Discrete Element Reduced-Order Modeling of Dynamic Particulate Systems

Amanda Rogers and Marianthi G. Ierapetritou
Dept. of Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ 08854

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One of the key technical challenges associated with modeling particulate processes is the ongoing need to develop efficient and accurate predictive models. Often the models that best represent solids handling processes, like discrete element method (DEM) models, are computationally expensive to evaluate. In this work, a reduced-order modeling (ROM) methodology is proposed that can represent distributed parameter information, like particle velocity profiles, obtained from high-fidelity (DEM) simulations in a more computationally efficient fashion. The proposed methodology uses principal component analysis (PCA) to reduce the dimensionality of the distributed parameter information, and response surface modeling to map the distributed parameter data to process operating parameters. This PCA-based ROM approach has been used to model velocity trajectories in a continuous convective mixer, to demonstrate its applicability for pharmaceutical process modeling. © 2014 American Institute of Chemical Engineers *AIChE J*, 60: 3184–3194, 2014
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Introduction

One of the key technical challenges associated with modeling particulate processes is the ongoing need to develop efficient and accurate predictive models. It is often the case that the models that best represent solids handling processes are computationally expensive to evaluate. For instance, discrete element method (DEM) models can provide detailed information about particulate processes by accurately representing process geometry and calculating particle movement based on particle–particle and particle–geometry interactions.[1] DEM can be used to obtain distributed parameter information, like particle velocities, which are often of interest in solids-handling applications.[1–4] However, these simulations can take hours or even days to run depending on the number of particles involved.[5,6] This makes it difficult to use them for applications like flowsheet modeling, where models that evaluate quickly may be needed to conduct dynamic simulation[7] and optimization[8] of manufacturing processes. For this reason models that incur a lower computational cost, such as population balance models (PBM) and reduced-order models (ROM) are frequently used to represent solids-handling processes in flowsheet simulations.[7,9–15]

PBM take into account distributed parameters like particle velocities or size distributions, but do so through the use of a population distribution function such that it is not necessary to consider all particle-level interactions.[11,16] A number of pharmaceutically relevant processes can be described using PBM,[17] including wet granulation,[18–20] milling,[10,21] and continuous blending.[11,16] PBM are useful as a means of representing these processes in a detailed fashion without requiring the extensive calculations that are implemented in DEM simulations. Recently, PBM models that are informed by DEM simulations have been developed for continuous blending processes.[11,22,23] These models couple particle velocity profiles obtained from DEM with PBM models, as it has been shown that incorporating information from DEM into PBM models can increase their accuracy.[11,22–24] However, this approach requires evaluation of an expensive DEM simulation for each realization of the process operating parameters. If the equipment operates at steady state, as in Sen et al.,[22] then the DEM simulation needs to be evaluated only once to obtain the particle velocity profiles for the PBM. However, if process dynamics are to be captured by the model, it is advantageous to have a ROM so that particle velocity profiles can be obtained without evaluating a DEM simulation every time the process operating conditions are modified.

Although PBM are faster to evaluate than DEM models, PBM can be difficult to solve as the dimensionality of the model increases. This can be addressed in part by a variety of order-reduction techniques[25] and the implementation of hierarchal solution methods.[18,19] Even with these, PBM may not evaluate quickly enough for applications where rapid model evaluation is needed, like model predictive control,[26] sensitivity analysis,[27] or surrogate-based optimization.[8] Therefore, it is desirable to have an alternative approach that can provide process response information in a matter of seconds. ROM can be developed to map process outputs to operating conditions using response surface modeling techniques. These can be used in conjunction with the previously described ROM for distributed parameter information. The

Correspondence concerning this article should be addressed to M.G. Ierapetritou at marianth@soemail.rutgers.edu.

combined models can provide both distributed parameter information and predicted process responses, and require less extensive calculations than PBM.

This work is concerned with the development of ROM that can represent distributed parameter information obtained from DEM in a computationally efficient way. The development of ROM is motivated by the need for models that can provide distributed parameter information quickly in process simulation and optimization applications. The developed ROM can be used to obtain velocity profiles for use in PBM models. They can also be implemented directly in flowsheet simulation applications, in conjunction with response surface models mapping process responses to process operating conditions. The development of such response surface models is also discussed in this work.

In the following section, the computational methods used in this research are described, including DEM simulation, principal component analysis (PCA) and response surface modeling approaches. Thereafter, the dynamic discrete element-reduced-order modeling (DE-ROM) methodology is described in detail. The proposed methodology is then applied to a series of case studies describing a continuous blending process. Finally, Conclusions and Future Work are presented.

Computational Methods

DEM simulations

DEM models are particle-level computational tools that can be used for detailed simulation of particulate processes. They account for individual particle–particle and particle–geometry interactions across very short time scales.[1] It is important to note that, although DEM simulations consider particle-level phenomena, the number of particles considered in DEM simulations is typically much smaller than the number of particles observed experimentally in a solids-handling process. That said, DEM is still used extensively in the study of pharmaceutical processes[4,24] including blending,[2,5] die filling,[28,29] and powder compaction.[30,31] This work uses DEM models of continuous powder mixing processes, which are of interest in pharmaceutical manufacturing applications.[3,5,32,33] DEM simulations of continuous mixing processes have shown good qualitative agreement with experiments in terms of mixing performance,[5] powder dispersion behavior,[34] and powder velocity profiles.[35] Powder velocity profiles from these simulations have been used to inform hybrid PBM models for continuous mixing processes as well.[22]

The DEM simulations used in this work include a model of a commercially available continuous mixer as well as models of a periodic section of a continuous blender. The use of periodic section modeling to study continuous blending processes has been discussed extensively in the literature.[32,33,35–37] Periodic section modeling is based on the idea that continuous blending processes can be viewed as consisting of two phenomena: powder movement and powder mixing. Powder movement is characterized by the number of periodic sections placed in series, while powder mixing is represented as a batch mixing process occurring within each section.[32] An advantage of using periodic section models relative to DEM simulations of an entire blender is that they can be evaluated quickly due to the smaller geometry and the fact that fewer particles are involved. For this reason, periodic section models are used for initial demonstration and evaluation of the proposed ROM methodology. Simulations of the entire continuous mixer are needed to obtain velocity profiles for use in hybrid PBM models and performance metrics for use flowsheet simulations. Thus, a final case study is presented in which ROM based on the entire continuous blender are developed.

