federal do Rio de Janeiro – COPPE/UFRJ, Cx. Postal 68505, CEP 21941-972, Rio de Janeiro, RJ, Brazil

Ground storage in stockpiles is the most used method for storage of granular materials, particularly for large volumes. The utilization of stockpiles enables the homogenization and buffering of the material. Homogenization occurs when the material being reclaimed mixes by the action stacking and reclaiming, reducing the variations in the properties of the solid. However, the homogenization is far from being perfect and variability in the properties of the solid are still expected due to the nature of the granular solids. A specific case of interest takes place inside metallurgical facilities in Brazil, where the sintering process is used. Sintering takes sinter feed as the main raw input and produces sinter product. The chemical and physical properties of the sinter feed presents large variations due to the diversity of the production and the availability of different production sites and suppliers Such variations cause operational problems, so that corrections in the operational set-up are constantly required to maintain the quality of the product. Furthermore, operational problems become more relevant in facilities where batches of sinter feed from different sources are stacked together, forming a single pile that is reclaimed to feed the process. In this regard, knowledge of the magnitude of the variations beforehand is a key information for the operation and planning of the process. Efforts have been made to model the variations of the properties of the sinter feed while being fed to the metallurgical process. A numerical method was developed by the authors to model the stacking of the different batches of sinter feed and the reclaiming of the previously formed stockpile. The numerical method utilizes a volume discretization approach called voxelization to discretize the volume of the pile and simulate the reclaiming operation. This work present a specific case of study where the modeling of the stacking and reclaiming operations was implemented and validated using industrial data from a metallurgical operation in Brazil. The objective of the study is the temporal prediction of the properties of the sinter feed while it is reclaimed and fed into the sintering process. The prediction is carried out by simulating the piling and reclaiming processes that take place in a stockyard with the aid of the previously mentioned numerical method. Each batch has been characterized previously by the supplier, thus, the simulation links known information to predictions. The numerical method used in this work is able to reproduce the stockpiling and reclaiming processes and demonstrates to be able to give a fair estimation of the different quality characteristics of the sinter feed while being fed to the process.

Modeling of stockpile drainage and seepage in real applications

Jairo Paternina[1], Francisco Cabrejos[2], David Craig[1], Rogerio Ruiz[3], Corin Holmes[4], Enes Kaya[4]

[1]Jenike & Johanson, Tyngsboro, Massachusetts, USA

[2]Jenike & Johanson, Viña del Mar, Chile

[3]Jenike & Johanson, Vinhedo, Brasil

[4]Jenike & Johanson, Belmont, WA, Australia

Stockpiles are widely used in many mining plants, ports and industrial processes to handle and store large quantities of bulk materials at rest. But they are not free of issues and may experience different flow and safety problems related to drainage and seepage. The purpose of this article is to highlight a simulation technique using COMSOL to model the flow of liquids within a porous media, and determine the final moisture retained in the bulk material after gravity drainage. In addition, two real examples of the application and usefulness of this approach are presented, including experimental results of a drainage pipe test with wet salts developed by J&J engineers, and the infiltration plus runoff of rainwater in iron ore stockpiles.

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MIXING AND SEGREGATION

Description of size segregation in multicomponent mixtures using a probabilistic continuum model

Monica Tirapelle[1], Silvia Volpato[1], Andrea C. Santomaso[1]

[1]Dept. of Industrial Engineering, University of Padova, Padova, Italy)

Particles of differing sizes under external agitation typically segregate rather than mix. This phenomenon, which is spontaneous and unavoidable in practice, represents an unending source of frustration for the bulk chemical, pharmaceutical, agricultural and food industries. In this work, we present a new continuum model aiming to develop a continuum framework for the modelling and the prediction of size-driven segregation in multidisperse granular mixtures. The magnitude of the segregation velocity is based on the combination of kinetic sieving (percolation) and squeeze expulsion mechanisms. Unlike the several formulations already existing in the literature, the segregation model relies on probabilistic assumptions combined to physical considerations in the formalization of the kinetic sieving mechanism. Each particle has different probabilities of falling into the underlying layer or remaining trapped in the original cage. These probabilities are dependent on the particle size, local diameter, packing density and magnitude of the local shear rate. As an effect of percolation, the force imbalance in the granular medium, the particles can also be squeezed upward in the upper layer. To solve the flow field of the granular medium, we employed an existing rheological model previously proposed by us, which is a generalized Newtonian model where the viscosity of the dense granular medium depends on the granular temperature. The rheology of the solid was fully coupled with the segregation equations. Such a continuum model was used to simulate the size-segregation in ternary mixtures of coarse, intermediate and fine particles (respectively 1.5, 2.4 and 3.4 mm), occurring during the discharge from a blast furnace hopper. Simulations, carried out on a commercial CFD code, were validated against independent experimental and DEM simulation data taken from the literature In particular we considered ternary mixture of particles combined in different proportions (5:24:71, 25:20:55, 25:30:45, 45:14:41 and 65:9:26 percent of fine, intermediate and coarse particles respectively) and with different initial configurations (flat surface or heap surface in the hopper). The comparison between model predictions and literature data led to satisfactory results. Some discrepancies arose only at the final stage of the discharge process. We found, however, that they were mainly due to assumptions made on the wall-particle friction coefficient. We found out also that the model can well predict the singly no-convex asymmetric behavior of the flux function. The main advantages of the proposed segregation model are that it is simple, it can be applied to mixtures made of any number of discrete solid phases that differs by size and it is potentially applicable to any geometry and flow configuration.

Solid state material driven turbine to reduce segregation effects in bunkers

Michael Denzel, Michael Prenner

Chair of Mining Engineering and Mineral Economics – Conveying Technology and Design Methods, University of Leoben, Leoben, Austria

For most applications and following processes an evenly distributed bunker outflow is desired in terms of particle size. Various discrete element simulations were performed to analyze the current state of an existing bunker used for storage of blast furnace sinter, which is simply filled with a discharging belt conveyor. Great segregation effects could be determined, which are mainly caused by the filling method and further intensified by the core flow effect and bunker geometry effects. Several concepts and devices to reduce segregation in bunkers were evaluated using DEM. Therefore, the particle size distributions at the bunker outflow were each compared with the current state without device. A solid state material driven turbine is presented, which reduces segregation effects during bunker filling and leads to a significant improvement while discharging. The results show a more evenly distributed bunker outflow in terms of particle size. As sinter is a very abrasive material, the wear at the turbine has also been evaluated. Furthermore, the power output in this case and the potential of energy recovery were investigated, which could be of interest in many other applications. Additionally, the particle degradation at the solid state material driven turbine is evaluated in this case. Therefore, a newly developed breakage model for DEM is used. The model is based on the particle replacement method, combined with the voronoi tessellation algorithm and replacement probabilities to achieve a high accuracy in terms of fragment size distribution. The fragments are further breakable, which also allows simulation of more complex conveying systems. The breakage model is calibrated with a specially developed single particle impact tester, which allows rapid analysis of breakage characteristics of bulk materials.

The development of new radial stress theory to predict segregation: The relationship between mass flow, segregation prevention, and stress and gas pressure gradients

Kerry Johanson[1]

[1]Material Flow Solutions, Gainesville FL, USA

Almost all products created in today's marketplace are a mixture of unique ingredients and many of these products are dry blends. Each ingredient has characteristics that are very different from the other ingredients in the blend. Thus, segregation is a significant problem with many of these mixtures. Segregation mitigation can be accomplished by modifying the product or by modifying the process. Solving segregation issues from a process point of view requires knowledge of the segregation pattern which can be measured for any mixture. However, it also requires an understanding of the velocity profiles in all pieces of the process equipment between the blending step and the packing step. The mode of operation of each process step is critical to preventing segregation. There are two modes of operation that influence segregation, depending on the pattern of the segregation induced during the filling process. In some process steps, the container is filled and then emptied. Therefore, the segregation which occurs during the emptying cycle must be known. In other process steps, the mode of operation is mostly continuous and the resulting segregation depends on the residence time distribution of material passing through a key piece of process equipment. In both cases, the velocity profile coupled with the segregation pattern determines the variation of key components as they pass through the handling system. Velocity profiles in a process depend on the geometry of the process and on the bulk material flow properties. If flow properties are measured, then mathematical theories such as the radial stress theory can be employed to estimate the velocities in process equipment and compute residence time distributions and segregation emptying profiles for fill-then-empty processes – as well as semi-continuous processes. However, the basic assumptions of the radial stress theory are limited and many real processes do not conform to the assumptions behind the standard theory. Therefore, the solids velocity profiles computed from the radial stress theory may not be sufficient to describe segregation profiles and residence time distributions for material leaving the process. This work examines the relationship that external gradients such as non-radial stress gradients or local gas pressure gradients in the process might have on the solids velocity profiles in process equipment. The work outlines calculations to compute velocities in bulk handling process equipment subject to these gradients and then applies those velocities to the calculation of segregation profiles. The ultimate goal and focus of the work is to relate the external force gradients to product consistency. A new radial stress theory to include non-radial stress and gas pressure gradients will be presented. Finally, the mass flow plots created by Andrew Jenike and Jerry Johanson were used to determine velocity ratios in process equipment, feeders stress loads, and even flow factors to describe arching effects. However, they do not contain a segregation index that could be used to determine what type of mass flow will give a certain degree of segregation prevention. Therefore, as part of this work new mass flow plots containing a segregation intensity number are generated for various nonradial solid stress gradients, local gas pressure gradients, effective internal friction angles, hopper angles, wall friction angles, and segregation patterns. These tools can assist practicing engineers design process equipment to more easily solve segregation problems.

Batch versus continuous powder mixing of excipients and active pharmaceutical ingredients

Maarten Jaspers, Pauline H.M. Janssen, Bastiaan H.J. Dickhoff

Dept. of Innovation and Technical Solutions, DFE Pharma GmbH & Co, Goch, Germany

The pharmaceutical industry is currently undergoing a transition from batch-wise to continuous manufacturing. This transition is driven by several benefits of continuous processes such as improved efficiency, improved product quality and increased flexibility for the scale of production. Continuous manufacturing is also encouraged by regulatory bodies, as it is in line with the quality-by-design (QbD) paradigm for pharmaceutical development. The main focus of pharmaceutical continuous manufacturing is on oral solid dosage forms such as tablets and capsules. The production process of solid dosage forms generally starts by blending the active pharmaceutical ingredient (API) with excipients. The addition of excipients is required to improve processability of the API and to provide the final dosage forms with desired properties. Blending of API and excipients is an important unit operation, as uniform blending is required to ensure accurate dosing of API in the final dosage form. Pharmaceutical powder blending is historically performed in a batch process, which suffers from some critical limitations including difficulty in scaling and flexibility, as batch size is determined by blender dimensions. A continuous blending process resolves these issues, as the amount of material is determined by process run time rather than blender size.

Although continuous powder blending is gaining interest both in academic research and the pharmaceutical industry, a direct comparison between batch and continuous blending of API and excipients is lacking. So far, most studies on continuous blending have been restricted to a particular material or formulation, even though powder material properties can have a large impact on mixing performance. In the current study, we show the advantage of continuous powder blending for API-excipient blends based on different functional excipients. Batch-wise and continuous powder blending are directly compared for combinations of six different excipients and two API's. Furthermore, blending is performed at varying API dosages and blending times. The excipients and API's used cover a broad range of relevant powder material properties such as particle size, morphology, density and flowability.

Blend uniformity analysis reveals how excipient properties, API dosage and blending time affect blend uniformity in both a batch and continuous process. Blends prepared in a batch process show a strong dependence of uniformity on material properties such as bulk density and flowability. Matching the material properties of the individual components and good powder flowability are key factors that determine blending performance in a batch process. For the continuous process on the other hand, the effect of material properties on blending performance is less pronounced. The continuous process is capable of producing uniform blends, even when the material properties of excipients and API are vastly different. Blending performance of the continuous process does show a minor dependence on powder flow and API dosage. Overall, the results presented here show that continuous powder blending is a robust process that is suitable for a variety of pharmaceutical excipients. This greatly reduces the complexity of excipient selection for continuous manufacturing of solid dosage forms.

Advantages of a continuous measurement of great mass flows in a mixing process for cement plant application using an electromagnetic + time of flight online massflow meter

Tiago Morais[1], Philipp Tretow[1], Lars Orzelkiewicz[1], Gilles Campagnola[2], Alexandra Schmedt[1]

[1]ENVEA Process SchlingenGermany

[2] ENVEA Spa Verano Brianza Italy

Cement production is a well-known process which is involving different raw materials in order to have an high quality product at the end of the process. High end cement products are coming from precise mixing ratio of different elements before high temperature phase. Achieving a good mixing step for production process leads to advantages in a wider range than a good final product. Typically, it avoids losses of batches and material, maintenance issues or optimization of the raw materials. All those points are strongly related to an economic aspects in term of cost reduction for wrong batches or maintenance issues. Typically, gravimetric systems like scales and baffle plates are used to give a feedback on the process in order to regulate mixing ratios. These systems are mechanical and take up a lot of room in the plant. One solution that can be adopted is using an online measuring device without moving parts; the ENVEA MaxxFlow

A silo plant was built at a cement plant. Three silos are filled differently.

Silo 1: cement

Silo2: fly ash

Silo3: white fine lime

The feed mixer flow is controlled by a dosing valve. This valve is feedback controlled by the ENVEA Maxx Flow. The mixer screw transports the material to a bucket elevator. The bucket elevator conveys the material upwards into a further transport screw and then into a truck which stands on a truck scale. Each device is calibrated with its related material for a “taylor made” configuration both on materials and flow range increase reliability and precision. The advantages on the plant side are at different levels; from the stability of the mixture to the information if one material is properly fed, from reduce maintenance to space saving.

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COMPACTION AND TABLETING

Modeling the shear sensitivity of lubricated powders in a paddle feeder

Daniel Puckhaber[1,2], Arno Kwade[1,2], Jan Henrik Finke[1,2]

[1]Institute for Particle Technology, TU Braunschweig, Braunschweig, Germany

[2]Center for Pharmaceutical Engineering (PVZ), TU Braunschweig, Braunschweig, Germany

The industrial production of pharmaceutical tablets is mostly carried out with rotary tablet presses which apply paddle feeder to enhance the powder flow into the dies. However, in addition to improving the filling yield, the shear forces acting due to the rotating paddle can lead to various negative effects. Besides particle abrasion, overlubrication of formulations is of particular importance. Overlubrication is the excessive distribution of lubricant particles, which deagglomerate due to shear stress. This excessive distribution exacerbates undesirable effects that occur when lubricants are added internally, particularly tablet tensile strength reduction. Although overlubrication is a known risk in the use of paddle feeder, no comprehensive model description of the underlying processes is available to date. In this study, the influence of different paddle speeds on the compactibility was systematically investigated and a model was developed to describe the kinetics of compactibility loss as a function of residence time in the paddle feeder. Binary mixtures of microcrystalline cellulose and magnesium stearate were used as model formulations. In order to evaluate the influence of the formulation parameters on the sensitivity of the formulation with respect to overlubrication, magnesium stearate grades with widely differing specific surface areas were also used. The mathematical model developed was proven to accurately describe the kinetics of strength degradation as a function of residence time. The model was adapted based on the equation of Ryshkewitch-Duckworth [1] and in this new form allows a prediction of the tablet strength as a function of the process parameters over the entire process time. In addition, characteristic parameters could be derived to compare the kinetics of the different formulations and to investigate the influence of the materials used. It was shown that the relative strength decrease depends significantly on the paddle speeds and that there are only minor differences in the kinetics for different lubricant concentrations. Furthermore, significant differences in the kinetics of strength loss for different lubricants were found, indicating considerable differences in the deagglomeration behavior of the magnesium stearate grades used. The results obtained in this work allow a quantitative description of the overlubrication in paddle feeder and thus, represent a useful extension of the existing process understanding in tableting. Building on the obtained results, the developed model is to be applied to industrially relevant formulations and, if necessary, further developed so that a quantitative prediction of the strength loss of tablets due to the paddle feeder passage can be prospectively made on the basis of rapidly accessible raw material data. [1] Ryshkewitch, E., 1953, Journal of the American Ceramic Society 36, 65-68.

