Institution: Edinburgh Research Partnership in Engineering

(ERPE: Edinburgh and Heriot-Watt Universities joint submission)

Unit of Assessment: UoA12 Engineering

Title of case study:

Advanced Particulate Simulation Modelling Supports Global Process Industries

Period when the underpinning research was undertaken: 2005-2017

Details of staff conducting the underpinning research from the submitting unit:

Name(s):	Role(s) (e.g. job title):	Period(s) employed by submitting HEI:
Jin Ooi	Chair of Particulate Solid Mechanics	01/09/1990 - present
Jin Sun	Reader	01/09/2010 - present
John Paul Morrissey	Postdoctoral Research Associate	01/12/2009 - present
Carlos Labra	Postdoctoral Research Associate	12/03/2012 – 03/03/2014

Period when the claimed impact occurred: March 2015 – December 2020

Is this case study continued from a case study submitted in 2014? No

1. Summary of the impact

80% of all industrial feedstocks are particulate-based. Underpinning research in ERPE has enabled the development of new disruptive particle analysis methods and technologies for powders, granules and pastes. Two key advances are: the development of a new coarse-graining method to analyse data produced by discrete element method modelling of particulates and the creation of a new numerical model named EEPA. These have been adopted into commercial software with subsequent worldwide utilisation across multiple industry sectors. The significant industrial impacts include:

(A) - Creation of the spin-out company Particle Analytics Ltd in 2015 that developed, and commercialised under licence, new 'IOTA' software. IOTA incorporated ERPE coarse graining methods to transform highly intense data from particle-scale to bulk-industrial-scale, and enabled new understanding of complex particulate flow processes and industrial innovation;

(B) - Integration of the the new 'EEPA' numerical model for particle analysis, into the globally-used software package EDEM® to simulate cohesive powders;

(C) - Development and application of an advanced Digital Twin for modelling powder mixing and granulation to optimise manufacture of pharmaceutical products, using EDEM®; and

(D) - Licencing of a new Uniaxial Powder Tester (UPT) to UK company Freeman Technology Ltd, now distributed widely in Europe, USA and Asia.

2. Underpinning research

Ooi and colleagues in ERPE at the University of Edinburgh (UoE) have performed world-leading research in Discrete Element Method (DEM) modelling techniques and software for particle simulation over the past 16 years. They developed an adhesive elasto-plastic contact model, termed the Edinburgh Elasto-Plastic Adhesion (EEPA) Model using DEM, with three dimensional non-spherical particles that enabled, for the first time, quantitative prediction of cohesive powder flowability [3.1]. Simulations were then able to be performed for the industrially-important example of uniaxial powder consolidation followed by unconfined

compression to failure. The model delivered the capability of predicting the experimental flow function (unconfined compressive strength vs. the prior consolidation stress). Contact plasticity was modelled and shown to significantly affect the flowability, which was demonstrated to be essential for producing accurate computations of the behaviour of a cohesive granular material. It proved that the contribution of the adhesive force to the limiting friction had a significant effect on the bulk unconfined strength. The results provided new insights and established a micromechanically-based measure for characterising the strength and flowability of cohesive granular materials.

The DEM method generates huge volumes of data describing particle locations, velocities and contact forces which creates significant challenges in the extraction and visualisation of the temporal and spatial characteristics of the bulk parameters of specific interest in targeted problems. ERPE research on the 'coarse graining' analysis [3.2, 3.3] developed techniques to transform the particle-scale data in the simulation into meso- and macro-scale parameters such as stresses, densities, concentrations and other application specific parameters.

Once integrated into the new software platform (IOTA), under licence, its use provided new insights into the underlying material, thermal and chemical flow processes across a wide range of industrial particulate systems. The coarse graining algorithm could, for the first time, convert and visualise discrete datasets from the solver applications into continuum data sets. This would provide key design insights and data for the pharmaceutical, mineral processing, bulk material handling and manufacturing industries to improve system designs. The simulation modelling would also enable the water, oil and gas sectors to predict wear and erosion in pipework and closed systems with greater confidence.

[3.4] reported a numerical study on the DEM modelling of cohesive solids using a visco-elasto-plastic frictional adhesive contact model. The capabilities of the contact model to capture the mechanical macroscopic behaviour of cohesive materials were investigated by means of cone penetration and unconfined compression simulations. The results showed that the simulations were able to reproduce qualitatively the typical trend of the penetration resistance profile in cohesive solids, characterised by steady-state at large penetration depths. It was also capable of capturing the dependence of the penetration resistance on the consolidation stress history. Results proved the ability of the model developed to simulate, for the first time, complex processes involving cohesive solids in large engineering applications.

