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"Simulations in Bulk Solids Handling: Applications of DEM and Other Methods"

By Professor Don McGlinchey (Leader, Engineering Simulation and Advanced Manufacturing Research Group, Glasgow Caledonian University, UK), Wiley-VCH, Weinheim, Germany, 2023, 272 pp, ISBN: 978-3-527-35010-0, £110.00, €124.30, US$156.36

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Introduction

Commonly, granular material properties and methods for understanding granular material processing are often omitted or given brief coverage in formal education. Skills and knowledge in this area tend to be developed postgraduate or within industrial roles. This book was compiled to provide insight into current simulation methods that are employed in bulk powder handling. Application examples in critical industrial transfer and transport processes are contained within and the book is best suited to those with some pre-existing knowledge of discrete element method (DEM) and related methods, as well as for experienced modellers. More specifically, the book is focused on simulation of granular solids transfer and transport operations within manufacturing environments whose nuances are often under-appreciated in plant design.

This book was edited by Professor Don McGlinchey, the Head of the Centre for Industrial Bulk Solids Handling at Glasgow Caledonian University. He has undertaken consultancy projects for both multinational companies and small to medium enterprises and delivered short courses in Europe, USA and the UK. He is a Chartered Physicist, with a PhD in the particle technology area, editor of two books and has authored over 50 research articles. His current research interests include multiphase flow pipeline transport measurement and modelling and pneumatic conveying system modelling. The chapter authors are recognised academics and industrialists in conveyance and particle processing, each offering expert insight into their respective focus of study.

The Application of DEM Modelling

This book is not a step-by-step tutorial through the various modelling packages available. Rather, it focuses on the application of DEM modelling and adjacent methods applied to transfer chutes, belt conveyors, DEM-coupled multibody dynamics, pneumatic conveyors, erosive wear and material packing, each of which are often under-appreciated but crucial operations for getting material 'from A to B' on a manufacturing plant or site. Only a single combined chapter (Chapter 7) is given to powder: mixing, segregation, blending, hopper filling and discharge, twin screw granulation, milling and powder inhalation. Furthermore, it does not go into the details of coding, needed for most modelling packages, nor the pros and cons of the numerous packages available (either open-source or commercial) where the nuances are left for those interested to discover!

Calibration in the context of DEM modelling is a parameter estimation activity whereby the DEM input parameters are evaluated to allow recreation of the calibration experiment, for example, the static angle of repose of poured powder. Selection of the descriptors and parameters can be achieved in a facile way or through extensive designs of experiments and various analytical fitting tools. In the first chapter of the book, Professor Corne Coetzee (Stellenbosch University, South Africa) and Professor Andre Katterfeld (University of Magdeburg, Germany) discussed calibration of DEM parameters. Common calibration experiments, methods and optimisation approaches were all covered in this chapter. A summary of DEM input parameter's sensitivities to material bulk properties (for non-cohesive powders) are given in **Table I**. This chapter, coupled with any modelling package-specific training, would give a good physical grounding for simulation work where readers are also encouraged to read other Johnson Matthey opinions on this topic (1).

There is a current lack of confidence in calibration for cohesive materials, attributed to difficulties in calibrating for cohesive parameters and the cohesive contact models not truly capturing the physics of the systems. Quantification of adhesion or cohesion and the kinetics of their evolution through processing increasingly utilises cross-discipline knowledge, is an under-developed area in the wider literature and beyond the scope of this book.

In the second chapter on 'Simulation of transfer chutes' by Dusan Ilic (University of Newcastle, Australia) and Professor Andre Katterfeld (University of Magdeburg, Germany), the authors advocate for optimised pairing of chute design and operation rather than considering them in isolation. They argue that this approach is more likely to result in efficient and reliable throughput. Beyond identifying approaches (including continuum and discrete modelling), emphases are given to discharge trajectories, belt tracking as a function of discharge forces from a chute to a conveyor belt, blockage, wear prediction and dust generation as illustrated through **Figure 1**.

The above phenomena are highly relevant to industrial operations with abnormal powder physical properties (high density, combustible).