Processing of living microorganisms: Fluidized-bed granulation and tableting

Karl Vorländer[1,2], Arno Kwade[1,2], Jan Henrik Finke[1,2], Ingo Kampen[1,2]

[1]Institute for Particle Technology, Technische Universität Braunschweig, Braunschweig, Germany

[2]Center of Pharmaceutical Engineering (PVZ), Technische Universität Braunschweig, Braunschweig, Germany

Producing tablets with living microorganisms is of special interest for the administration of probiotic microorganisms. These microorganisms provide health benefits to the patient when administered in viable form and adequate doses. Understanding the influence of different process steps, their specific process parameters and formulation aspects is crucial for improving the quality of probiotic tablets, especially with regard to microbial survival.

Different drying technologies can be used to dry microorganisms preserving their viability. In this study, fluidized-bed granulation was used to dry microorganisms at comparatively mild temperatures. A yeast cell suspension (*Saccharomyces cerevisiae*) enriched with protective additives was sprayed on typical tablet fillers and binders (dicalcium phosphate (DCP, DICAFOS A150, Chemische Fabrik Budenheim), isomalt (ISO, GalenIQ 721, BENEO), lactose (LAC, Granulac 70, MEGGLE) and microcrystalline cellulose (MCC, Vivapur 102, JRS Pharma)) to produce granules with dried microorganisms, which were tableted subsequently. The tablets were characterized regarding porosity, tensile strength and cell survival.

In general, compressibility and tabletability were improved in comparison to the pure fillers/binders, whereas compactibility was reduced during granulation. Exceptions to these phenomena were the compactibility of LAC and the tabletability of MCC. This could be explained by the carrier-specific deformation properties. During the granulation, the surface is covered with yeast cells and protective additives reducing the attractive forces and thus leading to the decreased compactibility. The compactibility of LAC seems to be lower than that of the dried formulation of yeast cells with protective additives, so the compactibility was improved when it was layered on the lactose particles. The observed reduction in tabletability of MCC granules is comparable to the susceptibility to lubricants due to the different deformation mechanisms. While MCC particles mostly deform plastically, mainly brittle fragmentation occurs for the other materials. In the latter case, newly formed surfaces are free of yeast cells or protective additives, so that these do not impair bond formation as in MCC.

A strong influence of the compression stress on the yeast cell viability was obvious. The higher the compression stress, the worse the survival rate as cells were mechanically destroyed. This is directly linked to the porosity as a decreasing porosity is accompanied by lower survival rate. Interestingly, the survival rate for LAC was significantly higher than for the other materials at the same porosity. Due to the low intra-particulate porosity of LAC crystals compared to agglomerated other materials, a higher inter-particulate porosity was present in LAC tablets, giving space to accommodate the yeast cells. Due to the different tabletabilities especially of MCC and LAC, the combination of both quality attributes survival rate and tensile strength suggests that both materials seem equally suitable for the considered process chain.

Material and Process Analyses for the Derivation of Process and Property Models in Food Compaction

René Rösemeier-Scheumann[1,2], Jan Henrik Finke[1,2], Ulrich Bobe[3], Annabel Bozon[3], Arno Kwade[1,2]

[1]Institute for Particle Technology (iPAT), TU Braunschweig, Brunswick, Germany

[2]Center of Pharmaceutical Engineering (PVZ), TU Braunschweig, Brunswick, Germany

[3]Department of Science & Technology, Nestlé Product Technology Centre, Singen, Germany

The compacting of powders is a process used to convert powdery materials into a suitable form for industry and customer needs, whereat the properties of resulting food compacts depend on the complex interplay of material, formulation and process parameters. Due to the high number of different materials and property variations, a general classification system of mechanical characteristics must be established to generalize this knowledge derived from experiments, which is supported by numerical simulations of the compaction process to understand underlying micro processes. Through the synergy of all three material, formulation and process parameters, property models shall be established to describe the entire compaction process to accelerate the whole development and production process in case of formulation adaption.

In this work, the influence of significant components on the final compact properties are investigated, especially taking the effect of varying moisture content into account. In addition to the dominating product property tensile strength, glass transition temperatures (T_g) of formulations of crystalline and amorphous components are determined by differential scanning calorimetry (DSC) to elucidate their effect on compaction processes.

The results pronounce the different extents of the influence of moisture content on the deformation behavior and resulting strength of the compacts of different component classes. The systematic comparison of compaction results of the individual components with those of specific formulations enable the derivation of essential rules of mutual influence. DSC measurements support the effect of T_g on the compaction results and clarify blend behavior based on the mixing ratios of crystalline and amorphous components.

Modeling of high-density compaction of pharmaceutical tablets using Multi-Contact Discrete Element Method

Kostas Giannis[1,2,*], Carsten Schilde[1,2], Jan Henrik Finke[1,2] and Arno Kwade[1,2]

[1]Center of Pharmaceutical Engineering (PVZ), Technische Universität Braunschweig, Franz-Liszt-Str. 35A, 38106 Braunschweig, Germany

[2]Institute for Particle Technology (iPAT), Technische Universität Braunschweig, Volkmaroder Str. 5, 38104 Braunschweig, Germany

*Correspondence: k.giannis@tu-braunschweig.de; Tel.: (+49-531-391-65554)

The purpose of this work is to simulate the powder compaction of pharmaceutical materials at the microscopic scale in order to better understand the interplay of mechanical forces between particles, and to predict their compression profiles by controlling the microstructure. For this task, the new framework of multi-contact discrete element method (MC-DEM) was applied. In contrast to the conventional discrete element method (DEM), with MC-DEM interactions between multiple contacts on the same particle are now explicitly taken into account. A new adhesive elastoplastic multi-contact model invoking neighboring contact interaction was introduced and implemented. The uniaxial compaction of two microcrystalline cellulose grades (Avicel® PH 200 (FMC BioPolymer) and Pharmacel® 102 (DFE Pharma)) subjected to high confining conditions was studied. The objectives of these simulations were: (1) to investigate the micromechanical behavior; (2) to predict the macroscopic behavior; and (3) to develop a methodology for the calibration of the model parameters needed for the MC-DEM simulations. A two-stage calibration strategy was followed: first, the model parameters were directly measured at the micro-scale (particle level) and second, a meso-scale calibration was established between MC-DEM parameters and compression profiles of the pharmaceutical powders. The new MC-DEM framework could capture the main compressibility characteristics of pharmaceutical materials and could successfully provide predictions on compression profiles at high relative densities.

Three-dimensional discrete element modelling of diametrical compression of annular tablet

Jiawei Hu, Chuan-Yu Wu*

Department of Chemical and Process Engineering, University of Surrey, Guildford, U.K.

*Corresponding author: Prof. Chuan-Yu Wu, Email: c.y.wu@surrey.ac.uk

Understanding the effect of material properties, interfacial properties and structure of the agglomerate on the strength of agglomerates is critical in many processes. For instance, for manufacturing of pharmaceutical tablets and pellets with dry granulation, understanding the relationship between the tablet properties and the properties of granules is critical in controlling the granulation behaviors, and the tablet properties (e.g. tensile strength and density distribution) is determined by the material properties of feed powders, interfacial properties between particles and the process condition, which determine the structure of the tablet. This study aims to study the dependence of the tensile strength of pharmaceutical annular tablet on surface energy and inner diameter, for which three-dimensional discrete element modelling (DEM) with a cohesive particle model based on the JKR theory was performed. Diametrical compression tests with specimens of different inner diameters and surface energies were modelled by DEM, as shown in Figure 1(a). It was found that there is a strong correlation between the tensile strength with the surface energy and inner diameter of specimens. In Figure 1(b), the maximum loads on the compression wall increase with the surface energy and hence lead to the tensile strength grow with the increasing surface energy. In addition, for specimens with the same outer diameter and thickness, the annular tablet with larger inner diameter has a smaller tensile strength than these with smaller inner diameter, as shown in Figure 1(c).

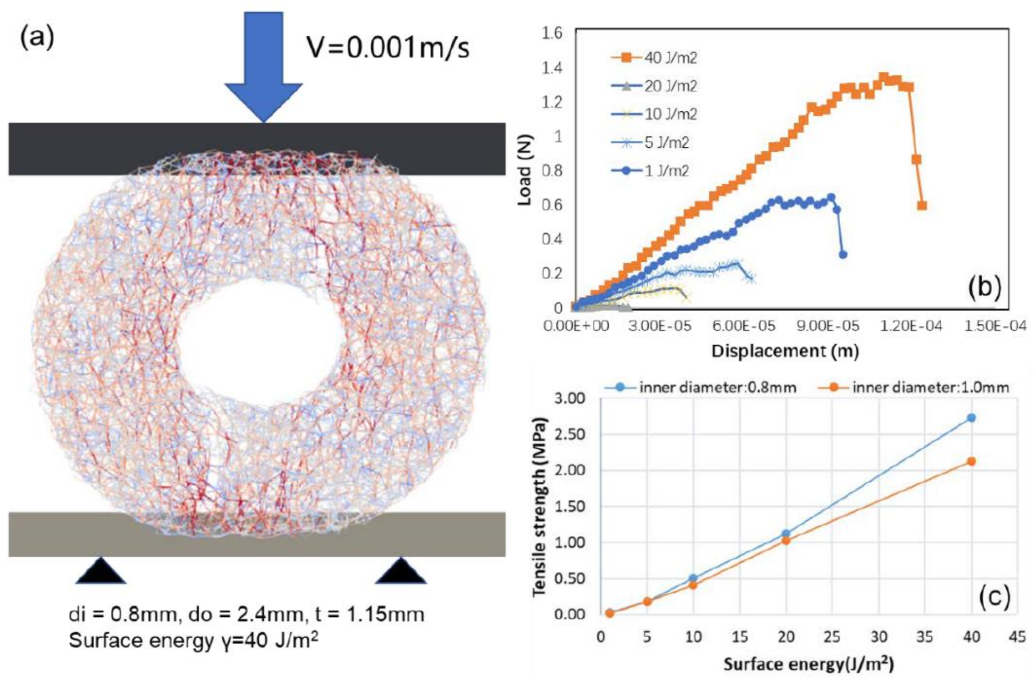

Figure 1. (a) Typical breakage pattern and force chain for annular tablet during diametrical compression; (b) Load-displacement curve during diametrical compression; (c)The variation of tensile strength with surface energy at different inner diameter.

Material-independent description of die filling in rotary tablet presses

Ann Kathrin Schomberg[1,2], Jan Henrik Finke[1,2], Arno Kwade[1,2]

[1]Institute for Particle Technology, TU Braunschweig, Braunschweig, Germany

[2]Center for Pharmaceutical Engineering (PVZ), TU Braunschweig, Braunschweig, Germany

Rotary tablet presses are used for the industrial production of pharmaceutical tablets. The filling of dies is one of the quality-determining sub-processes, since it determines the dose as well as the uniformity of the mass and the active ingredient. In addition, with varying weight, different compression forces act, so that the resulting tablet properties, such as the breaking strength and porosity, also do not correspond to the specifications. To achieve complete and consistent die filling, certain process parameter combinations have to be set depending on the material properties of the formulation. In order to enable a model-based description of the filling process in the future and thus reduce the time required for cost-intensive process development, an indepth understanding of the material influence is necessary. In this study, the die filling of pharmaceutical excipients with different bulk and solid densities and varying flow properties was investigated on rotary tablet presses with different scales (pilotscale: XL 100, production-scale: XL 400, X 3 (Korsch AG). The suction angle of the fill cam, which causes the formation of a temporary vacuum during suction filling, was varied on the pilot-scale rotary press. For comparison of the materials, the filling time was taken into account to calculate the volume flow rate into the dies for a given paddle speed. Comparisons with larger rotary presses (XL 400, X 3) showed that the volume flow rate provides a good basis for the model description. Thus, the volume flow necessary for complete filling can be calculated across scales and the required paddle speed can be determined. Despite the reference to the bulk volume, influences of the different materials were still evident. These could be attributed to the different flow properties. Furthermore, a positive correlation with increasing vacuum levels was demonstrated.

The effect of particle adhesion on die filling performance in a gravity filling device

Mohammadreza Alizadeh Behjani[1], Chao Zheng[1], Omar M. Ismail[1], Edward Yost[2], Ariel Muliadi[2], Chuan-Yu Wu[1]

[1]School of Chemical and Process Engineering, University of Surrey, Guildford, UK

[2]Small Molecule Pharmaceutical Sciences, Genentech, South San Francisco, USA

Die filling is one of the most critical stages during tableting processes in the pharmaceutical industry. Gravity die filling is the process of delivering powder into a die taking the advantage of its weight. This process can be generally performed by moving a feed shoe on top of a die. The die filling performance depends on many parameters, including the feeder type, the operational conditions, and powder properties.

In this study, DEM (Discrete Element Method) modelling is performed to explore the relationship between particle adhesion and gravity die filling quality in a linear die filling system fitted with a Huxley Bertram forced feeding shoe (HB system). The standard VIVAPUR® MCC Spheres 350 powder is used in the simulations as the model powder, and the DEM input parameters are selected based on the experimental measurements and the numerical calibration. Rocky 4.5 DEM software is utilised to simulate the die filling process. To do so, suitable contact models are used to take account of the particles' collisions and adhesion during the process.

Using the DEM simulations, the effect of particle adhesion on the performance of the die filling is investigated at various feeder speeds and stirrer rotational velocities. It is observed that increasing the powder cohesion leads to a less efficient die filling, i.e., the fill ratio decreases with a logarithmic fashion as the Cohesion number increases. The results also show that stirring the powder bed facilitates the die filling process, especially when the powder is highly cohesive.

The protective potential of cushioning coatings on enteric-coated pellets during tableting

Lara Stein[1,2,3], Sonja Bauhuber[3], Gernot Warnke[3], Jan Henrik Finke[1,2]

[1]Institute for Particle Technology, TU Braunschweig, Braunschweig, Germany

[2]Center of Pharmaceutical Engineering, TU Braunschweig, Germany

[3]JRS PHARMA GmbH & Co. KG, Rosenberg, Germany

gernot.warnke@jrspharma.de; jan.finke@tu-braunschweig.de

The protection of sensitive active pharmaceutical ingredients (APIs) against gastric conditions or the protection of the stomach against the API frequently requires enteric coating of dosage forms. The application of multi-unit pellet systems (MUPS), which comprise coated pellets in a solid, monolithic dosage form, adds the advantage of a quicker and less filling-dependent passage of the stomach and by that onset of effect.

As tablets are the most convenient dosage form for most patients, the compression of pellet blends to tablets is the most popular approach. However, due to the stresses necessarily applied during compaction, the functional coating of the pellets may be damaged. This is caused by the stress distribution through the external phase (e.g. filler, binders, disintegrant) to the pellet surface in combination with the deformation behaviour of the pellets themselves and the mechanical properties of the film coatings on these pellets. The latter properties of the coating can be influenced by coating formulation, coating process conditions causing specific changes in coating structure, and the applied coating thickness or weight gain.