In addition to the above numerical modelling, the ERPE team conducted physical modelling and experimental measurements to examine material rheological behaviour. The research in uniaxial testing of powders produced encouraging results in measuring powder compressibility and flowability for bulk handling applications. Between 2005 and 2009, the development of uniaxial handleability testers enhanced the design of cohesion testers, initially for coal handling applications with Australian (CoalTech Pty) and UK (UK Coal) companies [3.5, 3.6]. The uniaxial testing was further developed for application to chemical powder testing in two EPSRC Impact Acceleration Awards in 2015-16, involving Freeman Technology and DuPont (Chemours). A universal powder tester (UPT) was then developed in collaboration with both companies to provide an intuitive measurement of unconfined yield strength that (unlike other methods) was based on fundamental powder mechanics. The device would also facilitate efficient time consolidation and caking studies, that can often be the determining factors in industrial powder flow problems with organic chemicals and soft polymers, yet are difficult to characterise with conventional testers.

3. References to the research

[3.1] **Journal**. Thakur, S.C., Morrissey, J.P., Sun, J., Chen, J.F. and Ooi, J.Y. (2014) "Micromechanical analysis of cohesive granular materials using the discrete element method with an adhesive elasto-plastic contact model". Granular Matter, Vol. 16 (Issue 3) pp383–400. https://doi.org/10.1007/s10035-014-0506-4

[3.2] **Conference**. C. Labra, J. Y. Ooi and J. Sun (2013) "Spatial and temporal coarse-graining for DEM analysis" Proc. Powders & Grains, Sydney, Australia, June 2013, p1258-61. https://doi.org/10.1063/1.4812167

[3.3] **Journal**. Weinhart, T., Luding, S., Labra, C., Ooi, J.Y. (2016) "Influence of coarse-graining parameters on the analysis of DEM simulations of silo flow" Powder Technology, Vol. 293, pp138-148. https://doi.org/10.1016/j.powtec.2015.11.052

[3.4] **Journal**. Janda, A. and Ooi, J.Y. (2016) "DEM modelling of cone penetration and unconfined compression in cohesive soils" Powder Technology, Vol. 293, pp60-68. https://doi.org/10.1016/j.powtec.2015.05.034

[3.5] **Conference**. Bell T.A., Catalano E.J., Zhong Z., Ooi J.Y. and Rotter J.M. (2007) "Evaluation of the Edinburgh Powder Tester" Proc, PARTEC 2007, Nuremberg, March. https://www.research.ed.ac.uk/en/publications/evaluation-of-edinburgh-powder-tester-ept

[3.6] **Journal**. Zhong Z., Ooi J.Y., Rotter J.M. (2005) "Predicting the handlability of a coal blend from measurements on the source coals", Fuel, Vol. 84, pp2267-2274. https://doi.org/10.1016/j.fuel.2005.05.023

4. Details of the impact

The particulate products market is worth GBP180,000,000,000 per year in the UK, and approximately GBP1,000,000,000,000 per year in emerging global markets. Over 80% of industrial feedstocks are moved, transported or processed in particulate form (powders, granules, pastes etc.). Particulate movement can affect the long term structural condition of silos for material storage, degrade the performance of machinery and processes and influence the material properties from heat flow through particle contact. All of this has significant cost impact on the manufacturing and flow processes where powders are used, from continuous manufacture of synthetic materials, to mixing of powders or dispensing of tablets in the pharmaceutical industries. Increased knowledge and understanding from ERPE's improved modelling of the flow, compaction and movement of particulates has impacted an array of industry sectors including food, pharmaceutical, mining, construction, chemical energy storage and additive manufacturing. The impact summarised in Section 1 is expanded in A-D below. Industry descriptions of the ERPE impacts and outcomes achieved include '*best in class*', '*changing the way we look at DEM data*', '*enabled clients to model complex powders for the first time*', '*state of the art*', '*exceptional*' and '*ground breaking*'.

