

Simplifying Calibration of Powders by use of Numerical Methods

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Abstract

Area: Fluid Mechanics and Computational Fluid Mechanics

Purpose: We come across many materials that occur as fine chemicals. The behaviour of these can neither be described by fluid dynamics nor rigid body mechanics. Hence, we need simulations to study these. If we simulate all the forces on every particle, it will take exceedingly long time to converge to results. Hence, mathematical models are used to describe the particle flow. To use these models, one of these two (or a combination of both) methods needs to be used: Coarse graining using scaling laws or bulk Calibration. Calibration procedure currently used is quite tedious as it requires us to do a hit-and-trial of input parameters and repeated simulations till we reach the experimentally measured values. This work proposes a method to simplify this.

Method: A varied set of input parameters was taken and simulated. For this, ROCKY software was used. Important parameters were identified by finding the sensitivity of output parameters to those input parameters. Next, numerical methods are used to interpolate and create a polynomial that gives the input parameters upon substituting the experimentally determined values. The method used was Lagrangian interpolation. Note that the number of input parameters selected must be less than or equal to the number of experimental/measured variables selected so that a one-to-one function can be generated.

Results: Only a partial set of data could be simulated due to time constraints and a polynomial is available for this data. Thus, a polynomial for a limited range of data is available for use.

Conclusions: The work described above proposes a method to simplify the process of powder calibration. A small proof of concept is also available but, a complete analysis of a larger set of data is still pending. Other researchers are invited to use this idea and make a polynomial that covers the entire range of input parameters so that the idea can be put to commercial use. This procedure will reduce the net time for simulations manifold.

Duration: Three months

Contribution: Everything mentioned above was done by the author of this abstract.

References

[1] C.J. Coetzee, Review: Calibration of the discrete element method, Powder Technology, Volume 310, 2017, Pages 104-142, ISSN 0032-5910