In this study, the effect of coating thickness of an enteric pellet coating and the protective potential of cushioning coatings applied as outermost layer on the pellets are evaluated. It is shown that the susceptibility of the pellet coating towards compression stresses is dependent on the coating thickness of the enteric layer. The thicker the coating, the higher the resistance towards mechanical stresses and, by that, the lower the undesired immediate release of (model) API under gastric conditions. The addition of an additive outer layer – a so-called cushioning coating – on the enteric layer can shield it from the mechanical stresses to a certain extent. By that, the enteric coating thickness can be reduced to less than half of the of the best-performing sole enteric layer, while still performing better, especially at lower compaction stresses.

This protective and economic effect of the cushioning layer is independent of its filling material (titanium dioxide or microcrystalline cellulose) and also independent of the outer phase composition. Regarding the latter, cushioning-coated pellets perform equally well in either microcrystalline cellulose or dicalcium phosphate outer phase. Also, at single pellet scale, the improved resistance of the pellet coatings could be proved by micromechanical testing and scaled to tablet compaction results.

FRIDAY, 8 JULY 2022
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AGGLOMERATION AND GRANULATION

Novel approach for the characterization of powder caking

Alessandra Hausmann[1], Britta Buck[2], Lukas Blesinger[2], Frank Kleine Jäger[2], Daryl Williams[3]

[1]Department for Materials, Imperial College London, London, UK

[2]BASF SE, Ludwigshafen, Germany

[3]Department for Chemical Engineering, Imperial College London, London, UK

Storage and transport conditions such as temperature and humidity can have a wide range of effects on the physical properties of powders such as loss of pharmaceutical potency, food spoilage and powder caking. Powder caking is the undesirable process of a powder forming agglomerates, referred to as "cakes". Industrial methods of determining caking conditions are often time-consuming, require large sample volumes and provide little scientific insight. However, current analytical techniques rarely represent "real-world conditions" and may provide inaccurate data when compared to the storage and transport lifetime of the powder sample.

We have developed a novel characterization method for assessing the role of humidity in caking, allowing for in-situ measurements of powder flow while exposed to a tunable environment of humidities. It is faster than current industry standards and correlates to common methods used. The technique uses commercially available equipment such as the FT4 Powder Rheometer, correlates to common experimental methods used in solids handling industries and is easily reproducible due to its modular design. Among other parameters, the instrumental setup measures flowability energy, as a function of relative humidity. Powder flow energy is a measure for a powder's resistance to flow. Parameters that influence powder flow energy include particle size, shape, cohesivity, density, elasticity and electrostatic charge.

To further understand the interaction of relative humidity with the studied powders and the mechanism of caking, supporting DVS (Dynamic Vapor Sorption) experiments were performed. DVS is a gravimetrical analysis tool that measures a materials uptake of water vapour and potentially a variety of other gases while allowing tight control over the temperature in ranges typical for industrial storage and transport (10-50°C), (0-95% RH). We were especially interested in equilibrium sorption capacities and the kinetics of the water uptake. DVS can be combined with Raman and near IR spectroscopy to provide insight in phase transitions, swelling behaviour and deliquescence of materials.

Our measurement protocol is designed to assess caking conditions, but the flexibility of the setup has the potential to be utilized more broadly for determining the moisture-induced change in powder rheology. This way of characterization can be used for a wide range of powders differing in crystallinity, morphology and chemical structure.

Pellet screenings sintering

Helio Pereira[1], Phillipe Rocha[2], Antonio Peres[3]

[1] Iron Ore Agglomeration, Sintering and Pelletizing Consultant, Belo Horizonte, Brazil

[2] Technical Marketing Specialist, Anglo American, Singapore, Singapore

[3] Dept. of Metallurgical and Materials Engineering, Federal University of Minas Gerais, Belo Horizonte, Brazil

With the progressive deterioration in iron ore quality worldwide, steelmakers need to seek alternatives to mitigate the deficiency of this raw material. Investments in the use of high grade concentrate and the application of pre-agglomeration technologies are alternatives to make up for this deficit. As a possibility to avoid such high investment, the motivation for this study was to compare the behavior of pellet screenings, undersize product of sieving burned pellets at 6.35 mm, with current natural sinter feed available in the market. Pellet screenings presents advantages such as low alumina and silica contents, in addition to low loss on ignition (LOI) and suitable particle size distribution. Sintering tests were performed at the SGA (Studiengesellschaft für Eisenerzaufbereitung) laboratory in Germany to evaluate the performance of this product when added to typical sintering mixtures used in Western Europe. The test results showed gains in the chemical, physical and metallurgical quality of the sinter produced. Keywords: Pellet screenings; Sintering process; Sinter feed; Iron ore mixtures

Parametric study of residence time distributions and granulation kinetics as a basis for process modeling of twin-screw wet granulation

Timo Plath[1*], Carolin Korte[2], Rakulan Sivanesapillai[2], Thomas Weinhart[1]

[1] Multi-Scale Mechanics, TFE, ET, MESA+, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

[2] Process Technology Development, Engineering & Technology, Bayer AG, 51368 Leverkusen, Germany

t.weinhart@utwente.nl; carolin.korte@bayer.com; rakulan.sivanesapillai@bayer.com
*Correspondence t.plath@utwente.nl; Tel.: +31-53-489-3997

Twin-screw wet granulation is a crucial unit operation in shifting from pharmaceutical batch to continuous processes, but granulation kinetics as well as residence times are yet poorly understood. Experimental findings are highly dependent on screw configuration as well as formulation, and thus have limited universal validity. In this study [1][2], an experimental design with a repetitive screw setup was conducted to measure the effect of specific feed load (SFL), liquid-to-solid ratio (L/S), and inclusion of a distributive feed screw on particle size distribution (PSD) and shape as well as residence time distribution of a hydrophilic lactose/microcrystalline cellulose based formulation. An intermediate sampling point was obtained by changing inlet ports along the screw axis. Camera-based particle size analysis (QICPIC) indicated no significant change of PSD between the first and second kneading section, except for low L/S and low SFL where fines increase. Mean residence time was approximated as a bilinear fit of L/S and SFL. Moreover, large mass flow pulsations were observed by continuous camera measurements of residence time distribution and correlated to hold-up of the twin-screw granulator. These findings indicate fast granulation kinetics and process instabilities for high mean residence times, questioning current standards of two kneading compartments for wet granulation. The present study further was designed for simplified process modeling. Due to the repetitive screw design discrete element simulations can be performed efficiently and a population balance model can be coupled without simulating the whole screw setup. Moreover, residence time distributions will help in calibration of such models. Future work on this study will consist of developing a discrete element/population balance multiscale simulation approach which is able to include particle dynamics via coarse graining. Keywords: Agglomeration and Granulation, Multiphase flow and fluidization, Computational modeling References: [1] T. Plath, C. Korte, R. Sivanesapillai, T. Weinhart, Parametric Study of Residence Time Distributions and Granulation Kinetics as a Basis for Process Modeling of Twin-Screw Wet Granulation, Pharmaceutics. 13 (2021). [2] T. Plath, C. Korte, R. Sivanesapillai, T. (Thomas) Weinhart, Dataset as a basis for process modeling of twin-screw wet granulation: A parametric study of residence time distributions and granulation kinetics, (2021). https://doi.org/10.4121/14248433.v1.

Influence of spray configuration and material on particle formulation in fluidized beds with liquid injection

Maike Orth[1], Swantje Pietsch-Braune[1], Stefan Heinrich[1]

[1] Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology, Hamburg, Germany

The fluidized bed granulation or coating process is applied for the production of high-quality granular solids in various industries, including for example the food, pharmaceutical or chemical industry. The strong dependence of the granule properties on the overall process conditions allows the production of tailor-made particles for distinct and innovative applications. To design the process in such a way, that the desired product requirements for a specific application are matched, it is essential to understand, how the three phases – fluidization gas, solid particles and liquid droplets – interact with each other. For this, the transport processes and different micro mechanisms happening within the fluidized bed are of great importance.

To investigate this connection between the process configuration, the phenomena taking place on the interfaces of the three phases and the structure of the resulting product and to integrate these interactions into simulation cases, coating experiments are performed in a lab-scale fluidized bed (Glatt, Germany). Depending on the materials, different micro processes can occur and be more or less pronounced. After the injection of a solution for example, crystal structures can be observed on the surface of the product particles. In case of a suspension as a spray liquid on the other hand, crystallization does not occur. The coated particles are analyzed regarding their surface structure via confocal laser scanning and scanning electron microscopy in order to identify the phenomena that were involved in the formation of these structures. Since the characteristics of the injected droplets are a key part in the coating process, additional measurements of the spray cone angle at different spray parameter combinations are carried out, showing that the cone angle depends on the spray air pressure and liquid viscosity, among others.

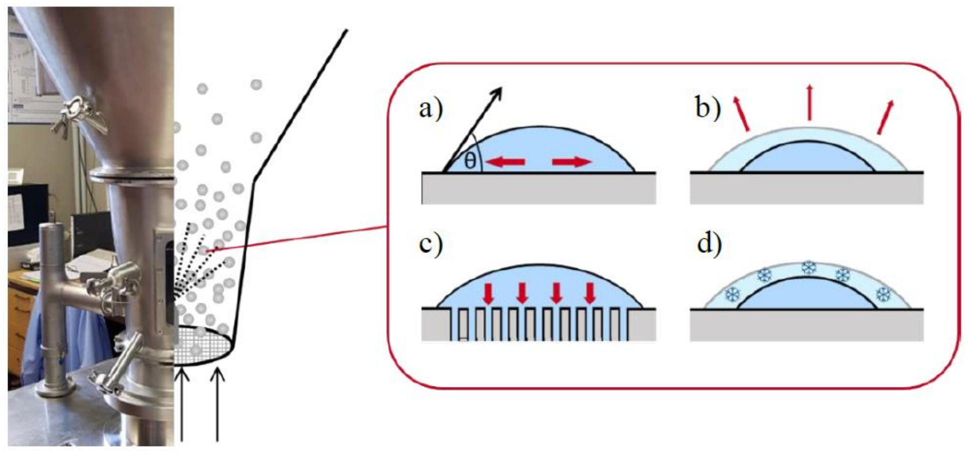

Fig. 1: Fluidized bed set-up and some possible micro processes on the particle surface: a) droplet spreading, b) evaporation, c) penetration into porous particle, d) crystallization.

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Structuration of plant-based milk powder for improved reconstitution

Kathrin Kramm[1], Jana Kammerhofer[2], Vincent Meunier[3], Swantje Pietsch-Braune[1], Stefan Heinrich[1]

[1]Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology, Hamburg, Germany

[2]Nestlé Product Technology Center Dairy, Konolfingen, Switzerland

[3]Nestlé Research, Lausanne, Switzerland

Food products in powder form are widely produced industrially due to advantageous properties including easy preservation, weighing, processing, transport and storage. Milk powder in particular has numerous applications in various products, but a growing number of consumers are tending towards plant-based alternatives. The plant-based milk powder investigated in the project, consisting of oil, sugar, plant protein and soluble fiber source, exhibits to lump formation upon reconstitution. This lump formation is most likely correlated with the powder bulk structure as well as the viscosifying and swelling properties of the plant ingredients.

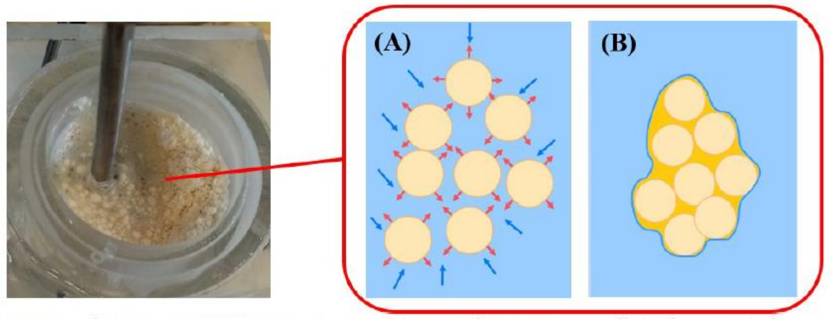

Figure 1: Lump formation during reconstitution process; (A) particles start to swell (red arrows) due to water contact (blue arrows); (B) formation of a viscous outer layer linked to the aggregation of swelling particles

For more efficient wetting behavior and facilitated water penetration due to capillarity between individual particles, the fine food powders are often agglomerated. The agglomeration enables defined reconstitution behavior, stability and flowability. To design targeted particle structure, fluidized bed processing is used by fluidizing the solid material with an upward gas flow and spraying water forms liquid bridges when the particles collide before drying. The solvent evaporates as the drying occurs and a solid bridge binds the particles together. In order to obtain an optimized agglomerated structure of plant-based milk powder for subsequent applications, the influence of material properties on the formation, structure and qualities of the agglomerated powder has to be investigated. The material characteristics have to be examined in dependency of the water content and temperature at different formulations due to the complex powder composition consisting of partially amorphous components. Since the supra-molecular structure of the individual components determines the behavior of the entire formulation. The study allows to further understand the micro and macro mechanisms of food particle agglomeration containing increased quantities of plant protein and fibers. The macro mechanisms are investigated by experiments in a laboratory-scale fluidized bed (Glatt, Germany). Thereby, the process parameters have to be selected in such a way that an agglomerate structure is formed which exhibits advantageous reconstitution properties.

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THERMOMECHANICAL BEHAVIOUR OF GRANULAR MATERIALS

Powder flow and heat transfer in a rotary kiln with baffles

Benjamin Glasser[1], Elaheh Ardalani[2], William Borghard[1], Alberto Cuitino[2]

[1]Dept. of Chemical and Biochemical Engineering, Rutgers University, Piscataway NJ, USA

[2]Dept. of Mechanical and Aerospace Engineering, Rutgers University, Piscataway NJ, USA

Rotary kilns and calciners are commonly used in the chemical, metallurgical, and catalyst manufacturing industries. Their practicality is evident in their ability to simultaneously mix and heat material as part of a manufacturing process involving the drying or calcination of solids. Powder flow and heat transfer in rotary calciners and dryers are difficult to predict, which can result in reduced product quality. Calcination and drying are also known to be extremely energy intensive processes and calcination alone is estimated to consume around 3% of the world's energy. An ongoing challenge is the scale-up of calcination and/or drying in rotating drums from the laboratory and pilot plant scales to the manufacturing scale. Developing such fundamental understanding of rotary calcination and drying can improve product quality and cut energy and material costs. Our research seeks to provide a methodology for scale-up through understanding of the effects of material properties, operating conditions and calciner/dryer size on the rate and uniformity of heat transfer.

Baffles or flights are often introduced on the walls of the drum in order to improve the rate and uniformity of heat transfer of the powder bed. However, the introduction of baffles is usually done using a trial-and-error approach as there is not a good understanding of how the baffle properties affect the rate of heating of the powder. In this work we carry out DEM simulation of heat transfer in a rotary kiln in order to investigate the effect of baffles on the rate and uniformity of heat transfer. We also investigate drums of different sizes in order to develop an understanding of scale-up.

In general, the heat transfer mechanisms include conduction through the solid, conduction through the contact area between particles, conduction through the interstitial fluid, convection by the fluid, radiation between the surfaces of particles and drum, and radiation between neighboring voids. At low temperatures (less than about 700K) and in the absence of highly conductive flowing fluid this results in a low Biot number ($Bi = hd/k < 1$), where h is the heat transfer coefficient of the gas, d is the size of the particles, and k is thermal conductivity of the particles, and the rate of heat transfer is dictated mostly by the thermal conduction through particle contacts. We used the non-linear spring-dashpot Hertz–Mindlin particle contact model which was coupled with heat conduction though particle contacts in our simulation. The extent of heat conduction was based on the overlap between particles. Operating conditions were altered by adjusting the following variables: particle fill level (3%-30%), drum size (15cm-120cm), three baffle sizes, number of baffles (0-16), and the speed of rotation (1rpm-30 rpm).