(A) Particle-Analytics Ltd (2015) and Coarse-Graining disruptive technology

To capitalise on the developments enabled by the underpinning research on course graining [3.2, 3.3] and previous application capabilities of the DEM [3.5, 3.6], Particle Analytics Ltd was spun-out of the University of Edinburgh in February 2015 to exploit commercially their particle engineering data analysis software 'IOTA' [5.1]. This provides users with the ability to perform rigorous root cause analysis on the design of new systems or review existing systems by combining data science methodologies with engineering decision making [5.1]. The main benefits include the course graining analysis and measurement of: mixing and segregation analysis; residence time calculation; solid fraction; bulk density; contact and kinetic stress. Clients include early-adopting multi-national organisations such as Procter and Gamble, Astec Industries Inc, Johnson Matthey and Pfizer. More recently, Particle-Analytics Ltd have been collaborating with oil and gas engineering company Schlumberger to exploit new applications in sub-surface engineering [5.1]. The Chairman of Particle Analytics endorsed the importance of the ERPE research to the quality of the software, stating *"We believe IOTA is the best in class predictive tool available in the market. This view is supported by various independent empirical data experiments and case studies, confirming that we can deliver a unique level of insight and discovery"* [5.2].

The licensing of the coarse-graining algorithm methodologies to Particle Analytics Ltd for use in the IOTA Software has, as intended, yielded a disruptive technology which allows vast amounts of complex particle data to be "coarse-grained" and transformed from particle scale to bulk-industrial scale [5.3]. This provided new understanding of particulate flow processes

and drove industrial innovation. The Chief Commercialisation Officer of Particle Analytics said, "*Particle's ground breaking coarse graining algorithm allows engineers and scientists to do proper root cause analysis on their designs to ensure they are fit for purpose and deliver long life extension. This allows engineers, such as in the Oil and Gas industry, to pinpoint failure modes in piping systems, caused by sand, which results in pipe erosion, at a cost to the industry of $2Bn per annum. Particle's front end interface capability provides for flexible developments of new models as yet undiscovered."* [5.3]

An example case study is Astec Industries, Inc. (USA) which manufactures more than 100 different products from rock crushing and screening plants to hot mix asphalt (HMA) facilities, concrete plants, milling machines, asphalt pavers, and material transfer vehicles. For their HMA equipment design and optimisation, they utilised the IOTA software designed by spin-out Particle Analytics, where the coarse-graining analysis has provided a more meaningful visualisation of the heat transfer in the complex and dynamic aggregate flow in a dryer. This resulted in the design, manufacture and supply of more efficient dryers to the road construction sector with significant fuel savings and future reduced carbon emissions [5.4]. The Head of Simulation and Modelling of Astec Industries USA confirmed that "*IOTA from Particle Analytics Ltd has changed the way we look at DEM data. We've used the coarse graining tools to gain better insight into particle behaviour in our equipment. It's enabled us to maximize heat transfer across a range of operating conditions for our clients in the road construction industry"* [5.4]

(B) EEPA modelling adopted within EDEM® software 2018 …and follow-ons

The EEPA contact modelling capability developed in [3.1, 3.4] was integrated into the commercial software EDEM® in 2018 [5.5]. EDEM® promoted the increased capabilities as '*More particles….faster with EDEM 2018*' across its multi-sector users, including pharmaceutical, equipment manufacturing and battery technology companies [5.5]. Altair Inc. is a Nasdaq (USA) registered global technology company that provides software and cloud solutions in the areas of data analysis, product development, and high-performance computing. They included the EEPA model in the Altair/EDEM® commercial particle simulation software in 2018. After acquiring EDEM® in 2019, the Chief Technology Officer of Altair endorsed, *"The recent adoption of the EEPA model has allowed our clients to model their complex cohesive powders successfully for the first time. The applications are wide ranging including pharmaceutical, manufacturing, battery technology, automotive design and have directly contributed to the Company securing new clients. The success of EEPA model is a contributing factor to Altair's decision to acquire EDEM® in 2019"* [5.6].

(C) Development of a Digital Twin for modelling powder mixing and granulation

Funded by Innovate UK, in collaboration with Centre for Process Innovation Ltd (CPI) and industrial partners AstraZeneca, EDEM®, Johnson Matthey, Pfizer, PSE, and Procter & Gamble, the EEPA model within EDEM® was successfully used to develop an advanced Digital Twin of a twin-screw granulator for modelling powder mixing and granulation to optimise, in advance of process, the manufacture of pharmaceutical and other high value products [5.7]. Dr Graeme Cruickshank, Director of Formulation at CPI, said: "*These projects are exciting developments in the application of digital design methods to the development of formulated products and manufacturing process. The leveraging of UK expertise across industry, academic centres of excellence and highly-specialised technology suppliers has been key to the success of this project and providing state-of-the-art capability to help UK companies benefit from developments in digital manufacturing"* [5.7].