DEM simulations were implemented in the commercially available EDEM® software package by DEM Solutions. The periodic sections used in this work are 0.08 m in diameter and 0.04 m in length with varying blade and shaft configurations and weir heights. The particles in these simulations are 1.5×10^{-3} m in diameter and each periodic section contains between 2400 and 3600 particles, depending on fill level. The periodic sections contain two types of particles, Material 1 and Material 2, which have identical properties and differ only in their numerical designation. Two particle types are defined so that mixing performance can be evaluated. The periodic section simulation approach used in this work is discussed at length in Gao et al.[32]

The proposed ROM methodology has also been applied to a DEM simulation of a commercially available continuous blender, the Gericke™ GCM250. This blender has a length of 0.33 m and a diameter of 0.1 m. In the current work, an all-forward blade configuration is considered. Particles enter the blender at a rate of 1990 per second, and the corresponding number of particles in the blender is between 20,000 and 60,000, depending on the blade rotation rate at any given time. Slower blade rotation rates correspond to lower outflow from the blender and, therefore, a greater fill-level. A normal particle size distribution with a mean radius of 1.0×10^{-3} m and a standard deviation of 2.0×10^{-4} m is used during particle generation, and the minimum and maximum particle size are 7.0×10^{-4} and 1.0×10^{-3} m, respectively. Again, two particle types with identical properties are used. Additional details pertaining to the development of this DEM simulation can be found in Dubey et al.[38]

Reduced-order modeling

ROM refers to the use of lower dimensional or lower cost models to approximate high-fidelity or high-dimensional simulations that are computationally expensive to evaluate.[39] ROM can be used to represent information obtained through experimental study or process simulation in an efficient manner.[40] The use of ROM in powder processing applications can enhance the accuracy of flowsheet models by incorporating information from high-fidelity simulations like DEM without incurring the corresponding computational cost.[6,41] In addition, ROM methodologies can be used to provide approximate representations of objective functions and constraints for applications in process flexibility analysis and optimization.[8,12,42,43]

A number of techniques for model reduction have been developed specifically for applications where distributed parameter information is of interest, as in DEM and computational fluid dynamics (CFD) simulations. ROM for CFD are extensively used in aerodynamics, where ROM based on the Volterra theory[44] and proper orthogonal decomposition (POD)[45,46] are prevalent.[47] POD, more often referred to as PCA in the statistics literature, is one of the most common methods used to reduce the dimensionality of distributed parameter information like that obtained from CFD.[6,47,48] Lang et al.[49,50] have described the use of a ROM based on PCA to incorporate information from CFD into a flowsheet

model for co-simulation and optimization of an integrated gasification combined cycle plant. Boukouvala et al.[6] have extended this PCA based ROM approach to information obtained from DEM simulations, introducing the DE-ROM methodology. In Boukouvala et al.,[6] particle velocity profiles in a continuous blender were modeled at steady state as a function of blender design and operating parameters including weir height, fill level, blade width, blade angle, and rotation rate. For dynamic simulation and process control applications, dynamic process models are needed. Therefore, the current work focuses on the development of ROM to describe the dynamic evolution of powder velocity profiles in a continuous mixer.

ROM methodologies include statistical techniques like latent variable methods, response surface modeling approaches, hybrid and semiempirical models, or any combination thereof.[6,12,49] In the current work, both latent variable and response surface models are used.

Latent variable methods

PCA and partial least-squares regression, also called projection to latent structures (PLS) create latent variable models. These methods involve the projection of input and response data into a reduced space on a set of orthogonal axes. The transformed variables are referred to as scores while the transformed axes are described as loadings.[51] In PCA, the objective is to find scores and loadings that represent the most variance in the original dataset subject to certain orthogonality conditions.[52] In contrast, PLS regression seeks a transformation that explains variance in both the input and response data while retaining directions in the input space which are useful in predicting the responses of interest.[53] Latent variables models are often used in pharmaceutical development to evaluate the relationships between material properties and process performance or product quality.[54,55] For these applications, the interpretability of the model parameters is helpful in terms of developing process understanding.[51]

Response surface modeling

Response surface techniques involve the development of a functional representation, or response surface, for a system output based on a set of input factors. The response surface is generated by sampling the process of interest and fitting model parameters based on the collected input-response data.[56] Unlike PCA or PLS, the model parameters may not be interpretable in terms of explicit relationships between individual factors and responses. In addition, the functional form of the response surface is not necessarily based on the underlying process physics or dynamics. The functional form of the response surface and the values of the estimated model parameters are selected to achieve the best fit to the given set of input-response data.[12,57] A variety of techniques can be used to develop response surface models, including Kriging,[14,58–60] artificial neural networks (ANN),[9,61] and high-dimensional model representation (HDMR).[62–64] In a number of recent works comparing response surface modeling approaches for pharmaceutical processes, Kriging outperformed other techniques like ANN and HDMR.[14,43,65] This may be due to the ability of Kriging to handle noisy data, which is often an issue in modeling solids-handling processes.[58,66] Kriging can also model complex nonlinear and dynamic processes.[12,58] Kriging is used as a response surface modeling technique throughout this work due to its ability to model the highly nonlinear dynamic process data collected from the continuous blender DEM simulations. In the remainder of this section a preliminary introduction to Kriging is provided. Interested readers are referred to the literature for a more detailed description of the method.[14,15,59]

Kriging is an interpolating method for mapping input-response data[60] that was originally developed for the purpose of predicting mineral deposit distributions.[67] Recently, it has been adopted in a variety of other fields due to its ability to model noisy, dynamic and nonlinear processes.[58] Kriging is especially attractive for applications like surrogate-based optimization because it provides prediction uncertainty estimations along with the predicted function value at each new test point.[43] The underlying assumption of Kriging is that given a previously untested data point x_k, the corresponding process response $\hat{f}(x_k)$ can be determined as a weighted sum of the known responses $f(x_i)$ for a set of data points x_i that are within some Euclidean distance r of the point x_k. This is represented mathematically in Eq. 1, where the weights w_i decrease as a function of increasing Euclidean distance between x_i and x_k[58,59]

$$\hat{f}(x_k)=\sum_{i=1}^{N} w_i f(x_i) \tag{1}$$

The weights in Eq. 1 are estimated using a fitted variogram model, shown in Eq. 2. In Eq. 2, h is the Euclidean distance between two points x_i and x_j and $\gamma(h)$ is corresponding semivariance between the points $f(x_i)$ and $f(x_j)$[58,59]

$$\begin{aligned} h &= \|x_i - x_j\| \\ \gamma(h) &= \frac{1}{2}\left[\mathrm{var}\left(f(x_i)-f(x_j)\right)\right] \end{aligned} \tag{2}$$