We observed that the simulation results can be categorized based on the ratio of the baffle height to bed depth and we introduced an optimum condition for adding baffles. A model was proposed to estimate the heating time for particles as a function of the number and size of the baffles for different operating conditions and particle properties, thus providing a method to predict heating in a rotary drum with baffles.

Hot or cool; powder characterization in non-ambient conditions – high- and low-temperature ring shear testing

Denis Schütz[1], Helena Weingrill[1]

[1]R&D Rheology (Anton Paar Gmbh, Graz Austria)

While the behaviour and mechanical coefficients of solids under the influence of temperature is well understood, how this translates to their behaviour when in the form of particulates is not studied in great depth. [1]

In this study, we will show both cryogenic as well as high-temperature measurements exploring the different ways that temperature influences the behaviour of bulk solids using dedicated measurement equipment.

The talk will focus on examples and strategies employed to solve industry centric practical problems. All of these effects have their distinct signatures upon the flow behaviour and of course, play a major role in their caking behaviour. Both the data, their influence upon silo and hopper design as well as interpretations of the underlying mechanisms will be shown.

Special focus will be given on the low temperature interactions, as these are the least understood and studied; here we will intersect specific points such as softening points and glass transition points from Dynamic Mechanical Analysis (DMA) and show their influence (or lack thereof). Finally, several possible thermal screening methods for using a ring shear tester will be presented and their respective merits and disadvantages discussed.

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Influence of temperature on the packing dynamics of powders

Aurélien Neveu[1], Geoffroy Lumay[2], Filip Francqui[1]

[1]Granutools SPRL, Awans, Belgium

[2]GRASP laboratory, CESAM research center, University of Liege, Liege, Belgium

Many parameters are influencing the behavior of powers such as steric repulsion, friction forces, cohesive forces and interaction with the surrounding gas. Both the surface state (rough or smooth surface) and the chemical nature of the grains influence the friction forces. Cohesive interactions may be due to the presence of liquid bridges, electrostatic charges, van der Waals interactions or more rarely magnetic dipole-dipole interactions. Environmental conditions can modify the predominance of these grain interactions. Indeed, moisture is known to influence both surface grains conductivity and capillary bridges formation leading to a modification of the static and dynamic behavior. Moreover, empirical observation seems to indicate that the temperature is affecting the interaction between the grains as well as grain breakage behavior. Precisely controlling the powder temperature during a process requires costly equipment and is almost impossible for large production facilities. Seasonal changes and production in different sites over the globe induce unavoidable variations of the environmental conditions at which the powder is processed. Therefore, understanding the influence of temperature on powder behavior is of great interest to predict a decrease in process performance and elaborate optimal processing conditions. However, previous studies have focused on processes that involve high temperature and mainly considered the influence of temperature on polymer[1] and metal powders[2]. In the present study, we explore the influence of temperature on the packing dynamics of common food and excipient powders. A novel characterization method allowing to accurately investigate the packing dynamics at different temperatures is presented. We show that even low variation of temperature leads to significant changes in the powder packing dynamics. The importance of evaluating the effect of temperature even for processes that do not involve powder heating is thus highlighted. Furthermore, we observe that the Hausner ratio, the common measure extracted from tapped density analysis, is not suitable to account for slight modifications of the powder properties at low variations of temperature. These new results are expected to motivate the development of future investigations to better understand the underlying physical mechanisms that lead to important changes in powder flowability due to temperature.

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The effect of temperature on the flow properties of SiC powders

Pablo García-Triñanes[1,2], Diego Barletta[3], Massimo Poletto[3]

[1]Materials and Chemical Engineering Group, School of Engineering and the Built Environment, University of Greenwich, Chatham Maritime, UK

[2]Wolfson Centre for Bulk Solids Handling Technology, School of Engineering and the Built Environment, University of Greenwich, Chatham Maritime, UK

[3]Dipartimento di Ingegneria Industriale, Università degli Studi di Salerno, Via Giovanni Paolo II, 132, 84084 Fisciano (SA), Italy

* Corresponding author email: p.garciatrinanes@gre.ac.uk

Gas-solids fluidised beds have been widely used in the process industries, due to their excellent mixing and heat and mass transfer performance. Recent thermal energy storage applications require high temperature operation to improve the throughput and controlling powder flowability in these systems is of paramount importance [1,2]. Despite the considerable studies of flow properties performed on ambient temperature fluidised beds, understanding the effect of elevated temperature on flow characteristics and regime transition is still quite insufficient, due to the difficulties in measurements of high-temperature fluidisation systems. In this research, powder measurements using Silicon carbide –SiC– consisting of the determination of bulk. quasi-static, dynamic and shear properties were carried out. The experiments were performed at different temperature conditions from ambient to 500 °C. The experiments considered try to simulate the different pathways taken by these powders as they are consolidated before being fluidised at a given temperature. Experiments at ambient temperature include original and literature data for these Geldart B particles obtained using the FT4 Freeman Technology Rheometer, the PFT Brookfield, the Seville Powder Tester (SPT) and the Schulze Ring Shear Tester while for elevated temperatures bespoke modified versions of the Seville Powder Tester (HTSPT) [3] and the High Temperature Annular Shear Cell (HTASC) [4] were used. Flow functions indicate that at room temperature the powder belongs to the "free-flowing" class and then passes gradually to the "easy-flowing" class at 300 °C and to the boundary between the "easy flowing" and the "cohesive" class at 500 °C. In order to understand the effect of temperature on interparticle forces, the procedure adopted by Tomasetta et al. [4] to estimate the tensile strength was the extrapolation of the linear yield loci to the traction quadrant. Estimated values of the tensile strength obtained in this work with a similar procedure are compared with the results provided by Gannoun et al. [4] on the tensile strength on a very similar powder at similar temperature and similar consolidation stresses. Keywords: Powder rheology; Shear testing; High temperature; Yield locus; Flow regime transition; Tensile strength

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DEM simulation study: the effect of temperature on powder spreading in selective laser sintering

Sina Zinatlou Ajabshir[1,2*], Colin Hare[2], Diego Barletta[1], Daniele Sofia[1], Massimo Poletto[1]

[1]Dipartimento di Ingegneria Industriale, Università degli Studi di Salerno, Fisciano SA, Italy

[2] School of Engineering, Newcastle University, Newcastle upon Tyne NE1 7RU, United Kingdom

*sizinatlouajabshir@unisa.it

Selective laser sintering (SLS) is powder-based manufacturing method that prototypes three dimensional sintered parts by feeding powders sequentially to the powder bed. The quality of spreaded layer of powder on the powder bed by the recoater is vital so that it controls the final mechanical properties of products. Features of spreaded powder layer at each run of the SLS process depends on several parameters, including the temperature achieved in the preheat stage. However, preheating to a higher temperature negatively affects powder flow behavior and can prevent proper spreading because of increasing interparticle forces. Therefore, it is important to analyze the effect of temperature on the powder layer to improve the SLS powder condition and achieve efficient parameters. In order to optimize the proper preheating temperature to enable a high-quality powder layer, and also reduce many experimental trials and errors, Discrete Element Method (DEM) could play an important role to simulate the spreading process in particle scale, where it can estimate the particle-particle and particle- geometry interaction, particles response compared to the situation and replicate the real powder distribution in SLS at powder bed by modelling. This study developed a DEM-based model to simulate the powder spreading process. Anton Paar shear cell experiments were used to calibrate the DEM simulation. The study's outcome made a complete set of experimental and modelling tools to correlate the powder flow properties with the final bed properties at high temperatures. This model considered the spreading powder thickness, the temperature, and finally, the spread tool shape and speed as parameters that affected the final spreading layer quality by DEM-based simulation. In conclusion, this will allow discerning on the powder suitability to be used in an SLS process and the best condition to optimize its layer process preparation at ambient and high temperature.

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DUST AND AEROSOL EMISSIONS

Optimization of a sampling method of airborne metallic ultrafine particles by cascade impactors

Virginie Matera[1], Naïma Gaudel[1], Sébastien Bau[1]

[1]Dept. of Pollutants Metrology, INRS (French National Institute of Research and Safety), Vandoeuvrelès-Nancy, France

For some years, the characterization of workers' exposure to airborne metallic ultrafine particles has been an increasing issue because of their effects on health, and as many activities are potentially concerned (welding, oxycutting, 3D printing ...) [MATERA V. et al, Hygiène et Sécurité du Travail, 2019]. The size distribution of an aerosol associated with its chemical composition and characterization provide a real contribution to the understanding of these effects [OBERDÖRSTER G. et al, Env. Health Perspectives, 2005; MAYNARD A.D. et al, J. of Nanoparticle Research, 2005].

In the framework of proposing characterization methods adapted to occupational situations, the optimization of metal aerosol sampling using cascade impactors is studied. These devices are a valuable aid since both the size distribution of an aerosol and its chemical characterization can be performed on the samples collected. A welding fume setup was used to generate a highly reproducible test aerosol of metallic ultrafine particles (mass median aerodynamic diameter MMAD=430 nm, ρeff =0.55 g.cm-3). Three different individual cascade impactors were studied (MARPLE, SIOUTAS and Minimoudi 135-8); the results obtained were compared to those from the DLPI+ , a static low pressure impactor, used as a reference (particles collected according to 14 size fractions in the range 16 nm – 10 µm) (Figure (a)). In these impactors, particles are mainly collected on impaction supports (PVC, PTFE, MCE membranes). Our results show that (i) the collection substrates have to be prepared beforehand by lubricating them, (ii) the nature and the quantity of the lubricating grease has an influence on the collection efficiency (iii) this optimization allows the phenomena of bouncing and re-entrainment of particles to be avoided/reduced/neglected [DZUBAY T.G. et al, Atmospheric Environment, 1976]. For the test aerosol under study, the cumulative mass distributions obtained by gravimetric analysis of the media on the different impactors used under optimized conditions show that the Minimoudi 135-8 leads to results very close to those of DLPI+ (Figure (b)), thanks to its high resolution in terms of number of stages (8) and low cutoff diameter (180 nm).

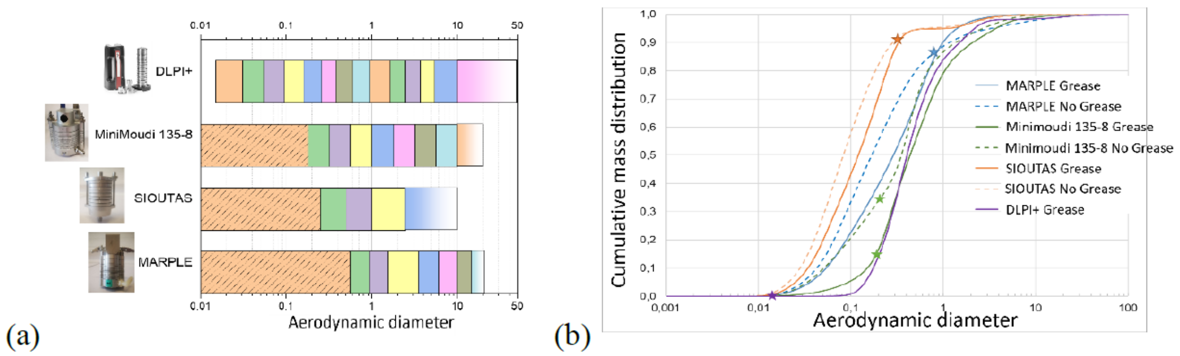

Figure: (a) Particle size classes and associated ranges, (b) cumulative mass distributions functions for supports with and without grease, and for the 4 impactors studied.

Novel technique for economic and continuous analysis of dust exposure levels in real-life production

Michael Pilz[1], Britta Buck[1], Jens Dittmann[1], Rainer Friehmelt[1], Frank Kleine Jäger[1]

[1]BASF SE, Ludwigshafen, Germany

Containment is a concept or technology to keep hazardous substances under control so neither environment nor operators will not be contaminated. Hazardous substances can be present as a solid (dust), fluid (aerosol) or gas depending on their state of aggregation. When handling powders dust containment is essential in protecting the employee and the environment. The proper dust containment strategy is influenced by machinery & apparatuses (MA), maintenance schedules and how often operators need to intervene in plant operations. Typically, the critical dust exposure moment is when an operator needs to interact with MA, such as loading / unloading stations, cleaning of MA and maintenance. In all cases, the occupational exposure limits (OELs) of hazardous products must be considered. Dust concentration and so the OELs are typically determined by gravimetrical measuring methods like the SMEPAC test (Standardized Measurement of Equipment Particulate Airborne Concentration). A defined air flow is sucked by a vacuum pump over a filter piece. This piece is analyzed by differential weighing and the dust concentration can be calculated. This method is slow and gives no time resolution. If there are dust peaks, these cannot be detected, because only the total dust amount can be analyzed.

We have developed a novel measuring method to determinate the dust situation in a much faster way. Therefore, an optical method was used and enhanced. The advantage is, that the dust concentration can now be analyzed with a high time resolution. This method uses optical particle counter, which produce a number-based concentration curve. This curve is then recalculated into a time dependent mass concentration by a specific calibration, based on density, form factor and refractivity. Since these calibration factors are typically not available for real-life dust of production plants, instead an environmental specific calibration factor can be determined by using the gravimetrical method. This gives a shift factor, which can be used to calibrate all other measurements. The filter piece can also be used for a chemical analysis, from which the element-specific concentration curves can be recalculated as well. This novel method is highly flexible and can be applied to multiple use cases: Within a production plant (e. g. powder filling unit) measurements are possible during running production. The results show critical processing steps for environment and operator.

The optical dust sensors can also be used for continuous monitoring of production plants. Several sensors can be integrated into a sensor network to monitor specific equipment or even the complete plant, implementing an early warning system, that evaluates the real dust situation in time. Optical sensors used are based on “low-cost sensors” (price ~ 20$ per sensor unit) and are shown to run stable for several month allowing fully automated monitoring and analysis of the particle size. This novel technique enables an economic and rapidly available view of the dust containment strategy compared to conventional methods.

Impact of powders flowability improvement on their dustiness generation

Maria-Camila Jiménez-Garavito[1,2], Maria-Graciela Cares-Pacheco[2], Fabien Gerardin[1], Véronique Falk[2]

[1]Institut national de recherche et de sécurité, 54519, Vandœuvre-lès-Nancy, France

[2]Laboratoire de Réactions et Génie des Procédés, 54000, Nancy, France

Powders are part of the design, production, and final products of different industrial sectors. Their handling, packing, and storage are subjects of interest because of the difficulties arising during manufacturing due to flow problems. Powders flow behavior can be improved by: modifying the facilities, which is a seldom universal solution; by the fluidization of powders, involving separation operations and so increasing process complexity; and by the addition of nanoparticles (NP), which is considered the more effective solution with the best benefit/cost ratio. Nowadays, nanomaterials (NM) are essential to the product conception of many industrial sectors, such as medical, cosmetic, food, and aerospace. The global production of NM has been estimated at 11 million tons per year with a market value of 20 billion euros in 2012. Among them, silica nanoparticles (S-NP) are widely used as food and pharmaceutical excipients for different purposes. According to the Handbook of Pharmaceutical excipients, S-NP work as a thickener and stabilizer in emulsions; they favor the particles suspensions in aerosols and enhance the flow behavior of dry powders. From a technological point of view, the addition of flow regulators in powders has been based on practical experience, trial, and error. Industrials add about 0.5 to 2% w/w of S-NP to their formulations. From a safety point of view, the US Food and drug administration (FDA) and the European food safety authority (EFSA) approve S-NP as a food additive. Nonetheless, even if the regulation entities still consider S-NP as nontoxic and nonirritant, their toxicity has been a recurring concern over the years. Several in vitro studies have shown that S-NP are toxic in different types of human and animal cell lines. In vivo studies have also demonstrated toxicity on rats. However, these results are not scaled to real human exposure and health effects because of the complications to represent a realistic exposure or the lack of epidemiological data. An exposure study done in Swedish foundries found that workers exposed to respirable silica presented elevated morbidity from strokes compared to the average morbidity, which to some extent evidences the relationship between exposure and the effect on human health. The results of the interaction of nanoparticles with humans and the environment have not yet been well evaluated, and this will only be effective with a scientific and legislative effort at the international level. In collaboration with the French National Research and Safety Institute (INRS), our project aims to determine the relationship between two end-use properties of powders, their ability to flow, enhanced by the use of glidants, and generate dust. Here, we study the improvement of the flowability of four industrial powders (microcrystalline cellulose, wheat flour, joint filler, and glass beads) by the addition of four references of S-NP. The flow behavior was determined using an Instron press through compactness measures. The effect of the flow enhancement on their dustiness generation was studied using a rotating drum and a vortex shaker. Our results show that increasing flow behavior using glidants increases the sample's dustiness considerably.

