Powder Technology 210 (2011) 230–240

Contents lists available at ScienceDirect

Powder Technology

journal homepage: www.elsevier.com/locate/powtec

Application of Taguchi methods to DEM calibration of bonded agglomerates

Kevin J. Hanley [a,*], Catherine O'Sullivan [b], Jorge C. Oliveira [a], Kevin Cronin [a], Edmond P. Byrne [a]

[a] Dept. of Process and Chemical Engineering, University College Cork, Cork, Ireland
[b] Dept. of Civil and Environmental Engineering, Skempton Building, Imperial College London, London SW7 2AZ, United Kingdom

ARTICLE INFO

Article history:
Received 19 August 2010
Received in revised form 5 March 2011
Accepted 25 March 2011
Available online 31 March 2011

Keywords:
Discrete element modelling
Experimental design
Simulation
Statistical analysis
Uniaxial compression

ABSTRACT

Discrete element modelling (DEM) is commonly used for particle-scale modelling of granular or particulate materials. Creation of a DEM model requires the specification of a number of micro-structural parameters, including the particle contact stiffness and the interparticle friction. These parameters cannot easily be measured in the laboratory or directly related to measurable, physical material parameters. Therefore, a calibration process is typically used to select the values for use in simulations of physical systems. This paper proposes optimising the DEM calibration process by applying the Taguchi method to analyse the influence of the input parameters on the simulated response of powder agglomerates. The agglomerates were generated in both two and three dimensions by bonding disks and spheres together using parallel bonds. The mechanical response of each agglomerate was measured in a uniaxial compression test simulation where the particle was compressed quasi-statically between stiff, horizontal, frictionless platens. Using appropriate experimental designs revealed the most important parameters to consider for successful calibration of the 2D and 3D models. By analysing the interactive effects, it was also shown that the conventional calibration procedure using a "one at a time" analysis of the parameters is fundamentally erroneous. The predictive ability of this approach was confirmed with further simulations in both 2D and 3D. This demonstrates that a judicious strategy for application of Taguchi principles can provide a sound and effective calibration procedure.

1. Introduction

In recent times, discrete element modelling (DEM) has become popular as a simulation tool. DEM simulations can replicate the often complex response of particulate materials by specifying a relatively small number of particle-scale parameters [1]. Although the fundamental algorithm for DEM was developed during the 1970s [2], the method did not become widely used until the 1990s, and its popularity has grown rapidly since. This increase in usage of DEM is commensurate with the rise in computational power, which has made it possible to run useful simulations on affordable desktop computers [1]. The availability of commercial software has also contributed to the increased popularity of the method.

A key challenge in DEM analysis is to select appropriate parameters so that the response of real, physical systems can be accurately simulated. Some of the input parameters, such as the particle dimensions or the density, can be measured or estimated with a large degree of confidence. However, the rheological parameters for input to the contact constitutive models are often more difficult to determine accurately by experiment. It is not generally possible to infer a complete set of appropriate parameters for a DEM simulation directly from properties of the physical material. Therefore a calibration approach is often used to select these parameters. Typically calibration involves varying the DEM parameters until the model response corresponds closely to the equivalent physical experimental response. This approach is widely used, e.g., [3–5]. This calibration is often conducted using a simple approach, where parameters are varied individually and the effect on the model response is monitored. While conceptually simple, this approach to calibration has many disadvantages: it may take a long time to obtain an appropriate set of parameters, it is impossible to know how many DEM simulations are required for calibration in advance, the final parameters obtained may not be optimal, and the mechanistic insight gained is limited.

Recently there have been proposals to develop more efficient DEM calibration approaches using design of experiments (DOE) methods. Yoon [6] applied a Plackett–Burman design and response surface analysis to determine suitable DEM micro-parameters for uniaxial compression of bonded rock particles. Favier et al. [7] used DOE methods to calibrate discrete element models for a mixer and a hopper, based on measurements of torque and discharge flowrate, respectively. Johnstone and Ooi [8] applied DOE methods to find appropriate model parameters based on experimental measurements of flow in a rotating drum device and mechanical response during a confined compression test. A large range of DOE methods is in use in the scientific field, but all these methods have the same objective: to find the relationship between the process parameters and the process

* Corresponding author. Tel.: +353 21 4903096; fax: +353 21 4270249.
E-mail addresses: k.hanley@umail.ucc.ie (K.J. Hanley), cath.osullivan@imperial.ac.uk (C. O'Sullivan), j.oliveira@ucc.ie (J.C. Oliveira), k.cronin@ucc.ie (K. Cronin), e.byrne@ucc.ie (E.P. Byrne).

0032-5910/$ – see front matter
doi:10.1016/j.powtec.2011.03.023

output by using a structured pre-planned methodology for obtaining experimental data that ensures an efficient balance between how much data is required (resource intensity) and the precision and confidence of the conclusions (information quality), which also implies minimising the bias that can be induced by the sampling design.

The Taguchi method has become very popular in industrial practise as a tool to achieve quality by design and minimise non-conformity costs, by establishing the optimum settings of a process that optimise its performance and the consistency of that performance [9]. As it has proved to be effective in ensuring robust operation in practise (i.e., obtaining the set of parameters that minimise system variability resulting from the inevitable variability of its inputs), it should be also ideal for calibration (identifying the set of model parameters that minimise the variability of model predictions). However, the authors are not aware of any published work which applies Taguchi methods to DEM calibration. In this paper, calibration of bonded agglomerates was chosen as an example application to illustrate the Taguchi method and to allow its effectiveness to be evaluated when compared to the simple *ad hoc* calibration approaches which remain in widespread usage.

