Multivariate Analysis and Reduced Order Modeling Based On Discrete Element Method (DEM) Simulations for a Powder Blender
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INTRODUCTION

Continuous powder mixing is a crucial unit operation in many industrial processes (e.g., pharmaceuticals, cosmetics, food, catalysts) since poor blend homogeneity can significantly affect the quality of the final products.

Current modeling approaches range from first-principle based models (Discrete Element Methods), data-driven models (Response Surface Methods, Kriging & Neural Networks), or hybrid models (Population Balance Models). However, a methodology which can combine mechanistic understanding, mechanistic and macroscopic information, design aspects, material property effects at low computational cost is missing.

OBJECTIVES

1. Investigate effects and significance of operating conditions (blade speed, fill level) and design variables (blade width, blade angle, shaft angle, weir height) on the performance of continuous particulate mixing.

2. Combine Discrete Element Method periodic section simulations with Proper Orthogonal Decomposition methods to develop a fast reduced-order model (ROM) to predict blending performance at unexplored operating regions.

METHODLOGY

Periodic section modeling

Whole mixer

Periodic section

Cross-sectional mixing as a function of location

Batch-like mixing as a function of time

- Discretization of process geometry for data extraction of 2_z variables.

Identification of variables which will form the data base (X, Y and Z spaces). Design of experiments for different input conditions based on Latin Hypercube Sampling.

- Is average number of particles inside bin large enough to get reliable mean value of 2_z?

YES

Is there few or no particles in the bin?

NO

Large enough number of particles: Consider as missing data

Few number of particles: Set equal to zero

Model training for input-output mapping using Kriging methodology:

\( y(x) = f(x) + \varepsilon(x) \)

where \( x = 1,...,N \) and \( j = 1,...,M \)

Model training for PCA using missing data imputation for dimensionality reduction of state variable space (KPCA or NIPALS algorithm):

\( P = \Gamma(x) \)

where \( x = 1,...,N \)

Periodic Section DEM Simulation design

Design of computer experiments

Design of computer simulations is based on Latin Hypercube sampling. A total of 64 samples are designed and simulated in order to cover the entire experimental region under investigation event.

RESULTS

Multivariate analysis of results using PLS

Two PC components capture 75% of the total variance.

Shaf angle and blade speed are the two most effective variables in improving continuous powder mixing performance.

PLS model provides good qualitative insight and is used to identify significant inputs, however, a ROM/POD based model can give better quantitative insights about distributed variables inside periodic section.

CONCLUSIONS

- Critical operating conditions and design parameters for the mixing performance of a continuous blender are identified through a POD model.

- Based on the leading scores of different variables, simultaneously increasing blade speed and decreasing shaft angle is the optimal strategy for the improvement of mixing performance.

- A reduced order model using data snapshots of the periodic section model based on PCA can predict distribution of particle properties inside mixer geometry.

- The discretization of the geometry for extraction of average particle information is a critical issue in DEM-ROM model. If not enough number of particles are inside each bin, it is preferable to treat it as missing data.

FUTURE WORK

- Experimental validation of optimal design strategy identified through this study.

- Use of DEM/ROM model in a flowsheet simulation environment, for process design, optimization and control.

- Implementation of proposed approach for full blender geometry where number of particles is significantly large and computational benefit will be greater.