SATURDAY, 9 JULY 2022
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FROM PARTICLE CONTACTS TO BULK BEHAVIOUR

Modeling snow deformation: from a meso grain to bulk behavior

Mohammed Hassan[1], Eelco Verhulp [2], Vanessa Magnanimo[3], Stefan Luding[4]

[1]MSM-ET-TFE, University of Twente, Enschede, Netherlands

[2]Apollo Tyres Global R&D B.V., Enschede, Netherlands

[3]CME -ET, University of Twente, Enschede, Netherlands

[4]MSM-ET- TFE, University of Twente, Enschede, Netherlands

Snow deformation behavior has been studied extensively. This interest arises from the importance of different encountered problems e.g., Tire Snow traction, avalanche release. Snow exhibits different deformation behavior under different strain rates. This wide range of behavior is due to intrinsic grain-grain collision, different types of existing bonds also known as bond matrix. To capture the plastic deformation and cohesion of Snow, an adhesive plastic viscoelastic contact model was used. Where we approximate different types of possible bonds to a single virtual bond. Two tests were performed on a representative volume element (RVE) of spherical particles. Meso-macro transition properties were obtained using a coarse-graining approach on the given RVE system.

First, a strain-controlled uni-axial compression test on a confined RVE under different strain rates was performed. Because of the difficulty of parametrization of the DEM model. A bulk calibration approach based on Machine Learning of strain-stress relation was used to tune the model parameters. Second, using the tuned parameters a simple direct shear test under different shear rates was performed.

Results reveal dependency of the adhesion also known as pressure sintering on the degree of Snow compaction. A good agreement between calibrated uni-axial compression and literature results was obtained. A classic granular rheology relation of macroscopic shear stress to the dimensionless inertial number was obtained.

A Study on the charge neutralising effect of Aluminium Stearate in triboelectrification

Jiachen Guo[1,2], Wei Pin Goh[1], Mojtaba Ghadiri[1]

[1]School of Chemical and Process Engineering, University of Leeds, Leeds, UK

[2]College of Civil Aviation, Nanjing University of Aeronautics & Astronautics, Nanjing, China

Aluminium stearate is a common metallic soap that is widely used as a thickener in paint, a water repellent and a lubricant in various industries. Depending on its synthesis process, aluminium stearate can exhibit three different crystalline forms of mono-, di- and tri-stearate, the most common one being aluminium di-stearate. Apart from having superior lubricating properties, it is also an excellent charge neutralising agent for preventing wall fouling in a fluidised bed reactor caused by electrostatic charge build-up. However, the underlying charge mitigating mechanism of this metallic soap is still not very well understood and hence it is a topic which requires further investigation.

The long stearic acid chains present are structured very differently for the three crystalline forms of aluminium stearate. The focus of this work is to study the role of structural difference of these surface stearic acid chains in electrostatic charge reduction. Assemblages of glass beads are made hydrophilic and hydrophobic through hydroxylation and silanisation. These glass beads are then dry coated with the three different stearates, separately and evenly, using the ProCepT, a high shear mixer. A novel method based on aerodynamic dispersion technique is then used to characterise the charge level of these blended mixtures of aluminium stearate and glass beads, of which the results will be presented and reported here.

Adhesive particle-particle contact and how it affects ceramic's bulk flow behaviour

Zohreh Farmani[1], Joshua A. Dijksman[1]

[1]Dept. of Physical Chemistry and Soft Matter, University of Wageningen, Wageningen, The Netherlands

Interparticle forces are very relevant for granular flow dynamics. Here we experimentally probe whether adhesive characteristics of particles also affect the rheology of such particle suspensions. We used ceramic microparticles with size distribution between 10-100 µm; these particles are base materials for porcelain stoneware. We characterize particle adhesion forces by using colloid probe atomic force spectroscopy. We find that acidic and basic environments can induce an increase in the adhesion capacity of certain types of ceramic particles. Additionally, the adhesion force can be contact time and retraction speed dependent; results repeat over many cycles. We attribute the adhesion dynamics to the presence of clay inside the ceramic microparticles. The adhesive properties of the ceramic microparticles also may affect their collective behavior in suspension, as we confirm that the rheology of ceramic microparticle suspensions is strongly pH dependent. Our results suggest that adhesive particle properties are relevant to consider in the analysis of suspension dynamics.

From particles to continuum: Review of micro-macro approaches

Stefan Luding[1]

[1]Multi-Scale Mechanics (MSM), Department Thermal and Fluid Engineering (TFE), Faculty of Engineering Technology (ET), MESA+, POBox 217, 7500AE Enschede, NL

Email: s.luding@utwente.nl; Website: http://www2.msm.ctw.utwente.nl/sluding/

The behavior of particle systems – like sand, powder, suspended particles, or colloids – is of considerable interest in a wide range of industries and research disciplines. These materials are intrinsically disordered, often come with a wide distribution of particle sizes or shapes and materials/mixtures and can behave both solid- or fluid-like. The related mechanisms/processes in particle systems are active at multiple scales (from nanometers to meters) and understanding them is an essential challenge for both science and application, i.e., finding the reasons for natural/industrial disasters like avalanches or silo-collapse, hampering industrial performance. In order to understand the fundamental micro-mechanics one can use particle simulation methods [1-5], where often the fluid between the particles is important, but neglected here. Large-scale applications (due to their enormous particle numbers) have to be addressed by coarse-grain-models or by continuum theory. In order to bridge the gap between the scales, socalled micro-macro transitions are necessary, which translate particle positions, velocities and forces into density-, stress-, and strain-fields. These macroscopic quantities must be compatible with the conservation equations for mass and momentum of continuum theory. Furthermore, non-classical fields are needed to describe the micro-structure [2-5] or the statistical fluctuations, e.g., of the kinetic energy [3,4], before one can reach the ultimate goal of solving application problems. Modern examples of multi-scale simulations and micro-macro methods involve additive manufacturing and other multi-phase flow processes, where particle- and continuum-methods are coupled, the dosing of cohesive fine powders in vending machines, avalanche flows on inclined slopes, segregation/mixing, rheology testing in ring-shear cells, as well as the study of non-linear elasto-plastic material mechanics related to the failure of solids.

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Implementation and Calibration of a Viscoelastic Bonded-Particle model: comparison of Burgers and Generalized Maxwell Relations and their flow prediction ability

Michael Mascara[1,2], Arno Mayrhofer[1], Stefan Radl[2], Christoph Kloss[1]

[1] DCS Computing GmbH, Industriezeile 35a, 4020 Linz, Austria

[2] TU Graz, Institute of Process and Particle Engineering, Inffeldgasse 13/III, 8010 Graz, Austria

The Discrete Element Method (DEM) is rapidly becoming the most used tool in industry, when dealing with granular materials. However, some processes involve materials which are granular in nature, but behave as a homogeneous solid and can flow. These materials are classified as “visco-elastic” and it is usually challenging to predict their behavior. In order to solve this problem, an innovation to the contact dynamics, called Bonded Particle Model, has been developed by Potyondy and Cundall [1], where the particles interact with their neighbours via a solid bond without necessarily overlapping. Moreover, a visco-elastic constitutive relation is solved in each bond, depending on the relative motion of the interacting particles.

Within the visco-elastic class, many different materials, such as slurries, pastes, asphalt, polymers, whose are used in various industrial processes, can be found. As of today, both experiments and mesh-based methods have been used to describe these materials. If experiments are limited by the fact that they can only give so much information of a material in specific conditions, mesh-based methods, on the other hand, need to solve complex tensormodified Navier-Stokes equations to solve the flow properties of a given material. Moreover, the use of a mesh makes it trickier to apply it to moving parts of a process machine, for example.

In this contribution, two constitutive relations, namely the Burgers and the Generalized Maxwell, are implemented. Oscillatory rheometer simulations are performed, highlighting the effect of lattice configurations and particles’ size on the material rheology. Moreover, using experimental results as input, a calibration is carried out to connect micro-scale parameters with meso/macro-scale behavior of the material.

At this point, given the results of the comparison between the two constitutive relations, the preferred one is chosen. Moreover, two visco-elastic materials, whose micro-parameters are obtained through calibration, are simulated in a simple extrusion process.

The latter shows how the predicted flow properties of the materials are in accordance to what is observed in the simulation, hence proving the reliability of the model in larger-scales.

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Concrete parts from the powder bed – Material modification for selective cement activation

Niklas Meier, Harald Zetzener, Arno Kwade

Institute for Particle Technology, TU Braunschweig, Braunschweig, Germany

Keywords: concrete, powder bed, 3D-printing, SCA, flowability, porosity

Concrete buildings are an indispensable part of modern life. However, there are some major drawbacks of concrete, such as large amounts of CO2 that are released during the production of cement. In theory, it is possible to produce load-bearing components with optimised shapes and thus reduce the amount of concrete used. These shapes are often too complex for conventional concrete manufacturing. Therefore, among other processes, additive manufacturing processes such as concrete 3D-printing using selective cement activation (SCA) are current research topics: SCA is a so-called powder bed process, in which the concrete part is built up layer by layer. For each layer, a mixture consisting of aggregate (sand) and cement is first applied to form a homogeneous and even powder bed. Subsequently, water is selectively sprayed onto the powder bed and hydrates the cement in the desired area. As SCA is a comparatively new process, there are some major challenges, currently: 1) the achievable strengths are still too low for structural use, 2) the shape deviations of the components from the initial design and 3) a high cement content must be used to achieve good component properties. To meet the above-mentioned challenges of the process, the powder properties of the aggregatecement mixture for the SCA process are investigated. One reason for the low strength is the high porosity of the printed components in comparison to conventionally produced structural concrete. Therefore, one goal is to improve the flowability of the powder since it leads to a reduced porosity of the compacted powder. To achieve this, the surfaces of the starting materials are modified in dry processes using nanoparticles or liquid additives. The effects of the modifications are characterised by means of the flowability, bulk density and tamped density. In addition, the density of the compacted bulk material is determined in an SCA prototype printer and compared to the previously mentioned characterization methods. The particle size distribution of the aggregate fraction is systematically adjusted to reduce the porosity of the compacted powder bed in the printer. Furthermore, by substituting cement with fine aggregate particles, the necessary amount of cement is to be reduced with as little negative influence on the component properties as possible, such as strength. To link the above-mentioned experiments with the SCA manufacturing process, test specimens are printed and evaluated by the project partner iBMB (TU Braunschweig). Initial tests have shown that both bulk and tamped density can be increased by surface modification and the compressive strength of printed components can be improved by more than 25 %.

Prediction of bulk flow properties using mechanical surface energy tester

Vivek Garg, Tong Deng, Richard Farnish, Michael Bradley

The Wolfson Centre for Bulk Solids Handling Technology, School of Engineering, Faculty of Engineering & Science, University of Greenwich, Central Avenue, Chatham, Kent, ME4 4TB, UK

Particle adhesion force plays a critical role in powder handling operations and processes. There are many widely used methods, such as atomic force microscopy (AFM) and centrifugal detachment. However, most methods have limitations when the measurements are correlated to the bulk behaviour of powders, such as powder flow with varied particle size distributions. The study focuses on a unique test technique for measuring forces between particles and surfaces using cohesive powders, which includes a mechanical surface energy tester developed at The Wolfson Centre. The work focuses on predicting the powder flow function using a novel technique in conjunction with common particle attributes, with the goal of predicting flowability problems at an early stage of formulation using only a small amount of powder sample.

A successful strategy has been devised by linking the aggregated particle Bond number (found using the innovative test procedure) with the flow function of the powder. The experiment was undertaken with a wide range of materials and particle sizes. Particle adhesion to a variety of surfaces (both compacted powder and solid materials) has been investigated. The methodology yields good outcomes.

A model has been developed and verified using a large variety of powders, and it is able to predict additional bulk flow property parameters such as unconfined failure strength, compressibility, the effective angle of internal friction, bulk density, and flow function.

SATURDAY, 9 JULY 2022
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ADDITIVE MANUFACTURING AND POWDER SINTERING

Surface tailored metal particles for additive manufacturing

Arne Lüddecke[1], Harald Zetzener[1], Jan Sehrt[2], Arno Kwade[1]

[1]Institute for Particle Technology, Technische Universität Braunschweig, Germany

[2]Hybrid Additive Manufacturing, Ruhr-Universität Bochum, Bochum, Germany

Keywords: Additive manufacturing, PBF-LB/M, Powder flowability, Nanoparticles

Additive manufacturing (AM) of metals is used particularly in the automotive, aircraft and medical industries. The advantages of additive processes are the realization of complex structures without geometric restrictions, especially in lightweight and prototype construction. Major challenges are still low productivity and high costs of the process, which is why an application in series production is not yet implemented as a standard. Among the many different AM processes, powder bed fusion of metals with a laser beam (PBF-LB/M) is considered a promising technique for the transition from rapid prototyping to series production. In PBFLB/M, a powder layer is applied to a build platform, selectively molten with a laser and finally building up the complete component layer by layer. Currently, an increase in productivity is achieved by higher laser intensities or the use of multiple lasers, i.e. this leads to an increase in investment and operating costs while less costly optimization methods are neglected. The approach of this work is to improve the efficiency of the process on the powder side by modifying the metal particle surface. For this purpose, a metal powder (stainless steel 1.4404) already established in PBF-LB/M is coated with silicon carbide (SiC) nanoparticles or graphene platelets. The coating is performed both in dry mode by dry mixing (high-intensity mixer and 3D shaker mixer) and in wet mode by a fluidized bed process. Previously published results show increased laser beam absorption, better flowability and improved component properties for wet coated metal powders with SiC. In the present paper, the surface quality of the coated powders as a function of mixing or spraying time is presented using among others scanning electron microscope measurements. In particular, the characteristic properties of the powders after wet and dry coating are compared. Furthermore, the influence of the coating quantity, as well as a changed additive particle size, will be analyzed. In addition to the surface quality, absorption measurements of the modified powders and the influence of nanoparticulate additives on the microstructure of manufactured specimens will be demonstrated. Another central topic is the improvement of the flowability caused by the surface modification, where especially the stress states of the real process are relevant. Measurements with the ring shear tester at low normal stresses are compared with dynamic measurement methods, such as the dynamic angle of repose, to show the differences between the measurement methods. In addition, a spreadability test rig that simulates the relevant stress conditions in the manufacturing process is used to investigate powder samples using X-ray microtomography (μCT) regarding i.e. porosity and surface roughness of the powder bed. Hence, the porosity of the bulk material can be determined as a function of the application speed and modification.