The variogram model is used to obtain the covariance function, Eq. 3. The covariance function can be used to determine the Kriging weights by solving the system of Eq. 4, where d_{ij} is the Euclidean distance between points x_i and x_j.[59]

$$Cov(h)=\sigma^2_{\max}-\gamma(h) \tag{3}$$

$$\begin{bmatrix} Cov(d_{1,1}) & \cdots & Cov(d_{1,N}) & 1 \\ \vdots & \ddots & \vdots & \vdots \\ Cov(d_{N,1}) & \cdots & Cov(d_{N,N}) & 1 \\ 1 & \cdots & 1 & 0 \end{bmatrix} \times \begin{bmatrix} w_1 \\ \vdots \\ w_N \\ \lambda \end{bmatrix} = \begin{bmatrix} Cov(d_{1,k}) \\ \vdots \\ Cov(d_{N,k}) \\ 1 \end{bmatrix} \tag{4}$$

$$\sigma^2_k=\sigma^2_{\max}-\sum_{i=1}^{N} w_i Cov(d_{i,k})-\lambda \tag{5}$$

Briefly, the algorithm for developing a Kriging response surface model is as follows:

1. Select an initial sample set x consisting of N_T sample points. Evaluate the process model at these points and collect the corresponding function values $f(x)$.
2. Calculate the Euclidean distances h and the semivariances $\gamma(h)$ using Eq. 2 for all $\frac{N_T(N_T-1)}{2}$ sampling pairs from the dataset collected in Step 1.
3. Smooth the $\gamma(h)$ vs. h data. Fit the smoothed data to a variogram model using a least-squares error minimization criterion and/or a secondary criterion for computational efficiency.
4. Use the variogram model to evaluate the covariance function as in Eq. 3

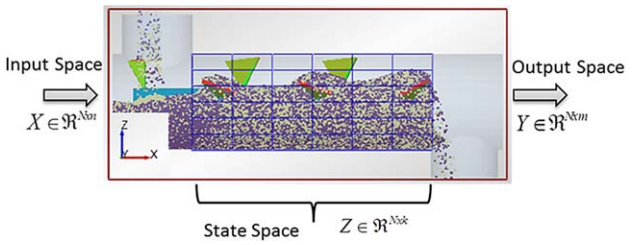

Figure 1. Space definitions for DE-ROM methodology.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

5. For a new point x_k, calculate the weights using Eq. 4, the prediction variance from Eq. 5 and the estimated function value $\hat{f}(x_k)$ from Eq. 1.
6. Optional—if the prediction variance is higher than a user-specified tolerance collect additional samples near the test point x_k and add those to the set N_T. Develop an updated Kriging model.

Kriging response surface models have been used in applications ranging from process simulation[12] to flexibility and feasibility analysis.[43] In the current work, Kriging has been used to develop a predictive model for distributed parameter information and for process performance as a function of operating conditions for a continuous convective mixer.

PCA based ROM methodology

To describe the proposed modeling methodology, it is first necessary to define the datasets used for model development. These include three relevant information matrices, the input space ($X \in \Re^{Nxn}$), the state space ($Z \in \Re^{Nxk}$), and the output space ($Y \in \Re^{Nxm}$). The three spaces are shown with respect to the process geometry in Figure 1. The input space consists of process design and operating parameters that can be controlled by the user or defined by the developer of the DEM model. Factors that are known to affect the state variables and process responses of interest should be included in the input space. The state space consists of distributed parameters, in this case particle velocities, and its dimensionality is defined by the discretization of the process geometry. Finally, the output space consists of process responses at the outlet of the unit. The goal of this modeling methodology is to develop predictive models for both the state variables and the process outputs as a function of the factors in the input space.

The use of PCA is motivated by the high dimensionality of the state space, as the rank of the state space tends to be significantly greater than that of the input space.[6,49] In the current work, the input space is of Rank 2 while the state space is of Rank 200 or more for all case studies. For this reason, it is difficult to use standard multivariate regression techniques to develop accurate models that directly predict the state variables from the input factors. If one were to instead model state variables in each discrete element independently, the number of models required to describe the full state space would be equal to the number of elements in the discretization. Such an approach is impractical and potentially time-consuming.

To address these challenges, the dimensionality of the state space is reduced using PCA. The original dataset, denoted as Z, consists of N observations of k variables, which may or may not be correlated. The principal components obtained through PCA are orthogonal to one another and are arranged in order of decreasing variance such that the first component explains the greatest amount of variance in the original dataset and the last component explains the least. The number of components in the model (α) must be less than or equal to the number of variables in the original dataset and can be selected such that the variance in the original dataset is well explained by the principal component model. The results of PCA can be expressed in terms of the component scores (T) and the corresponding loadings (P). The scores are the variables transformed into the latent space. This transformation is achieved by multiplying the original variables by the loadings to obtain the corresponding scores. The number of columns in the scores and loadings matrices is given by the number of principal components in the model (α). The original state data can be reconstructed from the scores and loadings as shown in Eq. 6, where ε is a matrix of residuals

$$Z = TP' + \varepsilon \tag{6}$$

A general overview of the algorithm for dynamic DE-ROM is presented in Figure 2. The method consists initially of sampling the input space, which contains operating parameters to be considered in the model. Design of experiments can be used to devise a sampling strategy to generate the input space.[68,69] The high-fidelity (DEM) model is evaluated for the set of conditions specified in the input space. Subsequently, the process geometry is discretized. This is an important step in the development of the ROM as too fine a mesh can result in noisy data due to a small number of particles in each discrete element. However, too broad a discretization could miss important features of the distributed parameter profiles within the process geometry. The discretization should ultimately be selected based on the intended application of the model. For instance, if the velocities obtained from the ROM are to inform a PBM, the discretization should be consistent with that used to solve the PBM.