This chapter leads well into the next on 'Belt conveyor design and troubleshooting' by C. A. Wheeler, P. W. Robinson *et al*., (University

Table I Relation between Discrete Element Method Parameters and Non-Cohesive Bulk Properties

DEM parameters	Bulk material properties: Bulk density and porosity including changes due to flow (dilatancy)	Bulk friction/ shear/ interlocking/ flow behaviour	Dissipation of energy (damping)	Bulk stiffness	DEM model computation time
Particle shape	Weak influences	Strong	Negligible	Negligible	Strong
Particle size distribution	Weak	Weak	Negligible	Negligible	Strong
Particle density	Strong	Negligible	Negligible	Negligible	Strong
Contact damping/ coefficient of restitution	Negligible	Negligible	Strong	Negligible	Negligible
Contact stiffness	Negligible	Negligible	Negligible	Strong	Strong
Contact coefficient of sliding friction: particle-particle	Weak	Strong	Strong	Negligible	Negligible
Contact coefficient of sliding friction: particle-wall	Negligible	Strong	Strong	Negligible	Negligible
Contact coefficient of rolling friction (particle-wall)	Negligible	Strong	Negligible	Negligible	Negligible
Experiments that are sensitive to the specific bulk material properties	Bulk density/ porosity, filled container dilatancy, direct shear test	Angle of repose, discharge rate, draw down test, direct shear test	Drop test, pendulum test, uniaxial compression	Uniaxial compression	–

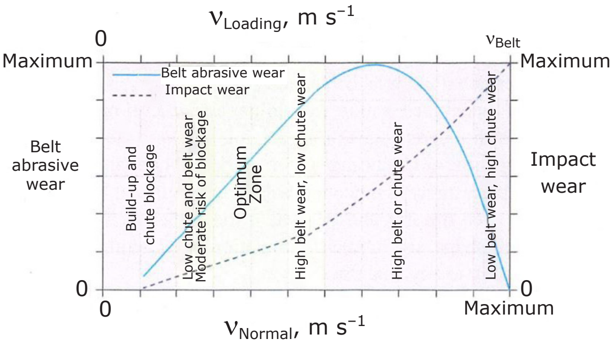

Fig. 1. Transfer chute and belt velocity, wear and flow relationships. Reprinted from (2) with permission from Wiley

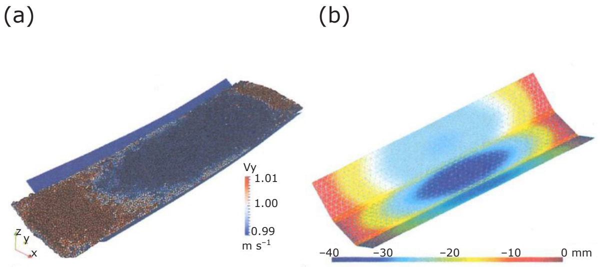

Fig. 2. Two-way coupling (FEM-DEM) showing: (a) particle velocities in LIGGGHTS; (b) belt deformation in Code_Aster. Reprinted from (2) with permission from Wiley

of Newcastle, Australia). A wealth of detail is provided in this chapter and introduces use of finite element method (FEM) and coupled FEM to account for the flexibility of the conveying belt itself. An FEM approach allows evaluation of indentation rolling resistance (IRR) of the idlers, belt flexure resistance, idler roller rolling resistance, idler roll misalignment resistance and bulk material flexure resistance allowing for energy efficiency calculations. Operationally, the modelling results can provide insight into belt start-up and shut-off, chute discharge point effects, belt wear, idler wear and belt roller wear. The sensitivity of belt tracking and wear to the chute discharge trajectory and contacting profile as well as the carry *vs.* return side belt tensions are highlighted in **Figure 2**.

The next three chapters then jump to considerations of 'Multibody dynamics and discrete element method co-simulations for large-scale industrial equipment' by Professor D. L. Schott (University of Delft, Netherlands) and M. J. Mohajeri (University of Delft, Netherlands), 'Simulation of pneumatic conveying' by Professor Don McGlinchey (Glasgow Caledonian University, UK) and 'Modelling and simulation of erosive wear and particle breakage in pneumatic conveying' by Professor R. Tarodiya (Ben-Gurion University, Israel) and Professor A. Levy (Ben-Gurion University, Israel) respectively.