Material properties and process parameter optimization in Selective Laser Sintering of polymers

Federico Lupone[1], Elisa Padovano[1], Francesco Casamento[1], Claudio Badini[1]

[1]Dept. of Applied Science and Technology (DISAT), Polytechnic of Turin, Turin, Italy

Corresponding author: Federico Lupone (federico.lupone@polito.it)

Keywords: Selective Laser Sintering; process optimization; isothermal laser sintering model; stable sintering region; attenuation melt ratio.

Selective Laser Sintering (SLS) is an additive manufacturing technology that is widely used for rapid prototyping and low-volume production of polymer based parts. SLS is a complex multi-physical process that involves various physical phenomena with different timescale (such as laser irradiation, thermal diffusion, coalescence and crystallization). Therefore, the optimization of process parameters represents one of the major drawbacks of the technique. Generally, an empirical approach based on iterative trial-and-error builds is used, but it is time consuming, costly and it ignores the properties of the raw powders. This presentation provides new results into the prediction of process parameters starting from material properties. The model of quasi-isothermal laser sintering and the stable sintering region approach has been applied to optimize the powder bed temperature (Tb) and laser exposure parameters respectively. A polyamide 12 powder reinforced with short carbon fibers (PA12/CF) was used to validate the method. The results show that the analysis of isothermal crystallization kinetics is effective to guide the choice of the powder bed temperature, thus avoiding distorsion of the printed parts. The stable sintering region defines the process window between polymer melting and degradation. This region can be conveniently expressed in terms of energy density using the attenuation melt ratio (AMR) parameter, which puts into relation material properties and process parameters. However, the analysis of void content, tensile strength and dimensional accuracy of the printed parts reveals that the range of laser energy density values suitable for optimal part properties is smaller than the stable sintering region. Benefits and drawbacks of the proposed method are highlighted along with suggestions on possible improvements on the basis of the analysis of the physical phenomena involved in the SLS process. In fact, increasing the predictive quality of the laser sintering process window will help to develop new materials, offering potential to save time and cost whilst maximizing part properties. An example of material development is presented in relation to the research activities performed at Polytechnic of Turin.

Fluidized bed machining of AlSi10Mg samples produced by additive manufacturing

Maurizio Troiano[1], Andrea El Hassanin[1], Alessia Teresa Silvestri[1,2], Fabio Scherillo[1], Fabrizio Scala[1], Roberto Solimene[3*], Antonino Squillace[1], Piero Salatino[1]

[1]Dipartimento di Ingegneria Chimica, dei Materiali e della Produzione Industriale, Università degli Studi di Napoli Federico II, Napoli, Italy

[2]Dipartimento di Ingegneria Gestionale, dell'Informazione e della Produzione, Università degli Studi di Bergamo, Bergamo, Italy

[3]Istituto di Scienze e Tecnologie per l'Energia e la Mobilità Sostenibili, Consiglio Nazionale delle Ricerche, Napoli, Italy

*corresponding author: roberto.solimene@cnr.it

Keywords: Selective Laser Melting, abrasive fluidized bed, roughness, surface finishing
Surface finishing of AlSi10Mg samples produced by Selective Laser Melting (SLM) technology has been investigated.

Surface roughness represents one of the most critical variables during the production of metal parts by powder bed-based additive manufacturing technologies, such as SLM. This issue affects in a remarkable way the mechanical, tribological and corrosion resistance properties of the final objects. As a consequence, objects produced by additive manufacturing technologies need to be further worked with post-process surface finishing techniques. The most common finishing methods such as Computer Numerical Control (CNC) machining, shot peening, electrochemical polishing and laser polishing are limited to objects with low geometrical complexity, while in principle, fluidized bed finishing (Fluidized Bed Machining) can be suitable also for parts with complex geometries, thanks to the mobility of fluidized particles and flowability of the emulsion phase.

In this study, the employment of the Fluidized Bed Machining technology is investigated for the surface finishing of AlSi10Mg parts. The fluidized bed apparatus consists in a Plexiglas fluidization column (inner diameter 0.21 m) which comprises a ceramic rings-filled windbox and an upper section 1.4 m high where the abrasive material is located. Two kinds of experiments have been carried out, while varying the abrasive material and some operating parameters. A first set of experiments is carried out with a stationary sample dipped into the fluidized bed under bubbling fluidization conditions, for different abrasive materials, process time and relative tilt angle between the sample surface and the fluidized material. A second set of experiments is carried out to evaluate the effect of the rotation on the surface finishing of the samples, with the abrasive material kept at minimum fluidization conditions. In this case, the rotation of the sample is provided by means of an electrical motor regulated by an inverter and the effect of the abrasive material, tilt angle of the sample and rotational speed is investigated. For both the experimental sets, the surfaces are characterized quantitatively before and after the tests by means of different surface texture parameters analyzed by means of confocal microscopy and weight loss measurements, while SEM images are acquired to establish the physical morphology evolutions experienced during the treatment. Results show that shear and energy dissipation induced by rotation of the sample significantly improve surface finishing, especially under specific operating conditions in terms of tangential speed and tilt angle.

Quantitative analysis of the powder layer quality in the Selective Laser Sintering process: Experiments and DEM modelling

Marco Lupo[1], Daniele Sofia[1,2], Diego Barletta[1], Massimo Poletto[1]

[1]Dept. of Chemical Engineering, University of Salerno, Salerno, Italy

[2]Sense square Srl, Salerno, Italy

Selective Laser Sintering (SLS) is an additive manufacturing process by means of which three-dimensional objects can be produced using a laser beam to selectively sinter powder particles. Many are the advantages of SLS, among which are the capacity to build high resolution and very complex shaped objects by using many materials. However, one drawback of SLS is the quality of the powder layer, which depends not only on the powder flow properties but also on the operating conditions. In particular, spreading of powder is a crucial step. Collecting information about the spreadability, that is the capacity of the powder to be spread, is relevant to optimize the distribution and the layering of powder.

A DEM model was created to simulate the spreading of powders with the future intent of understanding the mechanisms and the powder properties which are responsible for the good or bad quality of the layer. The Hertz-Mindlin (no slip) with JKR cohesive model was used to describe interparticle interactions. Three different approaches were tried to calibrate the model parameters and the one based on the comparison between the experimental bulk density and porosity with those measured from the simulations turned out to be the right one. The interfacial adhesive surface energy between the particles was estimated by assuming that the pull off force should provide the strength of the material under low consolidation. This latter was evaluated on the basis of shear test experiments. The particle rolling friction was calibrated considering the bulk density of the layer produced by the spreading tool.

The DEM model and the calibration procedure adopted were validated with the experiments by comparing the wavelet power spectrum applied to greyscale images of the layers obtained with the simulations and to grayscale images of the experimental layers illuminated by grazing light. Therefore, the DEM model allows to quantitatively evaluate the quality of the powder layer, i.e. in terms of dimension of surface asperities, obtained through deposition in the same spreading conditions of the experiment.

Keywords: Selective Laser Sintering, Powder layer formation, Discrete Element Method, Model calibration, Model validation, Quantitative analysis

Spreadability versus flowability: Transient jamming makes them different

Wei Pin Goh[1], Wenguang Nan[1,2], Mehrdad Pasha[1,3], Mojtaba Ghadiri[1]

[1]School of Chemical and Process Engineering, University of Leeds, Leeds, UK

[2]School of Mechanical and Power Engineering, Nanjing Tech University, Nanjing 211816, China

[3]UCB Pharma, Chemin du Foriest B-1420 Braine l'Alleud, Belgium

In additive manufacturing by application of radiation energy to a powder bed, fine powder is first spread by a blade or a roller to form a thin layer. The quality of layer in terms of the uniformity of the particle spread is critical for the quality of the final product, being free from defects. The ability of powder to be spread uniformly as a thin layer is described by spreadability. This depends on particle properties as well as the dynamic of the spreading process, and is commonly assessed by common flowability testing. However this approach might not give a full indication of powder spreadability because flowability testing is essentially a bulk testing method, where the failure in a natural bulk plastic zone gives an indication of flowability. There are two shortcomings in this approach which can affect the outcome, one is the absence of a narrow gap, in which transient jamming occurs, as prevailing in the powder spreading process, and another is the powder rheology in narrow gaps, which cannot be assessed not only by flowability tests, but also by powder rheometry. This requires an understanding of transient jamming and powder rheology in narrow clearances, a topic of investigation here. In this presentation, both experimental and numerical analysis by Discrete Element Method have been carried out comparing the outcomes of flowability and spreadability assessments using a powder rheometer (Freeman Technology FT4) and also spreading by a blade. A special methodology is suggested for assessing the spreadability of a powder.

Modelling of selective laser sintering of visco-elastic powders

Juan E. Alvarez[a], Bert Nijkamp[a], Hongyang Cheng[a,b], Stefan Luding[a], Thomas Weinhart[a]

[a]Multi-scale Mechanics, University of Twente, The Netherlands.

[b]Department of Civil Engineering, University of Twente, The Netherlands.

In laser 3D printing, the neck-growth determines the dimensional accuracy and surface quality of the final printed object. This industrial application employs a laser source to selectively irradiate particle surfaces, causing interparticle penetrations and densification of the powder bed. How to model this process numerically remains a challenge due to the different involved time scales and the accuracy of the energy absorption model. The present study provides a novel insight to computationally assess the neck-growth of visco-elastic particles caused by a laser source. First, an absorption model is built based on the transmission and reflection of visco-elastic powders. It provides the absorbed energy while particles are overlapping, and therefore the temperature evolution. Then, the discrete element method (DEM) for heat transfer problems is used with a new definition of a sintering regime map for visco-elastic materials. It describes the influence of both temperature and material flow during the sintering process. This approach is supported by MercuryDPM software and GrainLearning tool, both open-source packages. Finally, the present model qualitatively predicts the experimental observations on the laser sintering of PS and PA12. It is shown that the neck-growth kinetics is determined by the transient rheology caused by the finite relaxation times of visco-elastic materials and the time-dependent temperature evolution, which affects the fluidity of the samples.

Email address: j.e.alvareznaranjo@utwente.nl (Juan E. Alvarez)

A comparative study on polymeric materials for the selective laser sintering process

Daniele Sofia[1,2], Diego Barletta[1], Massimo Poletto[1]

[1]Dept. of Chemical Engineering, University of Salerno, Salerno, Italy

[2]Sense square Srl, Salerno, Italy

The Selective Laser Sintering process consists in the production of a product starting from a granular material. The object is formed layer-by-layer in an instrument which repeatedly places a layer of powder on a growing bed, on which a laser beam will selectively act. Therefore, in this process, energy is supplied only to the powder that occupies the portion of the surface identified as necessary for the formation of the final product.

In order to obtain a good results right sintering energy should be delivered on the powder planes so that it can connect the sintered parts in the underlying layers. To this purpose the most critical parameters are the temperature of the powder bed, the thickness of the layers and the laser scanning speed. Another important parameters are the properties of the powder, such as size, particle size distribution and the particle shape.

In this study, a commercial equipment with a laser source in the wavelength of 420nm was used to conduct the SLS process on different polyamide powders. The sintering results are compared with those obtained using PA12 with PA6, two of the most used material with laser sintering of polymers. The main purpose of this study was to evaluate the feasibility of using new types of powders by looking at the final mechanical properties of the artefact and relating them to the initial flow, optical and thermal properties of the powders.

Keywords : Selective Laser Sintering, Mechanical properties, Powder bed, Powder Properties, layer thickness.

A new approach to quantify powder's bed surface roughness in additive manufacturing

Hamid Salehi[1, 2], John Cummins[1], Enrico Gallino[3], Neil Harrison[4], Ali Hassanpour[5] and Michael Bradley[1]

[1]Wolfson Centre for Bulk Solids Handling Technology, University of Greenwich, Chatham, UK

[2]School of Engineering, University of Greenwich, Chatham, UK

[3]RICOH UK Products Ltd, Priorslee, Telford, UK

[4]Carpenter Additive, Widnes, UK

[5]School of Chemical and Process Engineering, University of Leeds, Leeds, UK

The quality of the final items created utilising powder bed Additive Manufacturing methods is influenced by the surface roughness of the powder bed. This study describes the development and usage of a new technique and prototype device for simulating the formation of a powder bed and revealing its surface features. The tester was successfully used to analyse powder bed relative packing fraction, change in particle size and shape across the build plate, and electrostatic charges over the powder bed. Different plastic and metal powders, Different recoater gap size as well as two recoater blade shapes, were used in this study. To assess powder bed surface roughness, an unique shadowgraphy technique based on lighting the surface with low-angle collimated light and analysing the image was used. There were two main measures that were discovered to be beneficial in quantifying the surface roughness of the powder bed. The first measure is the amplitude of variation in surface height, which is defined as the difference between the average surface height over 100 data points and the surface height at each data point. The wavelength of roughness, which is determined as the average horizontal distance between positive peaks across 100 data points, is the second metric. The surface roughness results demonstrated that the shadowgraphy approach, as well as the metrics generated by this method to quantify powder bed surface roughness, can quantify and discriminate diverse powder bed features (and therefore potential quality failures in the bed). These measures effectively reflected the effects of many spreading variables on the powder bed surface roughness, such as recoater shape, gap size, and especially the powder flow functions.

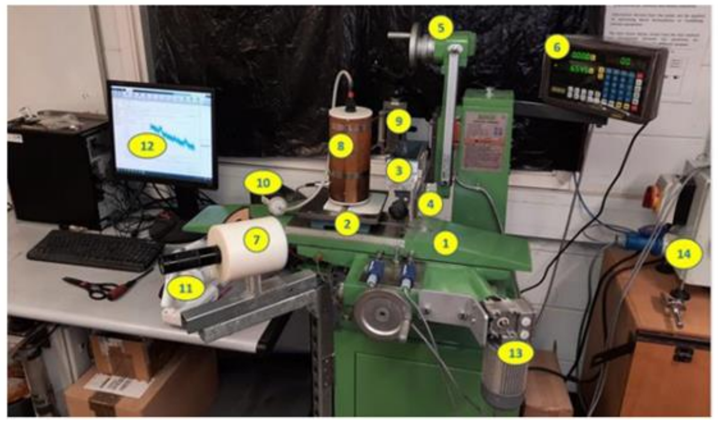

Figure 1. AM Powder Spreadability Tester based at The Wolfson Centre.

SATURDAY, 9 JULY 2022
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PARTICLE DEFORMATION

Particle-wall collision characteristics for non-spherical particles under normal impact: Numerical investigation

Rahul Tarodiya, Avi Levy

Dept. of Mechanical Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel

The particle-wall collisional behavior is known to be one of the critical factors influencing the particle motion during simulation of multiphase flow processes. The coefficient of restitution (COR) is generally used to characterize the particle-wall collisional behavior. The more accurate the COR considered for numerical simulations, the more accurate the resulting outputs will be. For spherical particles, determining COR is simple; however, for non-spherical particles, which are regularly encountered in real-world applications, determining COR is complex due to the unpredictable behavior of the particles after impact. In this paper, the COR during the normal impact of a rigid ellipsoidal particle on the target wall is investigated using the finite element method (FEM). The loss in kinetic energy of the particles after impact is used to analyze the COR. The simulations are conducted with a particle of sphericity 1, 0.9, 0.8, 0.7, and 0.5 impacted at different orientation angles (angle between particle major axis to the horizontal plane) in the range 0º to 90º. The effect of particle sphericity, particle orientation before impact, and impact velocity on COR is determined. Further, an understanding has been established to estimate the deviation in COR for the impact of non-spherical particles as compared to the COR for the impact of spherical particles. The present study helps to provide important engineering insights to calculate the motion of non-spherical particles in multiphase processes using the discrete element method (DEM).