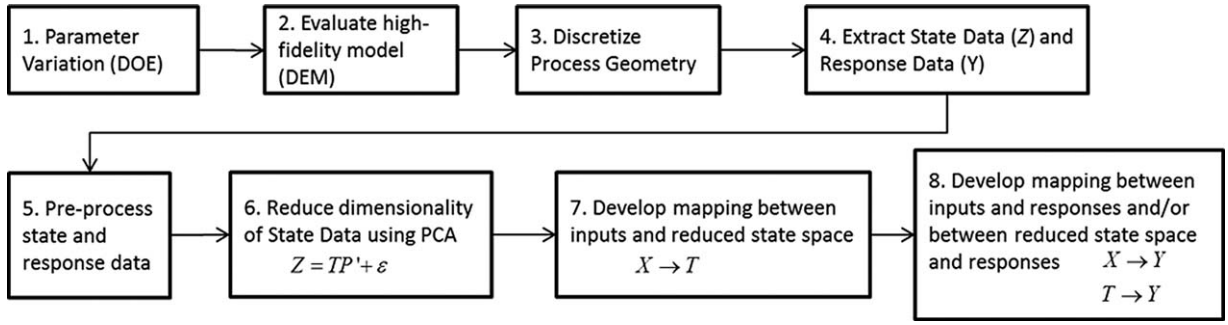

Figure 2. Algorithm for dynamic DE-ROM.

Subsequently, the state and response data are extracted from the simulation. In this step, it is important to determine an appropriate sampling frequency for the state space. Sampling too frequently can result in noisy data, similar to using too fine of a mesh in Step 3. However, infrequent sampling could fail to adequately capture the process dynamics. In some cases, preprocessing may be required to smooth the state and response data. State data may also be mean centered and scaled to unit variance prior to PCA.[52,53] PCA is then used to reduce the dimensionality of the state space. In this work, the number of principal components in the reduced state space was selected such that at least 95% of the variance in the original state data was explained. Because PCA is used to reduce the dimensionality of the state data without significant loss of information, a percent variance explained criterion was used to select the number of components. In general, the number of components in a PCA model can be selected through cross validation, such that the desired prediction accuracy is achieved by the principal component model.[69,70] In this work, the ROM, which includes the principal component decomposition and subsequent response surface modeling, is cross validated. In this way, it is verified that the selected number of components provides a ROM with acceptable prediction accuracy. Cross validation is discussed in greater detail in the *Case studies* section of the article. The reduced state space, given by the principal component scores (T), can then be mapped to the process inputs through any number of response surface modeling techniques. Lang et al.[49] have demonstrated the use neural networks, while Boukouvala et al.[6] have used Kriging.

Once the dynamic DE-ROM model has been developed, it is possible to predict the principal component scores (T_{pred}) corresponding to a new set of inputs (X_{new}). The predicted scores and the loadings determined in Step 6 can be used to calculate the distributed parameters corresponding to the new input (Z_{new}), as shown in Eq. 7. It should be noted that the predictions may not be valid if the predicted scores do not fall within the score space of the original model[49]

$$X_{\text{new}} \xrightarrow{\text{Kriging}} T_{\text{pred}}$$
$$Z_{\text{new}} = T_{\text{pred}} P' \tag{7}$$

A separate ROM may also be developed to predict the process outputs (Y) as a function of the inputs (X). This can be accomplished using any of the previously mentioned response surface modeling techniques. In the current work, Kriging is used to develop a response surface model for mixing performance as a function of blender operating conditions.

The process outputs (Y) can also be modeled as a function of the reduced state space (T). Such a model explicitly connects process performance to the distributed parameters in the state space. In this case, it may be preferable to use a latent variable technique like PLS to develop the model so that the model parameters are interpretable. Such a model can be used for process simulation and also to assess the way in which distributed parameters influence process outcomes.

Case Studies

All simulations were carried out on a desktop computer with a 2.93 GHz Intel® Core™ i7 (Vpro™) processor and 16 GB of memory.

Table 1. Design Parameters for Periodic Section Case Studies

	Fill Level (%)	Blade Angle (°)	Weir Height Ratio (w/d, %)	Blade Width (mm)	Shaft Angle (°)
Case 1	40.39	13.29	67.41	29.04	−7.38
Case 2	27.26	36.31	61.71	25.7	−19.34

Periodic section case studies

DEM modeling has been applied extensively to the study of granular mixing processes.[4,35,71] Thus, a continuous convective mixer provides a useful case study for the dynamic DE-ROM methodology. Initially, periodic section models of a continuous blender were used to test the dynamic DE-ROM methodology. These models evaluate quickly relative to models of the entire blender, and are thus preferable for preliminary evaluation of the proposed modeling approach. Periodic section modeling is well established in the literature as a means of characterizing and optimizing continuous blending processes.[3,32,33,36] As previously mentioned, the underlying principle of periodic section modeling is that the continuous mixing process consists of two phenomena; powder flow, which is characterized by the residence time distribution and powder mixing, which can be viewed as a batch mixing process occurring in a single periodic section of the mixer.[32] In this case study, mixing performance was characterized using the relative standard deviation (RSD). The RSD describes variability in mixture composition relative to the average composition. It is calculated as shown in Eq. 8, where C_i and $\bar{C}$ represent the concentration of a given component in sample i and the average concentration of a given component over N samples, respectively

$$RSD = \frac{\sigma}{\bar{C}} \quad \text{where} \quad \sigma = \sqrt{\frac{\sum_{i=1}^{N} (C_i - \bar{C})^2}{N-1}} \tag{8}$$

Two different periodic section case studies were considered in this work, each with a different shaft, blade and weir configuration. The specific design and operating conditions for each periodic section are shown in Table 1. The two periodic sections are hereafter referred to as Case 1 and Case 2, respectively.

