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. pharmaceutical, cosmetics, food, catalysts) since **poor blend homogeneity** can significantly affect the quality of the final products.

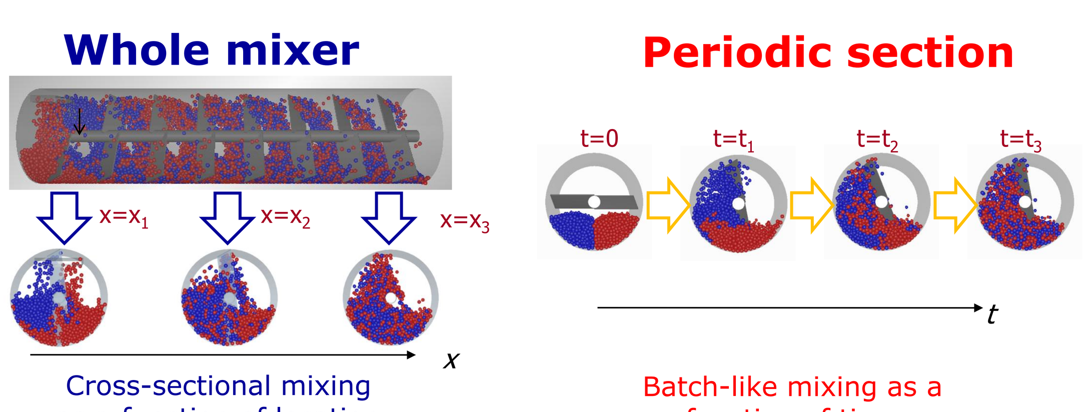
Current modeling approaches range from first-principle based models (Discrete Element Methods), data-driven models (Response Surface Methods, Kriging & Neural Networks), or hybrid models (Population Balance Models). However, a methodology which can combine **mechanistic understanding**, **microscale** and **macroscale** 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.

Methodology

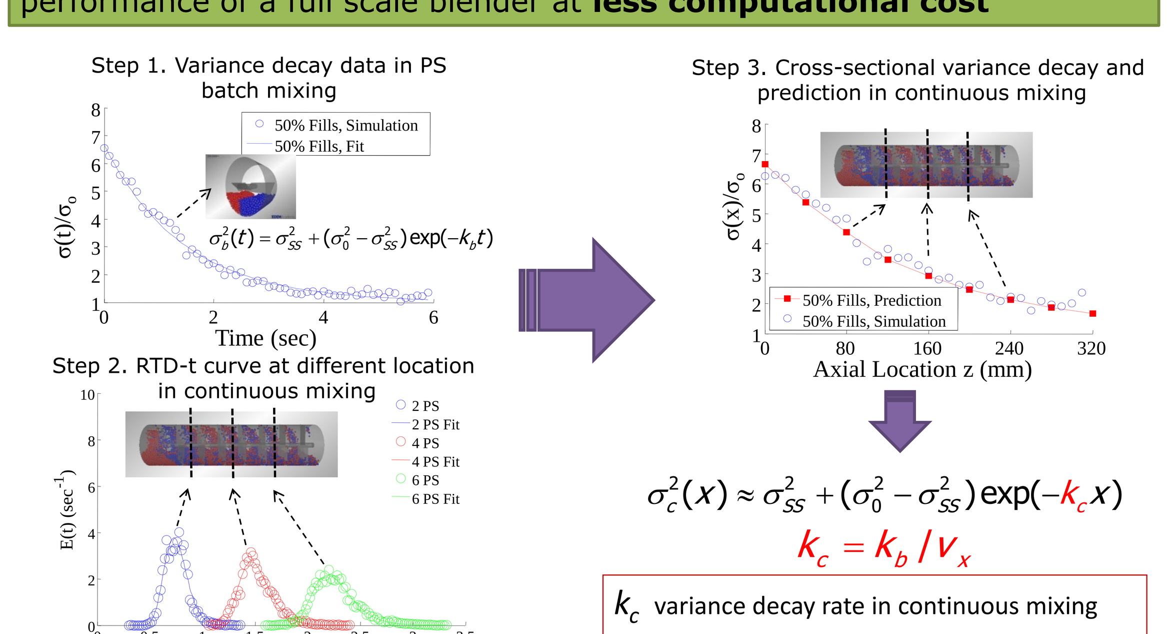
Periodic section modeling



$$\sigma_c^2(x) \approx \int_0^\infty \sigma_b^2(t) E(t,x)dt$$

$\sigma_c^2(x)$ variance decay in *continuous mixing* as a function of location *x*
$\sigma_b^2(t)$ variance decay in *periodic section* mixing as a function of time *t*
E(t, x) residence time distribution measured at location *x* in *continuous mixing*