Keywords: Particle-wall collision; Normal impact; Coefficient of restitution; Non-Spherical particle; Granular materials

Discrete Element Modeling of strongly deformed particles in dense shear flows

Nazanin Ghods[1], Payam Poorsolhjouy[2], Marcial Gonzalez[3,4], Stefan Radl[1]

[1] Institute of Process and Particle Engineering, Graz University of Technology, Inffeldgasse 13/III, 8010, Graz, Austria

[2] Department of the Built Environment, Eindhoven University of Technology, 5612 AZ Eindhoven, Netherlands

[3] School of Mechanical Engineering, Purdue University, West Lafayette, IN 47907, USA

[4] Ray W. Herrick Laboratories, Purdue University, West Lafayette, IN 47907, USA

Soft solid or fluid particles, such as gels, rubber, cells, droplets, bubbles, are ubiquitous in many industries and applications. Taking into account the deformability of soft particles is essential for correct understanding of their bulk and mechanical behaviour. The discrete element method (DEM) is a powerful, widely used numerical approach to study particulate systems at the particle scale. In the current study, we introduce a new formulation of the multi-contact (MC) force closure [1] for the DEM. The response of this new force closure has been verified by comparing the results for various compression cases with the results of a reference simulation [2]. This reference simulation uses a highly accurate nonlocal formulation of contact mechanics in the quasi-static limit, in which the interplay of deformations due to multiple contact forces on a single particle is considered. The comparison of the results shows a significant improvement over the existing multi-contact model. The calibration of the parameters in our new MC force closure is also presented.

In order to to probe the effect of particle volume fraction and the shear rate, an extensive campaign of simple shear flow simulations of dense packings of particles was performed. These simulations show that the pressure at particle volume fractions greater than a critical value depends not only on the friction coefficient and particle stiffness, but also on the Poisson's ratio of the material. Finally, a response surface for the pressure in granular shear flows as a function of key parameters is reported. This response surface is highly beneficial for calibrating DEM model parameters in extremely dense configurations.

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Water content related changes on wood pellet properties

Abdullah Sadeq[1], Swantje Pietsch[1], Maksym Dosta[1], Stefan Heinrich[1]

[1]Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology, Hamburg, Germany

Constantly rising prices for heating oil and natural gas in households and their environmental impact lead to a rising interest in renewable raw materials. Wood pellets are small cylindrical compacts from natural wood, primarily from sawdust and wood shavings. They are used as a versatile biofuel with a significant lower emission of the climate-relevant carbon dioxide compared to fossil fuels. These pellets can be burned using a variety of technologies, such as home heating stoves or institutional boiler systems. To ensure the burning efficiency of the pellets, their quality must remain constant during preceding processes such as transport and storage. However, an increased water content due to storage under conditions with high humidity can lead to a reduction in quality, e.g. by a decrease of their mechanical strength. Together with the stresses and friction caused by the subsequent transport, an undesirably high level of fines is produced, which can block the conveying systems. According to DIN EN ISO 17225-2, a critical water content of 10 wt.-% should therefore not be exceeded. When considering storage processes, the influence of increasing water content on the changes in wood pellets has been extensively studied so far. However, the process of storage is very dynamic in terms of environmental conditions, because just as the water content can increase with high humidity, it can decrease again due to low humidity. By humidifying and re-drying pellets, it can be shown that changes in density, porosity, surface roughness and or the loss of mechanical stability are reversible if a water content of 12 wt.% is not exceeded. The reversible changes can be attributed to swelling and shrinkage properties of individual wood shavings as well as the amorphous binding components such as lignin and hemicellulose. The binding components form the solid bridges between the wood shavings during the densification process. As humidity increases, they transition from a solid to a rubbery state making the pellet less durable. This transition is reversible when humidity decreases again. However, a water content above 12 wt.-% could be achieved by exceeding the saturation vapor pressure, which caused changes to be only partially reversible due to disintegration of some wood shavings from the pellet matrix.

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Understanding structured particle breakage using population balance modeling coupled with FEM calculation and phase-field model (PFM) prediction of crack propagation

Kerry Johanson[1]

[1]Material Flow Solutions, Gainesville FL, USA

Many products are created with a prescribed shape and porosity to accomplish the end-user requirements for the final product. Potato chips are designed to be sufficiently robust to survive packaging as well as a trip to the beach and are often made of powders that conform to a certain shape. Likewise, catalytic converter substrates are made of fine ceramic powder and of a complex shape to accommodate the optimal flow and temperatures during operation. Pet treat powders are formed into bone-shaped particles. Even drug dry blends have unique shapes that make the pill easier to swallow or to break at a prescribed location. Once we have created a structured shape from bulk powders we typically do not want that prescribed shape to change between the time it is formed and the packing step in the process. In some cases we want the shape to remain intact as the end-user handles it. Population balance models are powerful tools to relate the breakage observed to the probability that stress-stain events may induce the breakage of a given size particle. In addition, the population balance models relate the observed breakage to how a particular particle might break. The model helps determine how, or how much of, a particle of size bin 1 will break into size bin 2, size bin 3, size bin 4, etc. The trouble is that these population balance models are not predictive. They can analyze a set of batch breakage data and determine how and at what rate the various size particles might break, but they cannot provide guidance regarding how key powder properties, final structured particle shape, size, or other bulk properties might influence the breakage rate and breakage stoichiometry. Many of these structured particles are created by compressing the powder, followed by some processing to strengthen the green compact. Therefore, a FEM analysis of structured particles may tell us how particles might break when exposed to stress-strain events. The problem is that FEM analysis requires a continuum to compute the stress and strains and the act of breakage induces gaps in this continuum, thereby making a FEM analysis difficult to do without complex and continual regeneration of meshes as new particles are fractured or as cracks grow in the particle of interest. This complexity can be modeled using a phase-field model (PFM) to represent a crack geometry in a diffusive way without introducing sharp discontinuities. This enables PFM to model crack propagation using standard FEM. Thus, how a crack will form and propagate in a particle of a given configuration can be predicted. Applying a series of allowable contact points and positions to structured particles, and then using PFM to determine the location of the crack, allows engineers to develop a model that relates shape, powder properties, and potential particle-particle contact patterns to the breakage of structured particles. The powder flow properties help predict the breakage rates in the population balance model while the PFM crack propagation pattern helps predict the breakage stoichiometry.

Modelling of surface erosion for polymers and polymer composites due to solid particle impact

Rahul Tarodiya, Avi Levy

Dept. of Mechanical Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel

Polymeric materials are having wide engineering applications for handling solid particulate flow. Erosive wear of the materials is one of the major problems encountered while handling solid particles. To assess the material loss due to solid particle impact a semi-empirical model is developed by assuming the surface erosion due to elastic-plastic collision of the particles at oblique and normal impact angles. The model considered the material removal due to ploughing and fracture governed mechanisms and shows the capabilities to correctly capture the angle of maximum erosion for different erosion modes of polymeric materials. It has been identified that the ratio of the target material hardness (H) to notched Izod impact strength (I) is the parameter that governs the erosion mechanism and consequently the angle for maximum erosion. The model indicates the variation in velocity exponent to the mechanism of material removal. The theoretically derived model for single-particle impact is correlated to the available experimental results of multi-particle impacts through the empirical coefficients. The relation between the developed model empirical coefficients to target material mechanical properties is studied for polymers and polymer composites and correlations between model coefficients to the material properties are established. The predictions are in good agreement with the extensive literature data for polymers and polymer composites. The newly developed model can be found in its application to the numerical prediction of the erosive wear performance of the components of polymers and polymeric composites.

Keywords: Erosion model; Polymers; Polymer composites; Erosive wear; Solid particle impact

Modelling particle breakage using a bonded particle model

John P. Morrissey[1], Xizhong Chen[2], Li Ge Wang[3], Jin Y. Ooi[1]

[1] School of Engineering, University of Edinburgh, Edinburgh, UK.

[2] Department of Chemical and Biological Engineering, University of Sheffield, Sheffield, UK

[3] Process Systems Enterprise, Hammersmith, London, United Kingdom

Particle size reduction, either intended or through damage, is a process that is common across a wide range of industries. Whether intended or not, the effect of this breakage can be significant and predicting the breakage process in simulations can be a challenge. The Discrete Element Method (DEM) has seen a significant increase in usage in recent years due to advance in both the underlying hardware being more capable and through advances in the modelling techniques. However, despite these advances the inclusion of breakage in DEM is still in its infancy due to the significant computational cost and simplicity of proposed methods. Several techniques have been proposed such as the Bonded Particle Model (BPM), Particle Replacement Method (PRM) and Discrete Grain Method (DGM). The Particle Replacement Method (PRM) instantly replaces a particle with a predefined size distribution of child particles once the failure criteria are met for that particle. This is typically a single maximum compressive force, but more complex failure criteria can be implemented. This method suffers from and inability to incorporate natural breakage patterns (chipping, splitting, etc.) and does not account for weakening from repeated loading events. A BPM approximates the material as a bonded DEM particle fabric at a suitably chosen particle length scale which gives a greater degree of freedom in simulating smaller and irregular-shaped fragments. This method does not impose any predetermined limitations such as failure planes or crack initiation points and allows the model to be used to study the complex phenomena that arise in breakage. This study investigates the effectiveness of the BPM at simulating particle breakage and predicting the breakage size distributions. A rigorous Beam Bond Model is utilised to form the bonded fabric. The study demonstrates that the BPM model is capable of capturing breakage phenomena under both static and dynamic loading conditions and can be used to study damage due to varying levels of impact velocity and cumulative damage from repeated loadings. By tracking the development of bond breakage, the evolution of crack propagation through the material can be visualized.

Numerical investigation of hydro-abrasive erosion of Pelton turbine injector

Rahul Tarodiya[1], Subodh Khullar[2], Avi Levy[1]

[1]Dept. of Mechanical Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel

[2]Dept. of Mechanical and Industrial Engineering, IIT Roorkee, Roorkee, India

Erosion of turbine components due to sediment-laden water is one of the major sources of reduction in the operational economy for hydro-power generation. In Pelton turbines, the injector assembly is one of the most affected components due to sediment erosion. The surface erosion of the injector assembly due to solid particles has a detrimental effect on the water jet characteristics and hence, the turbine efficiency. An understanding of the erosion phenomenon in jet assembly can help to minimize the erosion and optimize the turbine performance. The erosion phenomenon depends on a large number of parameters including impact conditions, the properties of the target material and abrasive particles. The present study aims to numerically investigate the erosion of the Pelton turbine injector using CFD coupled discrete element method (DEM). The particle rotation and the collisions between the particles have been considered to simulate particle motion. Multi-size sand particles in the range of 75 µm to 300 µm have been selected to conduct the study. The particle collision characteristics and erosion distribution on the nozzle and spear have been studied for different spear positions and injector designs. A semi-empirical erosion model calibrated for turbine steel (CA6NM) has been adopted to estimate the erosion rate. The numerical model captured the asymmetrical erosion pattern on the Pelton injector parts similar to the field erosion pattern. Further, the zone of maximum erosion has been identified for different spear positions and injector designs. The present study helps to establish important engineering insights to control the problem of jet breakage due to erosion of injector assembly.

Keywords: Pelton turbine; Injector; Sediment Erosion; Turbine steel; CFD-DEM

Simulation of surface abrasion in DEM

R. Capozza and K. J. Hanley

School of Engineering, Institute for Infrastructure and Environment The University of Edinburgh, Edinburgh EH9 3JL, UK

e-mail: rcapozza@exseed.ed.ac.uk; k.hanley@ed.ac.uk

Abrasion is the process of wearing down particles due to contact interactions. Fines are produced during abrasion which are much smaller than the particle's size. Particles usually become smoother over time through the preferential removal of protrusions on their surface. Industrial applications are strongly affected by abrasion. Fines can reduce flowability, which can impair processing operations such as conveying, blending or tableting [1]. Attrition affects the bulk density, specific surface area, segregation behaviour and dissolution rate which can have major implications for product quality [2, 3]. Therefore, understanding and quantifying abrasion in order to predict and better control it are of fundamental importance. DEM simulations have made an important contribution to our understanding of granular materials in recent years [4]; however, simulations of abrasion in DEM are scarce and mostly limited to specific applications, e.g., [5]. We present a novel, comprehensive approach for modelling abrasion in DEM, which simulates explicitly the evolution of an abraded surface. The surface is discretized by a set of points and is abraded by a non-deformable particle. When the pressure on the surface overcomes a threshold, abrasion starts which is captured in the simulation by displacing points along the normal to the surface. The model describes both the abrasion due to scratching and normal/oblique impact as a function of velocity and applied load and shows a good qualitative agreement with experimental data. All sources of energy dissipation are naturally included in the model, with no need of fitting parameters. The implementation of this novel method in the open-source LAMMPS code is presented along with possible sources of performance improvement.

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POSTERS

A numerical assessment of different bend geometries for reducing erosion during pneumatic conveying

Eric Drescher[1], Shoya Mohseni-Mofidi[2], Claas Bierwisch[2], Harald Kruggel-Emden[1]

[1]Chair of Mechanical Process Engineering and Solids Processing, Technische Universität Berlin, Berlin, Germany

[2]Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

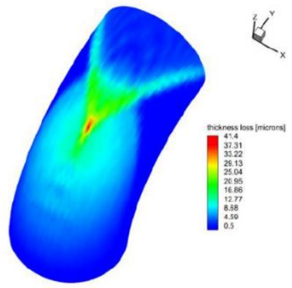

Fig. 1: Typical erosion pattern in a standard 90°-bend.

Erosion is a severe problem associated with pneumatic conveying. Thereby depending on the mode of transportation, particle properties, gas velocity and solids loading the extent of erosion can vary significantly. Erosion is especially encountered in bends where particles are forced to change their direction and are thereby slowed down with intensive particlewall contacts (see resulting erosion pattern in a standard 90°bend in Fig. 1). To overcome or at least reduce problems associated with wear in bends, wear reducing bend geometries Fig. 1: Typical erosion pattern have been proposed [1] and are commercially available such in a standard 90°-bend. as blinded tee, vortex chamber, gamma bend or pellbow which are also applied in industrial applications. Although several studies have compared individual bend designs in terms of erosion (see e.g. [2–4]), a comprehensive analysis of the advantages and disadvantages of the different available wear reducing bend designs is still lacking.

Aim of this investigation is therefore the benchmarking of the aforementioned available bend designs in terms of their erosion behavior, pressure loss and particle stressing by coupled DEM/CFD simulations. Based on them in an ideal manner recommendations in terms of the utilization of the wear reducing bend designs should be given.

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Pneumatic handling of bio and recycled solids (PHOBARS project)

Manuela Quezada Henry[1], Mikel Leturia[1], Elias Daouk[1], Thierry Destoop[2], Fabrice Bonny[2], Antoine Flament[2], Mathieu Morin[3], Sina Tebianian[3], Khashayar Saleh[1]

[1]Université de Technologie de Compiègne, ESCOM, TIMR (Integrated Transformations of Renewable Matter), Centre de recherche de Royallieu, Compiègne, France

[2]NEU-JKF Process, La Chapelle d'Armentières, France

[3]IFP Energies Nouvelles, Solaize, France

Current environmental issues have increased the need for new and more sustainable energy sources as well as the development of efficient waste recovery processes. Frequently, these recovery processes require the use of solids in divided form (biomass, plastics, etc.), considered as non-conventional solids due to their irregular shape and heterogeneity in terms of physical and physico-chemical properties (*e.g.*, Fig. 1). These non-conventional solids must be transported efficiently and reliably through pneumatic conveying between each step of the process, so as to prevent malfunctions. However, while the transport methods for conventional materials have been widely studied and are fairly well controlled, the same does not hold true for the emerging transport methods for non-conventional materials, which hinders the optimization of these processes. Therefore, there is a need to better understand and model the behaviour of these solids during pneumatic transport in order to improve its control and performance.