The periodic sections were simulated at 19 different blade rotation rates, randomly sampled from a uniform distribution with a lower bound of 40 rpm and upper bound of 250 rpm. These correspond to the operating limits for the Gericke™ GCM 250. The simulation was carried out for 4 s at each blade speed, as it is was found that the performance metric (RSD) does not continue to change after 4 s over the range of design and operating conditions considered. The periodic section was divided into 4 axial slices, which were further discretized into an 8 by 8 grid, resulting in a total of 256 elements, as depicted in Figure 3. This discretization was selected such that each element contained, on average, more than 10 particles. A minimum of 10 particles was selected based on previous work, in which it was found that state data from elements containing fewer than 10 particles tended to be noisy.[6] State data corresponding to the average particle velocities in the x, y, and z directions (u_x, u_y, and u_z, respectively) were extracted from the periodic section simulation every 0.1 s. This sampling frequency was observed to capture the rapid change in particle velocities and RSD

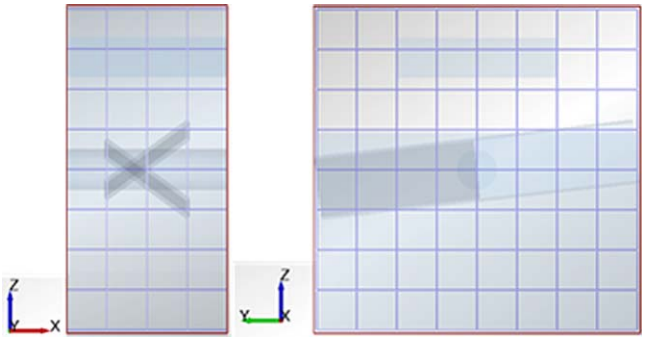

Figure 3. Discretization of periodic section for extraction of state data.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

occurring immediately after a change in blade rotation rate. The dynamic velocity profiles were smoothed using a Savitzky–Golay[72] filter prior to state space reduction.

The output space consisted of a single performance metric, the RSD. RSD was calculated as in Eq. 8 using only elements in the periodic section which contained more than 30 particles. This corresponded to 50 elements, or $N = 50$ in Eq. 8. PCA of the state space data was completed in Matlab® using singular value decomposition. 18 principal components were required to capture 95% of the variance in u_x, while only three components were needed for u_y and u_z. The fact that so many more principal components were needed for u_x is consistent with prior findings that a periodic section model is not ideally suited to represent the axial motion of particles in a continuous mixer.[6] The input space in this work consists of blade rotation rate (rpm) and time, in seconds, since a change in blade rotation rate was initiated. In this context, $t = 0$ corresponds to the moment when blade rotation rate is changed. The principal component scores were mapped to the input space using Kriging, with a unique Kriging response surface developed for each score vector. A Kriging response surface was also fitted to predict RSD as a function of blade rotation rate and time for each periodic section. Finally, PLS regression was used to develop a predictive model for RSD as a function of the reduced state space. PLS was preferred over response surface methods because examination of PLS weights can be used to gain insight into the relationship between the state variables and process performance.

Table 2. Percent Mean Square Error of Prediction for Velocities in Continuous Blender Case Studies

Percent mean square error of prediction	U_x	U_y	U_z
Case 1	0.13%	1.21%	0.48%
Case 2	0.22%	1.12%	0.65%

The accuracy of the velocity predictions was examined using k-fold cross validation with $k = 10$.[70] The percent mean square error of prediction, hereafter abbreviated as MSE, for the state data in Case 1 and Case 2 are summarized in Table 2. The MSE is less than 1.3% for the velocity predictions in both Case 1 and Case 2. This compares favorably with prior work in which steady-state ROM were developed to predict particle velocities in a periodic section of a continuous mixer as a function of design and operating parameters. These steady-state models for distributed parameters reported mean square prediction errors from 7 to 24%, as determined by leave-one-out cross validation.[6] The lower MSE achieved in this work is likely due to the larger datasets considered in developing the dynamic ROM. A visual representation comparing the velocities obtained from the ROM with those extracted from DEM simulations is shown in Figure 4 for Case 1 and in Figure 5 Case 2. Each figure corresponds to a snapshot in time, and shows velocity profiles for each of the four axial slices in the discretization shown in Figure 3. Figure 4 shows velocity profiles for the z component (u_z) for Case 1 while Figure 5 depicts velocity profiles for the x component (u_x) in Case 2. It can be seen from Figures 4 and 5 that the contours of the velocity profiles predicted using the ROM are comparable to those obtained from the DEM simulation.

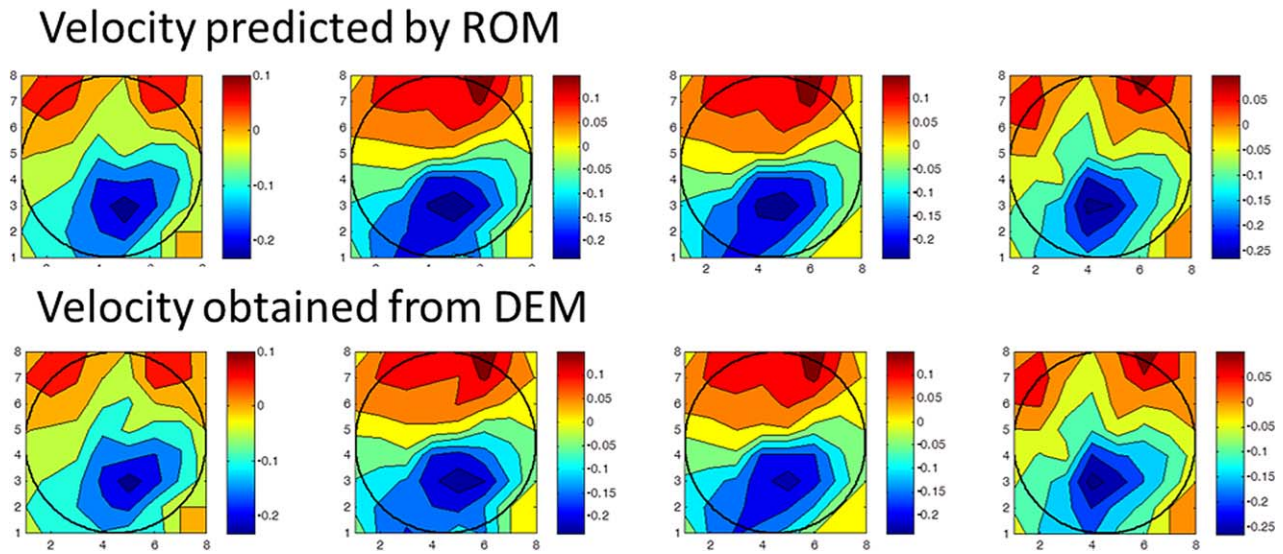

Figure 4. Predicted u_z obtained from ROM vs. u_z obtained from DEM simulation for the periodic section in Case Study 1.