- Cross-sectional mixing performance is determined by the competition between **local mixing** rate and **axial forward velocity**.
- By simulating a periodic section DEM simulation combined with the RTD information along the axis of the mixer, we can predict the mixing performance of a full scale blender at **less computational cost**



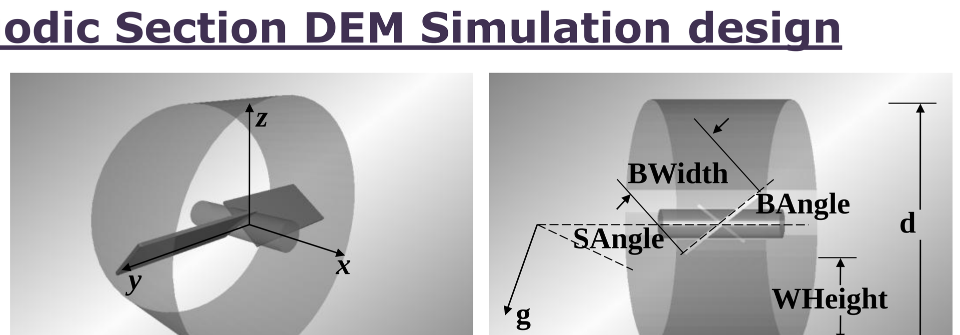
$$\sigma_b^2(t) = \sigma_{SS}^2 + (\sigma_0^2 - \sigma_{SS}^2)\exp(-k_b t)$$

$$\sigma_c^2(x) \approx \sigma_{SS}^2 + (\sigma_0^2 - \sigma_{SS}^2)\exp(-k_c x)$$

$$k_c = k_b / v_x$$

k_c variance decay rate in continuous mixing
v_x mean axial velocity

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 evenly.

Design/ Operation parameters	Low bound	High bound
Blade speed (RPM)	40	250
Blade angle (deg)	10	40
Blade width (mm)	10	40
Weir height ratio *w/d* (-)	0%	75%
Fill level (-)	25%	75%
Shaft angle (deg)	-30 (upward shaft)	30 (downward shaft)

Reduced Order Modeling using Proper Orthogonal Decomposition

- POD aims to obtain low-dimensional approximate descriptions of high-dimensional processes through modal decomposition of an ensemble of functions or data
- POD has been used successfully in literature for building reduced order models of complex CFD simulations[1] to be used for control, optimization and flowsheet simulation.
- When building a POD model using data 'snapshots' of the process, the method is equivalent to Principal Component Analysis

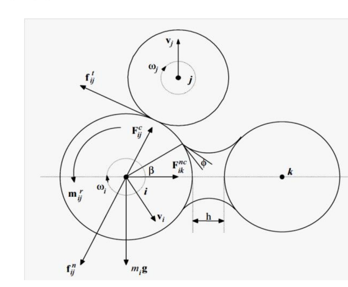
[1] *Lang, Y., et al. Energy and Fuels. (2009)*

Identified challenges

- Data extraction from DEM simulations is in form of discrete values for each individual particle movement
- Highly **non-linear** and **non-smooth** data

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_j \mathbf{F}_{ij}^c + \sum_k \mathbf{F}_{ik}^{nc} + \mathbf{F}_i^f + \mathbf{F}_i^g \qquad \forall i=1,\ldots,N_p \qquad (a)$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_j \mathbf{M}_{ij} \qquad \forall i=1,\ldots,N_p \qquad (b)$$



•**Discretization of DEM** geometry and **total number of particles** play a huge role in the quality of the extracted data based on which the reduced order model is built

Methodology

X_i $i=1,..,N$ Input variable Space (operating and design variables)
Y_j $j=1,..,M$ Output variable Space (blend homogeneity parameters)
Z_k $k=1,..,L$ State variable Space (distributed particle properties)

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

Discretization of process geometry for data extraction of Z_k variables.

Is average number of particles inside bin large enough to get reliable mean value of Z_k?