The PHOBARS project (Pneumatic Handling Of Bio And Recycled Solids) focuses on the study of the pneumatic transport of non-conventional powders resulting from plastic wastes or second-generation biomasses. This study considers both the system hydrodynamics and the electrostatic phenomena that occurs during transport and aims to achieve a better understanding of the mechanisms involved in order to describe, control, optimize, and predict their behaviour. There are two main axis to the project: the determination of the properties of the chosen materials and the relevant descriptors to characterize the transport, and the multi-scale modelling of the results using different approaches (CFD, MP-PIC, DEM-CFD). The ultimate goal of the project is to set up predictive experimental tests and their respective digital twins to describe the flow of powders at different conditions and thus optimize the design and implementation of the transport operation.

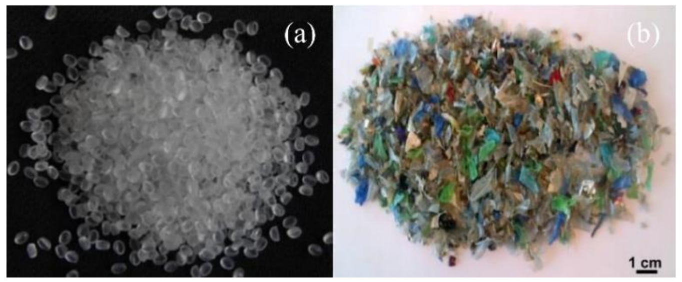

Fig. 1. Example of conventional (a) vs non-conventional (b) plastic solids.

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Impact of powder and tableting parameters on tablet properties

Amine Ait Ouazzou[1], Yogesh Harshe[2], Vincent Meunier[3], Stefan Heinrich[4]

[1,4]Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology, Hamburg, Germany

[2,3]Nestlé Research, Route du Jorat 57, CH 1000 Lausanne, Switzerland

Powders are extensively used in a wide range of industries such as food1 , pharmaceutical2 and also in chemical industries3 . The characterisation and understanding of powder behaviours is therefore crucial in order to ensure consistent product quality either when used powder in dry form and /or used for reconstitution4,5 . The process compaction is a common unit operation administered on powders to facilitate theirs storage and transport6 . The compacted powders can have many intended uses and can vary drastically from one industry to another7,8. It is therefore important to understand the powder behaviour as a subject of parameters concerning this unit operation. In this work we focus on systematically exploring the influence of maltodextrin powder, commonly used in food and pharmaceutical industry8,9, characteristics and tableting process parameters on the final compacted tablet. The compacted tablets are evaluated in terms of brittleness, porosity and reconstitution as a function of the powder and process variables. Using different experimental techniques, physiomechanical and surface properties of the produced tablets have been evaluated. The study therefore provides a better insight into inter-correlation of powder characteristics and tableting parameters on the properties of a tablet. Thus, this work is highly relevant for shelf-life study and downstream processing of the tablets.

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Experimental investigation on the role of particle shape and cohesion in the bulk flow behaviour of glass particles in a rotating drum

Wei Pin Goh, Mojtaba Ghadiri

School of Chemical and Process Engineering, University of Leeds, Leeds, UK

Rotating drums are common in many industrial processes for the purpose of mixing, coating, granulating and drying of particulate solids. The rheological behaviour of bulk powders and grains in a rotating drum is dependent on their physical characteristics, such as particle size, shape, surface roughness, adhesion/ cohesion. External factors such as the drum rotational speed, vibration, humidity are also of importance. In this presentation, we report on a systematic investigation of the role of particle shape and cohesion by studying the flow behaviour of four particulate solids systems in a rotating drum. Spherical glass beads and irregular shaped glass shards are surface-treated by acid washing (to remove any surface contamination and make them hydrophilic) and subsequently by silanisation (to make them cohesive). This makes four systems of glass particles: cohesive, non-cohesive, spherical, and irregular-shaped. Their flow behaviour is then investigated in a rotating drum. The results show that the effect of cohesion is very dominant for the spherical glass beads, but not for glass shards. Evidence of triboelectric charging is also found to influence the flow behaviour of silanised glass particles.

Preliminary investigation of fluidized bed reactors for carbon dioxide methanation by TPSIM Win software

Cesare Saccani, Marco Pellegrini, Alessandro Guzzini

Department of Industrial Engineering (DIN), University of Bologna, Bologna, Italy

To achieve the "Fit for 55" targets for 2030 in Italy, renewable energy generation is expected to increase in the next years. However, while traditional energy generation is programmable following market demand, most of energy production from renewable sources, such as solar and wind plants, are not forecastable, resulting in a potential issue for the stability of the existing electric grids. Therefore, to make possible the operation of an energy system based mainly on renewables, an energy storage infrastructure is also required to match energy demand and production. Batteries can play a role, but the availability of raw materials and their disposal at the end of life may limit sustainability at large scale. Power to Gas (P2G), i.e., converting renewable electric energy into a gaseous fuel, represents a strategic alternative. The national gas network represents a potential storage infrastructure for renewable gases, which are those produced from the conversion of renewable electricity in case of energy surplus production, thus realizing what is called "sector coupling". Accounting for more than 290,000 km of gas grids, Italy can have large benefits from P2G strategy adoption. P2G includes the conversion of renewable power into hydrogen (P2H) and synthetic methane (P2M). However, while the hydrogen blending percentage in existing gas grids is limited to avoid potential degradation and safety issues in industrial and domestic gas appliances, lower limitations exist for synthetic methane injection. However, developments are required to make P2M cost-competitive with other technologies. P2M is based on the well-known exothermic Sabatier's reaction and consists of the chemical conversion over Ni catalysts of hydrogen and carbon dioxide into methane and water. To improve the performances of P2M plants, new reactor design and control strategies have to be investigated as regards thermal and fluid dynamic parameters. For this purpose, the multiphase flow simulation software TPSIM Win was used to investigate the dynamic of the contact between solid catalyst and gases in fluidized bed reactors. Therefore, after describing the state of the art, the results of TPSIM Win simulations are discussed. Finally, preliminary observations deriving from the application of the software are shown.

Investigation of the agglomeration of particulate matter in chimneys using acoustic flow

Kristina Kilikevičienė[1*], Rimantas Kačianauskas[1], Vytautas Rimša[2], Artūras Kilikevičius[1]

[1] Institute of Mechanical Science, Vilnius Gediminas Technical University, Vilnius, Lithuania

[2] Department of Aviation Technologies, Vilnius Gediminas Technical University, Vilnius, Lithuania

* corresponding author

Key words: acoustic agglomeration, silica micrproparticles, CFD

The air pollution by micrometer-sized solid particles is becoming an increasing environmental problem on an industrial scale. Emphasis on the reduction of the micron-sized pollutants in the atmosphere is a challenge for many industries and the research community.

In this study, the acoustic agglomeration of fine particles is investigated experimentally and numerically. Acoustic agglomeration is the process by which acoustic waves are used to affect the movement of particles in the air. Promoting particle collisions and facilitating the formation of larger agglomerates to subsequent removal by filtering is the main idea of acoustic agglomeration.

The focus of this report is on the investigation of acoustic pretreatment to reduce the pollution of the atmosphere by harmful combustion products. Capturing fine silica particles of diameter ranging between 2 and 10 being discharged via chimneys of industrial plants may be seen as an important technological innovation.

The experimental part of this research is performed by the original experimental facility. The main parts of the facility are a wind tunnel, a particle dosing unit, an agglomeration chamber, and a particle volume measurement at the end of the stand. A loud speaker was used to estimate the effect of sound pressure in the frequency range of 500 to 3000 Hz. Experiments were performed in a small-scale wind tunnel to investigate the potential efficiency of acoustic agglomeration.Sound pressure and particle concentration measurements were performed at different acoustic frequencies: 500, 750, 1000, 1250, 1500, 1750, 2000, 2250, 2500, 2750, and 3000 Hz. The numerical contribution comprises the CFD simulation of the motion of the particles. The binary interaction of 8-micrometer particles is studied on the particle scale. One of the findings is that well-known long-range orthokinetic and acoustic wake agglomeration mechanisms are not valid when the interparticle distance approaches the thickness of the fluidised particle layer. contribution of the differently located third particle is also illustrated.

A detailed CFD study of the scale of very fine particles, including the boundary layer, was performed, which allowed a better understanding of the behaviour of the particles and their potential for agglomeration. The conducted experimental studies on particle agglomeration affected by the acoustic field in the frequency range from 500 to 3000 Hz have revealed the efficiency of the agglomeration of particles with different diameters. The particle agglomeration efficiency in the test at sound pressure values of 130 to 135 dB was up to 80% and the highest efficiencies were found at excitation frequencies of 1500 and 3000 Hz, respectively.

Meso-scale DEM for flowability assessment of weakly consolidated fine powders in industry

Rahul Sharma[1], Massimo Poletto[1], Diego Barletta[1], Jin Ooi[2], Stefanos Papanicolopulos[2], Marina Sousani[3]

[1]Department of Industrial Engineering, University of Salerno, Salerno, Italy

[2]School of Engineering, The University of Edinburgh, Edinburgh, UK

[3]Altair EDEM, DEM Solutions Ltd, Edinburgh, UK

Granular materials are ubiquitous in many industries such as pharmaceutical, food, chemical and find use in many processes namely mixing, granulation, transport and discharge, milling, and are quite often an end-product of these industries. In order for these industries to be working efficiently and without any interruptions or stoppages, it is necessary to ensure the adequate flowability of the powders through the various bulk handling equipment. The powders processed by the various bulk solid equipment are subjected to a range of stresses dependent on the quantity of the powder and the scale of the equipment with the range of stresses often classified as low, moderate, and high. The limit for powders to be subjected to low stress has been considered as lower than or around 1 kPa. Often, the powder mass being handled, and the scale of the process equipment cause the powder to be subjected to stresses lower than 1 kPa. Such low stresses or powders under very loose consolidation state or consolidation stress are found in applications such as dosing, filling of powders in pharmaceutical and food industries, small scale silos/hoppers for storage or discharge, powder feeders for tableting and during powder spreading process in layer-by-layer fabrication of parts by sintering or melting.

Powders having very fine particle size and subjected to such low stresses, can undergo selfaggregation or self-agglomeration because of the higher cohesive forces in comparison to the gravity forces. There is a need to study the effect of agglomeration on the flowability of very fine cohesive powders as it can influence the design of the process equipment. The principles of shear testing as first established by Jenike [5] and later elucidated by Schulze [6], calculate or capture the flow of powders at the steady state flow condition. The powder is assumed to achieve the steady state conditions under the action of it's own weight which may not be necessarily true when the powder mass or quantity under consideration is low and for the various low stress conditions. The shear stress the sample is subjected during flow may be a fraction of the steady state shear stress. There is a need to characterize powder flowability under low stresses while considering the possibility that the powder may not be subjected to the steady state flow conditions.

The project aims to test the powders at the low consolidation state and at the condition where it does not achieve the steady state (un-steady state condition). To find a link between agglomeration and flowability, powder will be tested at a base state where powder is sieved and then tested on Schulze RST at steady and un-steady state conditions, further the powder will be agglomerated by mixing/vibration equipment and then tested on Schulze RST at steady and unsteady state conditions. Subsequently, a DEM model would be developed, calibrated and validated for replicating the experimental powder flow behaviour.

DEM (meso-)particle property calibration with powder rheometry and other flow characterization techniques

Assem Zharbossyn[1], Diego Barletta[1], Massimo Poletto[1], Vanessa Magnanimo[2], Stefan Luding[2], Anthony Thornton[2]

[1]Department of Industrial Engineering, University of Salerno, Salerno, Italy

[2]Multi Scale Mechanics (MSM), University of Twente, Enschede, The Netherlands

*dbarletta@unisa.it

An accurately calibrated set of parameters of any discrete element method (DEM) model is indispensable part of any DEM simulation, which will determine the behavior of the modeled bulk material. As reported by Marigo et al. [1], calibration of the input parameters is considered as a major issue in the application of DEM by the industry. In a number of instances, the calibration process can make up the largest portion of a research using DEM simulation. Thus, more exertion has to be dedicated to obtaining robust calibration protocols that are accurate and effective in both experimental and modeling part. In addition to parameter calibration, another barrier to extensive industrial application of DEM is a large particle number participating in the industrial processes. For modeling full sized industrial installation primary size of a particle cannot be used as a consequence of restricted computation capability. In coarse graining particle size is increased while maintaining the same geometry size, accordingly the reduced total number of particles is attained [2]. This study aims at elaborating robust calibration protocols of DEM parameters both for primary and meso-particles with an individual approach for different interparticle interaction models (e.g., van der Waals, capillary or electrostatic interparticle forces, or any other interparticle contact mechanics) as well as in relation to mono- and bi-component powders. The Schulze ring shear tester (RST) will be used as a calibration test due to its several advantages as unlimited attainable shear strain, less complex and less operator-dependent procedure. First, the influence of particle and material properties (such as the particle size, the particle material, the amount of liquid available for capillary bridges) on powder rheology will be explored experimentally in order to minimize the number of parameters that should be considered in the calibration procedures. After that, sensitivity analysis of the DEM model parameters will be conducted followed by the application of grain learning in order to derive the relationships that will predict the parameter to system relationship [3]. Finally, primary and meso-scaled DEM modeling of the experiments will be performed to elaborate calibration procedures. Moreover, it is also planned to extend the characterization of the material by Anton Paar rheometer for the validation of the calibrated model.

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Analysis of the interaction of a fine particle as a droplet on a specific surface

Tim Tofan[1,*], Rimantas Kačianauskas[2,3], Raimondas Jasevičius[1,3]

[1]Department of Department of Mechanical and Materials Engineering, Vilnius Gediminas Technical University, Vilnius, Lithuania

[2]Department of Applied Mechanics, Vilnius Gediminas Technical University, Vilnius, Lithuania

[3] Institute of Mechanical Science, Vilnius Gediminas Technical University, Vilnius, Lithuania

With the rapid growth in demand for printing on different materials, the digital inkjet printing method is becoming increasingly relevant in the manufacturing process. The application of the method of digital inkjet printing of different materials and the study of their mechanics is a novelty of this work. The object of research is a droplet of ink used in the process of digital inkjet printing. Printing on various polymers can cause adhesion problems due to their low surface energy and adhesion strength. The printing is important part for many industries when we especially consider influence/contact with a food.

This work is to determine the surface wettability of polymers suitable for contact with food. This study examines the effect of energetic surface treatment on the bond strength of highdensity substrates. These plastics have been treated with various pre-treatment methods to improve surface tension and good inkjet adhesion and avoid any visual changes. It is important to determine the adhesion of ink to the polymer surface in order to improve the recycling of waste.

The presented model can be solved using either a set of levels or a phase field method to track the fluid interface. Here, the leveling method is used to determine the interface between ink and air. The work presented focuses on demonstrating how to test the suitability of ink for nozzles in inkjet printheads, for example, for use in printers.

The aim is to study the dynamics of a droplet and its interaction with the certain surfaces. Numerical modeling and analysis comprise the movement of the droplet in air until contact with the surface. The droplet as fluid is modeled considering moving boundary conditions by the equations of Incompressible Navier-Stokes fluid with added surface tension. The impact of the jet droplet on the treated and untreated surface was also investigated using the COMSOL computer simulation program. It could be mentioned that a final stable shape has been carried out as it expected in physical printing conditions. The shape is depended on various parameters. These parameters reflect on results, where are presented such as speed, size change, and volume versus time of the ink droplet. Described model could be adjusted to examine different inks impact of the printing process. Recommendations are also given on the use of specific inks.

Keywords: drop-on-demand inkjet; surface energy; droplet; measurement of droplet contact angle, droplet impact

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info@mcmcongressi.it