Specific objectives of this work were as follows:

1. To introduce and outline the Taguchi method for DOE, evaluating its advantages as well as its limitations.
2. To evaluate the Taguchi method as a tool for calibrating agglomerates of bonded disks (2D) and spheres (3D).

2. Overview of the Taguchi method

Genichi Taguchi is widely regarded as pioneering the modern quality-by-design approach [10]. The basic features of the Taguchi method are the use of orthogonal arrays to establish the experimental requirements and of Analysis of Variance (ANOVA) to analyse the results, without using any inference (interpolative) model to relate the system factors (inputs) with responses (outputs). Taguchi's practical approach led him to conclude that inference models are often underpinned by patterns (surfaces in the solution space) that do not reflect the real system behaviour. This results in the identification of points of optimum operation that are due to mathematical artefacts and do not exist in reality. Furthermore, using inference models pools the lack of fit with all other sources of error (unexplained variability), and as analysing sources of variability is one of the main reasons to use the Taguchi method, adding lack of fit (which is a limitation of the method of analysis and not a system characteristic) would not be helpful.

The first step in establishing a “Taguchi design” is to identify the factors to be tested and decide on the number of levels to be used for these factors. A two-level design, in which two different settings are tested for each factor, will minimise experimental requirements, but will not identify points of optimum operation within the solution space, rather only at its limits. Therefore, a three-level design is effectively the minimum for a typical optimisation procedure. Once the factors and levels have been decided upon, an appropriate array must be selected. The number of rows in the array corresponds to the number of trials or experiments to be performed, while the number of columns gives the maximum permissible number of factors which may be tested. The arrays are designated by the letter L followed by a number which indicates the number of rows in the design (L_4, L_8, etc.). Each factor is allocated to one column of the array, so that the number of different settings in each column is equal to the number of levels of that factor. The researcher does not need to develop these arrays, since the commonly-used arrays are provided both in literature and in many statistical software packages. As the Taguchi method does not use inference models, it only considers as solutions combinations of those factor settings used in the design (though the optimum combination itself may be one that was not tested).

It is conventional to denote the factor levels numerically so that the lowest level of any factor is 1, the second-lowest is 2 etc. If the actual levels of a factor are 5, 20 and 30, then these would correspond to 1, 2 and 3 in a three-level array. Levels are not required to be numerical, and if a factor is discontinuous, such as colour, then the levels may be assigned arbitrarily. If all columns of an array contain factors, the array is saturated; however, columns may be left unused, in which case, they may permit some interactive effects to be tested for significance, e.g., the interaction between the factors in columns 1 and 2 is contained in columns 3 and 4 for three-level arrays. A relatively small set of basic arrays is used for the Taguchi method, although a range of techniques are available to modify these arrays without loss of orthogonality. This is the defining property of orthogonal arrays, and ensures balanced comparison of all factors. In an orthogonal array, each factor is tested at each level the same number of times, and for any pair of columns, all possible permutations of levels are tested, and each permutation is tested an equal number of times.

The main advantages of using the Taguchi approach are that the experimental designs chosen minimise the amount of information needed and the analysis methods clearly identify what is being analysed and relate only to actual system behaviour. However, a theoretical analysis of the implications of Taguchi's choice of statistical tools identifies a number of limitations [11,12]; the most important is that the DOE with orthogonal arrays generates very intricate confoundings. This means that a column may contain a number of partial or full interactions, in addition to a factor. As an example, it was already stated that the interaction between the factors in columns 1 and 2 is distributed between columns 3 and 4 for three-level arrays. If factors are allocated to columns 1, 2 and 3 of this array, it would become impossible to distinguish between the effect of the factor in column 3 and the partial interactive effect due to the factors in columns 1 and 2, both of which are contained in column 3. The presence of confounding has significant implications for analysis of the results. For this reason, the initial allocation of factors to columns should ideally be done with the knowledge of which interactions might be relevant or negligible. For realistic Taguchi designs, it is inevitable that many of the effects being analysed are not individualised and actually pool a complex mix of effects. More information (experiments) would be needed in order to distinguish and separate those effects, if desired. Of course, in systems where interactions are all negligible, the method works perfectly with no complications.

The ANOVA applied to the results is a well-established statistical method that quantifies the total variability in terms of its variance, and then establishes how much of it can be explained by the influence of each factor or interaction between factors (many of which are pooled with the orthogonal array designs).

3. DEM simulations

In particulate DEM, the most computationally efficient particles are disks and spheres. By glueing disks or spheres together to create bonded agglomerates, more realistic particle geometries can be created and particle damage can be simulated. This approach has been applied by a number of researchers, e.g., Thornton and Liu [13] simulated agglomerate fracture for process engineering applications, Cheng et al. [14] and McDowell and Harireche [15] both used agglomerates composed of spheres to study the relationship between sand particle breakage with the overall mechanical response of sand, and Lu and McDowell [16] simulated the abrasion of railway ballast. Given the range of potential applications and level of interest in the modelling of particles using bonded agglomerates, it was chosen here as an exemplar application of the Taguchi method to DEM calibration. Real particulate materials of interest in engineering applications are