Snapshot at $t = 3$ s after a change in blade rotation rate from 144 to 44 rpm.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

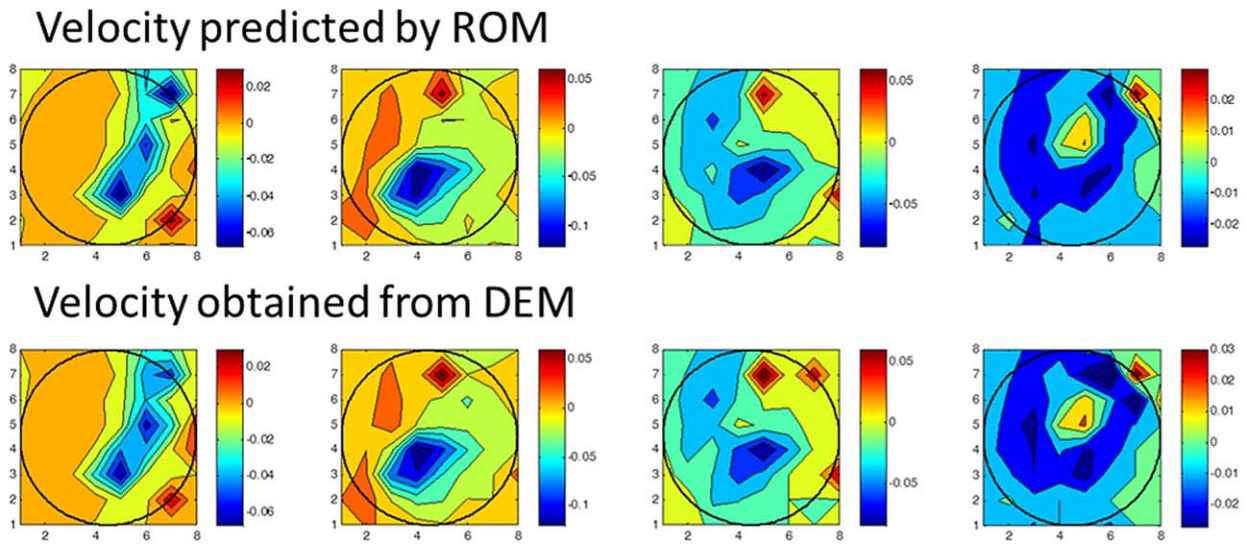

Figure 5. Predicted u_x obtained from ROM vs. u_x obtained from DEM simulation for the periodic section in Case Study 2.

Snapshot at $t = 0.7$ s after a change in blade rotation from 170 to 115 rpm.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

The performance of the mixer, as indicated by the RSD, was modeled dynamically as a function of the blade rotation rate. Kriging was used to develop a response surface relating RSD to blade rotation rate over time. These response surface models were also validated using k-fold cross validation with $k = 10$, and the percent mean square error of prediction for the RSD was found to be less than 1.0% for Case 1 and Case 2. This compares favorably to the accuracy previously reported for PCA based ROM in DEM and CFD applications. In Lang et al.,[49] predicted process performance was generally within 1% of the value obtained from the detailed process model, as determined via leave-one-out cross validation. However, for some process responses prediction errors were as high as 5%. In prior work on DEM-based ROM for continuous blenders, a prediction error for blender RSD of 1% is reported at steady state.[6] However, the prediction error is reported only for a single set of design and operating conditions, so a mean square error of prediction is not available for direct comparison. Prediction errors for the Kriging response surface models are summarized in Table 3, in the column titled "PMSE-Kriging." Figure 6 shows the predicted RSD values for Case 1 as a function of time on the same axes as the RSD values obtained from DEM. These are generally shown to be in good agreement, although the model tends to under predict RSD outliers. These outliers occur immediately after a change in blade rotation rate, when the RSD is greatest. Kriging is an interpolating method, and as such prediction variance tends to be greatest when the gradient of the response surface is steepest. The gradient of the RSD with respect to time is steepest immediately after a change in operating conditions, and as a result the prediction error is greatest in this region. Specifically, the model under predicts in this case because a majority of data fall below these RSD outliers.

The proposed modeling approach can also be used to examine the mixing performance in a periodic section as a function of the various velocity components (u_x, u_y, and u_z). This can be accomplished by modeling the RSD for the periodic section as a function of the state data. PLS regression was used to develop a model for the RSD as a function of the reduced state space. PLS was selected due to the interpretability of the model parameters.[54] The regressor in this case was chosen as a matrix containing the first two principal component scores for each velocity component, as shown in Eq. 9, where the vectors t_{x1} through t_{z1} correspond to principal component scores obtained by conducting PCA on the

Table 3. Percent Mean Square Error of Prediction for RSD in a Periodic Section of a Continuous Convective Mixer

	PMSE—Kriging	PMSE—PLS
Case 1	0.51%	0.80%
Case 2	0.55%	1.52%

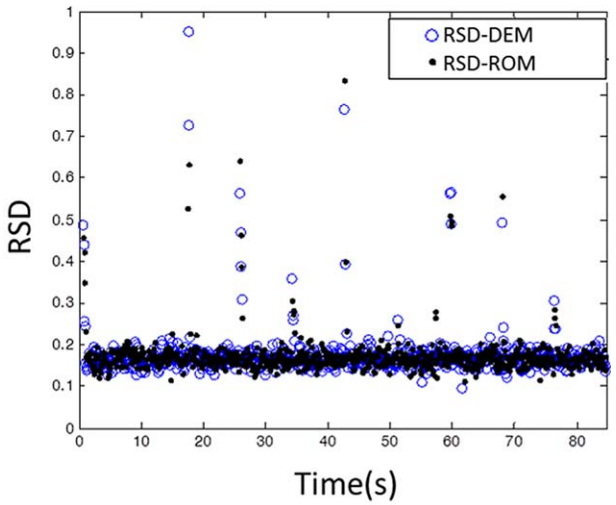

Figure 6. Predicted RSD obtained from ROM (RSD-ROM) and RSD obtained from DEM (RSD-ROM) as a function of time for periodic section simulation in Case 1.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