(D) Uniaxial cohesive powders tester (UPT) – license, launch and reach

In addition to the numerical modelling- and simulation-driven impacts above, ERPE research in measurement, characterisation, prediction and test of particulates has underpinned the development of a uniaxial tester for cohesive powders [3.5, 3.6] and, in later EPSRC-funded collaborative research, developed a universal powder tester (UPT), with DuPont (Chemours) and Freeman Technology. The UPT was licensed in 2016 to Freeman Technology, the

leading UK company operating in Europe, Asia and USA. The Freeman UPT Tester, is marketed on their website [5.8]. This UPT is now used to provide rapid, repeatable and accurate assessment of powder flowability for industrial powder handling applications worldwide. The UPT also overcame [5.8] many of the previous engineering and implementation constraints across many industry sectors including (i) the design and construction of a free-standing powder column; (ii) that ensured a uniform density and stress throughout the entire powder column, resulting in (iii) a user-friendly, dependable powder tester that is now used on a wide range of powders. The new UPT technology [5.8] developed a sleeve design that enabled the creation of a free-standing column of powder, and used a double-ended consolidation method to ensure uniform density and stress. The Operations Director at Freeman Technology stated *"The uniaxial tester contributed significantly to the development of the Freeman Technology Uniaxial Powder Tester. This instrument is now installed at powder handling organisations in the USA, Europe and Asia where it is used to assist with product development and optimisation in applications as industrial chemicals, household goods and pharmaceuticals"* [5.9].

An example case study is Chemours Inc (USA) which is a global chemical engineering company, employing around 7,000 staff across 37 manufacturing plants/laboratories, with a client base in 120 countries. Its work supplies the automotive, paints, plastics, electronics, construction, energy, and telecommunications industries. They use the UPT widely for quality control and product development of titanium dioxide (TiO_2) powder used in products such as paints, glazes, enamels, plastics, paper, fibres, foods, pharmaceuticals and cosmetics. The lead Particle Technology Principal Consultant at Chemours USA, stated, "*Having conducted over 2,500 tests with the UPT, the reproducibility has been exceptional; more than 10 times better than its 'competitor' in measurement of unconfined yield stress. This high degree of reproducibility minimizes the need for replicate tests and allows confident detection of subtle differences in flowability that affect the value of millions of dollars' worth of TiO2 pigment"* [5.10].

5. Sources to corroborate the impact

[5.1] Particle Analytics Ltd spin out company from University of Edinburgh (Feb 2015), multinational clients (by Dec, 2020) http://particle-analytics.com/about/

[5.2] Comments by Particle Analytics Ltd Chairman as 'best in class' software from comparisons with other softwares (Jan, 2020) http://particle-analytics.com/kevin-hart/

[5.3] Statement from Particle Analytics Ltd, Chief Commercial Officer.

[5.4] Statement from Astec Inc. Head of Simulation, USA.

[5.5] EDEM promotion to various industry sectors of the capabilities of the EEPA software now embedded in EDEM 2018 version. *More particles….faster with EDEM 2018* (Oct, 2017) https://www.edemsimulation.com/blog-and-news/news/more-particles-faster-edem-2018/

[5.6] Statement by Chief Technology Officer of Altair Inc (USA) on the success of EEPA model as a contributing factor to Altair's decision to acquire EDEM® in 2019.

[5.7] CPI Press release: Creation of the CPI Digital Twin with the EDEM software incorporating EEPA modelling and University of Edinburgh expertise. (March, 2019)

www.uk-cpi.com/news/cpi-collaborates-on-project-to-create-digital-twin

[5.8] Launch of the Uniaxial Powder Tester (UPT), sold by Freeman Technology Ltd stating developed in partnerships with University of Edinburgh (Jan, 2016)

https://www.freemantech.co.uk/news/freeman-technology-launches-a-new-ground-breaking-powder-tester-for-cost-effective-industrial-measurement

[5.9] Statement by Freeman Technology, Operations Director, on the significance of the uniaxial testing in the development of the Freeman UPT tester, and deployment in organisations across USA, Europe and Asia.

[5.10] Statement by Particle Technology Consultant, Chemours Inc USA on the importance of the Freeman UPT tester.