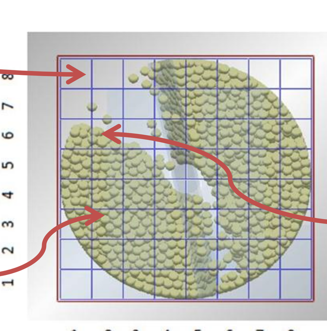
YES

NO

Discard value and regard as **missing data**

Very few or no particles: Set equal to zero

Large enough number of particles: Use average value



Few number of particles: Consider as missing data (impute)

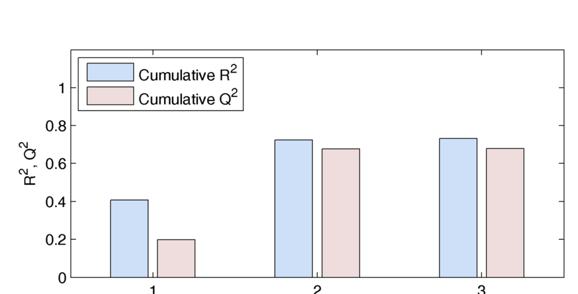
Model training for input-output mapping using Kriging methodology.
$Y_j = f(X_i)$ where $i=1,..,N$ and $j=1,..,M$

Perform PCA with missing data imputation for dimensionality reduction of state variable space (EM-PCA or Nipals algorithm)

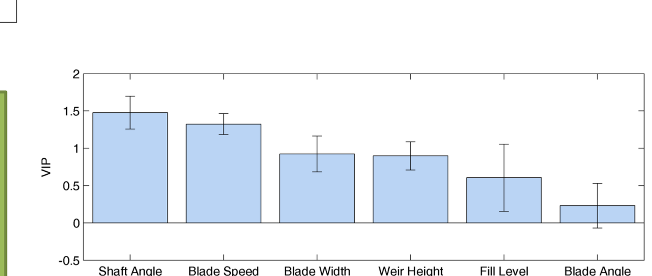
Model training for input- PCA loadings mapping using Kriging methodology.
$p_i = f(X_i)$ where $i=1,..,N$

Results

Multivariate analysis of results using PLS



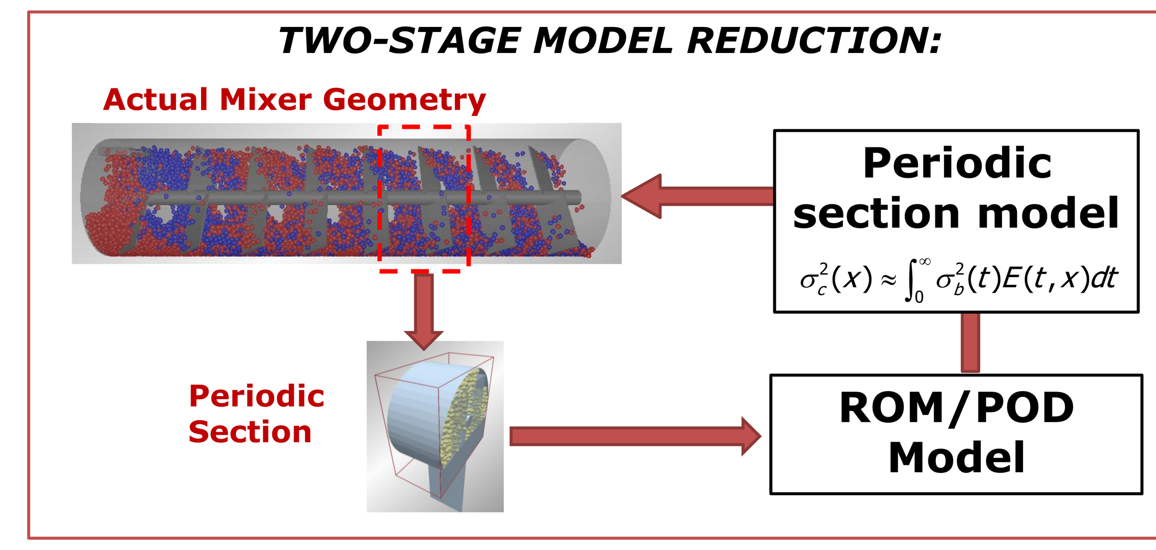
Two PC components capture 75% of the total variance.



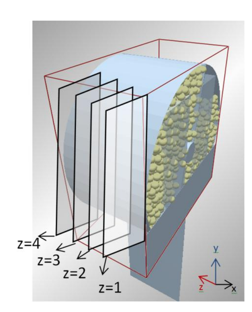
Shaft angle and **blade speed** are the two most effective variables in improving continuous powder mixing performance.