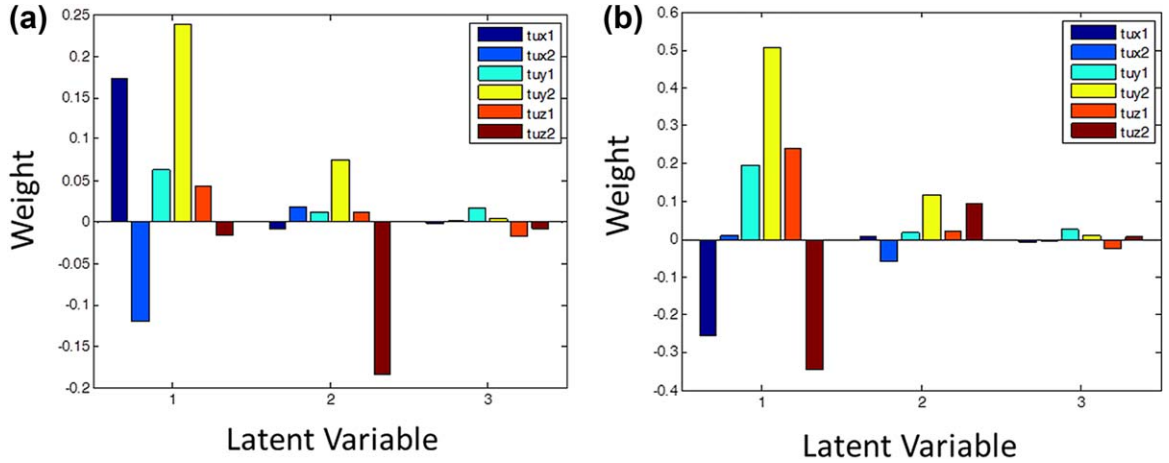

Figure 7. PLS weights for velocity components in PLS-regression model for prediction of RSD as a function of state space scores for (a) Case 1 and (b) Case 2.

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state space. This regressor was selected to facilitate interpretation of the results with respect to the particle velocities

$$[t_{x,1}t_{x,2}t_{y,1}t_{y,2}t_{z,1}t_{z,2}] \rightarrow RSD \tag{9}$$

The PLS models for RSD were validated using k-fold cross validation with $k = 10$. The percent mean square error of prediction for each case study is summarized in Table 3, in the column titled "PMSE-PLS." For both Case 1 and Case 2, the MSE is found to be less than 1.6%. Although it is not as accurate as the Kriging model, the PLS model can still be used to gain insight into the relationship between velocity components and blending performance. Examination of the PLS weights, shown in Figure 7 indicates a strong contribution of the y and z components of the velocity (u_y and u_z) to variability in RSD for both Case 1 and Case 2. This is consistent with the theory of periodic section modeling, as velocity in the x-direction tends to correlate most with the residence time in the periodic section while powder movement in the y and z directions is indicative of batch mixing within the periodic section.[32] The velocity in the x-direction plays a more significant role in mixing performance for Case 1 than for Case 2. This may indicate that back-mixing is more prevalent in Case 1, which is consistent with the blender geometry. The blender configuration in Case 1 has a larger weir height and increasing the weir height tends to promote back-mixing in continuous blenders.[13] Information about the dependence of mixing performance on the various velocity components may be used to identify important mixing mechanisms for various blender configurations. It can also be used to identify which velocity components are most influential with respect to RSD. This in turn can be used to adjust mixer configuration to enhance either axial or radial velocity with the aim of improving mixing performance.

Full blender case study

Periodic section modeling is useful for characterizing mixing performance with respect to design and operating parameters. However, in process simulation applications velocity profiles within the entire blender are of interest. Therefore, the proposed methodology has also been applied to a complete blender case study. The DEM simulation used for the full blender is a model of a Gericke™ GCM 250. The blade rotation rates are sampled from a uniform distribution between 40 and 250 rpm, as these are the operating limits for this equipment. The process geometry was divided into 6 axial sections and each was further discretized into a 6 by 6 grid in the y-z plane. The discretization of the process geometry was selected to be consistent with an existing discretized PBM for the continuous blender, so that the predicted velocities can be used in the PBM if desired.[22] The discretized geometry is depicted in Figure 8. The complete blender was simulated for 90 s at each blade rotation rate, as this was greater than the residence time for the blender even at the lowest blade rotation rate. RSD was calculated at the outlet of the blender, the section corresponding to $x = 6$ in Figure 8, over a total of 36 elements. In this case, 23 principal components were required to capture 95% of the variance in u_x, while eight components were needed for u_y and u_z.

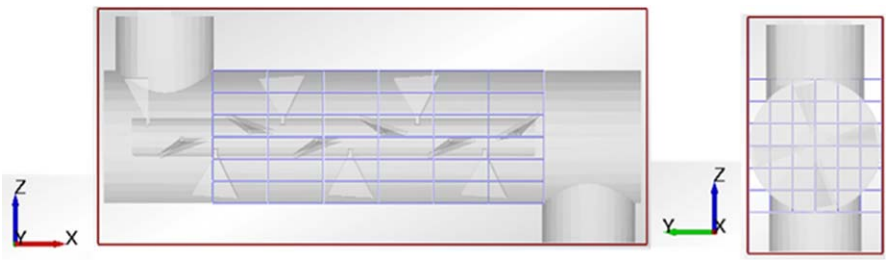

Figure 8. Discretization of process geometry for complete blender simulation.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 4. Percent Mean Square Error of Prediction for Velocity Components and RSD for the Complete Blender Simulation

	U_x	U_y	U_z	RSD
Percent mean square error of prediction	0.55%	0.96%	1.13%	1.07%

Model development and cross validation were carried out as in the periodic section case study, using k-fold cross validation with $k = 10$. In this case, a PLS model relating the reduced state space to the blender RSD was not developed, as only a single blender configuration was considered. Percent mean square error of prediction for the particle velocities and RSD are summarized in Table 4. The MSE is less than 1.2% for prediction of all velocity components. This compares favorably to previously reported prediction accuracies for ROM of state data using a PCA-based approach, which report MSE ranging from 7 to 24%.[6] The MSE is 1.1% for the RSD predictions, which compares well to the prediction error of 1% reported for the RSD in Boukouvala et al.[6] Good agreement between predicted RSD values and those obtained from DEM can also be seen in Figure 9, which shows the RSD predicted from the ROM as a function of time on the same axes as the RSD values obtained from the DEM simulation. Figure 10 compares the velocity profiles for u_x predicted by the ROM with those obtained from the DEM simulation. Each segment in Figure 10 corresponds to an axial slice of the mixer, as described in the discretization for the full blender, Figure 8. The velocity contours shown in Figure 10 correspond to a snapshot in time, as in Figures 4 and 5. Good agreement is observed between the velocity contours predicted by the ROM and those obtained from the DEM simulation.