The first of these chapters focuses on the multibody movement effects of granular material movement on the movement of the operational equipment (and *vice versa*) the forces on a scoop as it picks-up powder from a static pile. This chapter is mainly on considerations for civil engineering and mining equipment design and operation (diggers) though some considerations are given to high-pressure grinders and tamping equipment. The second of these chapters, the author provides a series of relevant definitions prior to case studies of different models of increasing complexity (as summarised in **Table II**).

Ultimately, the modelling approach taken is dependent upon a combination of the operational

Table II Overview of Recommended Conveyance Modelling Approaches (2)[a]

Model	Typical use	Resource requirements
Single fluid	System pressure drop	Low
1D CFD	Velocity profile	
DPM (discrete particle model)	Dilute (lean) phase solid interactions (e.g. bend erosion rate estimation)	Medium
Two-fluid model	Dense phase, component level fine particle/powders, moving bed flow behaviour, volume fractions, velocity profile, transient effects	
DEM-CFD (coupled)	Dense phase, component level granular material, plug/moving bed flow behaviour, plug formation/collapse, local gas pressure, particle level stress, particle breakage, transient effects, particle shape effects.	High

[a]Reprinted with permission from Wiley

regime, the level of detail required and the resource allocated to completing the work.

The last of these three chapters focuses on methods of constructing coupled breakage and wear models in pneumatic conveyance. Building from an overly simplistic population balance model type (which follow a simple $PSD_{output} = f(PSD_{input})$ where PSD = particle size distribution and f = operational parameters). More complex models incorporate both the flow model and a breakage algorithm (that accounts for impact force, collision frequency and distributed particle mechanical properties). Whilst the more complex models are advised, obtaining accurate calibration or parameterisation (as per Chapter 1) of these models may be time-consuming and require specialised equipment. Notably, the calibration and implementation of equipment wear models into DEM is an active field (3).

Chapter 7, 'Discrete element modelling of pharmaceutical powder handling processes', by C. Zheng, C.-Y. Wu *et al.,* (University of Surrey, UK) is more extensive and provides a wide range of example applications of DEM and related modelling to various powder unit operations: mixing, segregation, blending, hopper filling and discharge, twin screw granulation, milling (4) and powder inhalation where observations are relevant beyond pharmaceuticals, despite the chapter title.

The final chapter from J. Xiang and J. P. Latham (Imperial College London, UK) on 'Algorithms and capabilities of Solidity to simulate interactions and packing of complex shapes' specifically discusses the use of Solidity, a finite-discrete element method package developed by Imperial College London, UK, for the purposes of more accurate prediction of complex particle packing and is a chapter well-suited to modellers with active interest in understanding fixed bed packing catalytic reactors, absorbent beds.

Contact mechanics and models describing them are not truly within the scope of the book though for DEM modelling they are fundamental to model accuracy and a primary route for incorporating cohesion. This is an active sub-field within the literature where readers are initially referred to the work of O'Sullivan (5) and Thornton (6) for their implementation.

Conclusions

The book provides concise chapters and expert insights into granular solids transfer and transport operations with extensive reference lists comprising a mixture of seminal and contemporary works. It is not an introduction to the fundamentals of DEM for which there are numerous tutorials already available. Alternatively, it collates together underappreciated particle processing steps that are critical to the economics of industrial powder processing alongside recent advanced method development approaches. It correctly asserts, without dwelling on, the benefits and limitations to the approaches used. The two-fold challenges of exceptionally large particle numbers and complex interparticle forces (including cohesion) in the modelling of industrial processes mean the generation of completely accurate and validated models remains elusive, though improving. The famous aphorism of George Box "all models are wrong, but some are useful" (7) is still pertinent and modellers are encouraged to use DEM and related approaches as part of 'Un Bouquet de Fleurs' (a bouquet of flowers (of evidence)) alongside analytical and empirical methods.

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