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

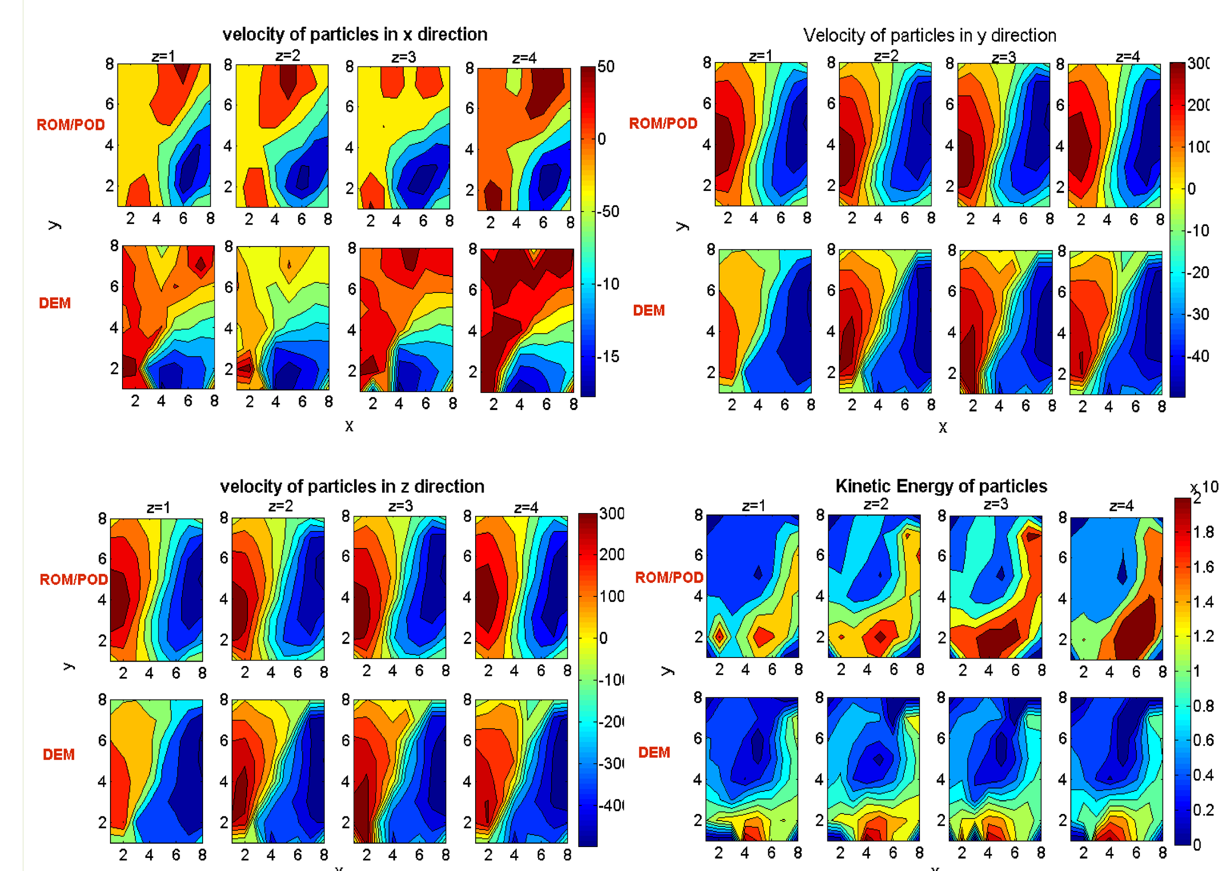
POD- based Reduced Order Model



Distributed State Variable	Importance
Velocity fields in x,y,z direction	• Movement of particles within section • Velocity terms input to Population Balance models (PBM)[2] [2]*Boukouvala et. al, MAME (2011)*
Kinetic Energy	• Energy of particles • Prediction of stagnant zones
Total Force	• amount of applied force on particles modifies material properties (i.e. cohesiveness)



Variable	Number of PCs	Total Variance (raw data)	Total Variance (imputed missing 10%)
u_x	2	43.88	45.90
u_y	1	67.76	65.42
u_z	1	47.67	57.37
Kinetic energy	2	42.74	58.21
Total force	1	41.60	57.02



- Total computational time ~ **60sec** as opposed to **~2days** for a single DEM simulation
- Method manages to capture trends of distributed state variables sufficiently with a very few number of Principal components
- Further improvement in predictions can be achieved by increasing the number of total particles of DEM simulation

Conclusions

- Critical operating conditions and design parameters for the mixing performance of a continuous blender are identified through a PLS model.
- Based on the loading 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 an 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.

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