The prediction accuracy for the models developed in this case study are comparable to those reported in previous implementations of ROM developed based on CFD or DEM simulations.[6,49] The developed ROM can thus be used in dynamic simulation applications to determine particle velocity profiles and RSD for a continuous blender. The ROM can provide significant savings in computational cost relative to the DEM simulation. The ROM evaluates in a matter of seconds, while the DEM model for the Gericke™ GCM250 takes 12 or more hours to run on the same computer.

Conclusions and Future Work

In this work, a method has been introduced for dynamic ROM of distributed parameter information in particulate systems. Distributed parameters, or state data, include things like particle velocity profiles within processing equipment and are often high-dimensional in nature. In the proposed method, PCA is used to reduce the dimensionality of state data and Kriging, a response surface technique, is used to map the reduced state space to process operating parameters. The ROM developed in this work are intended for use in process modeling applications in place of detailed simulations like DEM to improve computational efficiency. The performance of the ROM was thus evaluated relative to the detailed (DEM) simulations. Case studies related to continuous blending of particulate materials were used to demonstrate and evaluate the proposed method. The distributed parameters of interest in these case studies were particle velocity trajectories within a continuous convective mixer. The ROM performed well, predicting particle velocity profiles similar to those obtained from DEM simulations and evaluating quickly as compared to the more detailed process model. The prediction accuracy of the ROM for state variables developed in this work was improved relative to that reported in prior implementations of ROM for state data obtained from DEM simulations.[6]

ROM were also developed to relate process performance to operating parameters. In this work, the RSD was used as an indicator of mixing performance. Kriging was used to map RSD to the blade rotation rate in a continuous mixer. The dynamic response of the RSD to changes in blade rotation rate was well-represented by the developed ROM. Prediction accuracy for this ROM was comparable to that reported in prior applications of DEM and CFD based ROM.[6,49]

The developed ROM have numerous potential applications in process simulation and optimization. The prediction of distributed parameters can be used to enhance the accuracy of PBM for continuous mixing by incorporating estimations of particle velocities comparable to those obtained from DEM.[22,23] Using a ROM, particle velocity predictions can be obtained in a matter of seconds as compared to the several hours required to simulate the continuous blender using DEM. In addition, the ability to directly evaluate performance metrics like RSD as a function of process operating parameters has potential applications for surrogate-based optimization,[8,40] and model predictive control,[26] where rapid model evaluation is necessary.

ROM have also been introduced to connect distributed parameter information (particle velocities) with mixer performance through PLS regression of the RSD onto the reduced state space. Analysis of the model features, such as the PLS weights, can be used to identify key velocity components in a variety of mixer configurations and suggest modifications to design parameters like blade configuration or weir height to improve mixing performance.

The ROM approaches used in this work are data-based and as such have several limitations. It is not recommended

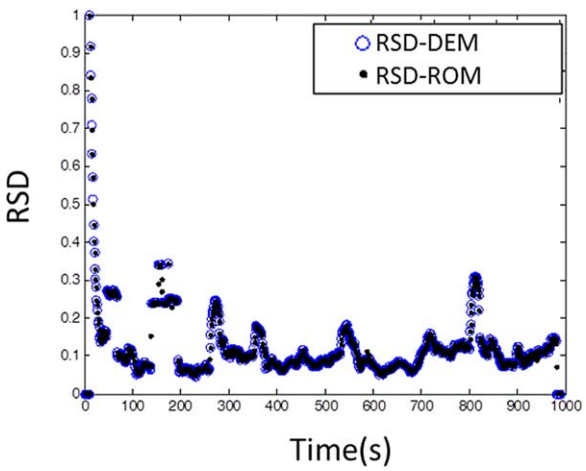

Figure 9. Predicted RSD obtained from ROM (RSD-ROM) and RSD obtained from DEM (RSD-ROM) as a function of time for complete blender simulation.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

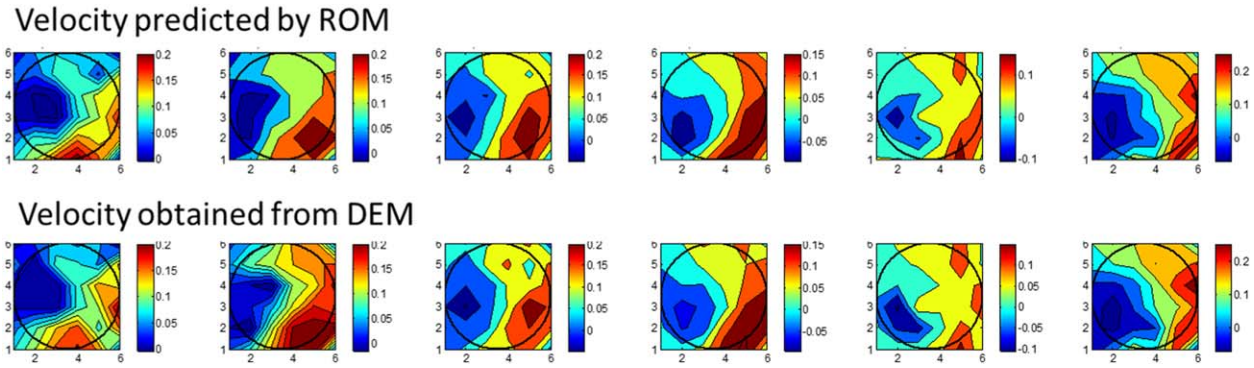

Figure 10. Predicted u_x obtained from ROM vs. u_x obtained from DEM simulation for the full blender case study.

Snapshot at $t = 23$ s after a change in blade rotation rate from 160 to 250 rpm. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

extrapolate using models developed with this method. Kriging is an interpolating method and as such is limited in its ability to extrapolate. In addition, the model for the state data relies on a principal component decomposition, which is only valid if the scores corresponding to a new data point fall within the score space of the dataset used to develop the model. In implementing this approach, it is thus recommended to sample within the full range of operating conditions for the unit operation of interest so that the model is used for interpolation rather than extrapolation. In addition, the developed ROM are fitted using information obtained by sampling a more detailed process simulation based on DEM or CFD. As such, the developed ROM will only be as accurate as these detailed process simulations.

Future work will focus on extending the proposed methodology to additional blender configurations and geometries. This will allow additional design and operating parameters to be incorporated into the existing ROM. As additional blender configurations are explored, the process discretization required to adequately represent the state space may also vary. This will facilitate the development of additional understanding with respect to the effect of process geometry discretization on the quality of the ROM in terms of its ability to accurately represent information obtained from more detailed process simulations.

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