Hybrid DEM-Compartment Modeling Approach for Granular Mixing

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A new hybrid approach to model powder mixing based on the use of discrete element method (DEM) and compartment modeling is presented. The main motivation behind the proposed approach is to reduce the computational expense of modeling powder mixing by partitioning the mixing system into high shear areas that are modeled using detailed DEM simulations, whereas the remaining process is simulated using stochastic models. The approach can, thus, be used to model complex geometries, as well as a large number of particles that is typically unfeasible with the existing approaches. The results of a horizontal convective mixing vessel are used to illustrate the applicability and efficiency of the proposed approach. © 2006 American Institute of Chemical Engineers *AIChE J,* 53: 119–128, 2007
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Introduction

Powder mixing processes are typically difficult to characterize since powders cannot be classified as either solids or liquids.[1] The unusual flow behavior of powders is of particular importance since segregation and agglomeration reduce the powder uniformity of powder blends used in a large number of applications. In order to model powder flow and improve the characterization of powder processes, several models have been proposed. Wightman and coworkers,[2] and Ottino and Khakhar[3] distinguished the following groups of mixing models: Monte Carlo simulations, particle-dynamic simulations, heuristic models, and models based on kinetic theory. Although these models have proven successful in describing the mixing behavior in many case studies, there are a number of remaining challenges that are briefly summarized here. In Monte Carlo simulations it is difficult to correlate real mixing time to simulation time. In the case of particle-dynamic simulations, the computational requirement for realistic mixing systems is extensive, thus, the computational power required limits the beneficial usage. The main limitation of the heuristic models is that they are based on ideal conditions, whereas the models based on kinetic theory are capable of simulating only binary and tertiary mixtures. Another method well suited to model deforming solid materials is smoothed particle hydrodynamics (SPH).[4] This method was originally developed for fluid mechanics, but has been applied to solid mechanic problems where there is fracturing, shattering, and possible phase change. It has, however, not been used to model solid mixing except where particle fractures occur.

In our previous work,[5] we demonstrated the use of compartment modeling as a tool to efficiently model and characterize powder mixing. Although compartment modeling is a very powerful analysis tool for mixing characterization, it does not predict the details of particle behavior, such as particle location and particle trajectory, which can be determined using a particle-dynamic simulation, such as discrete-element method (DEM).

Discrete-element method (DEM) is a simulation methodology that predicts the trajectories of individual particles by solving Newton's equations of motion.[6] A number of studies have been performed using DEM, including modeling tumbling mixers[7,2,8] and convective mixers.[9,10,11] An excellent review of the recent advances in the field of powder mixing and DEM can be found in Bertrand et al.[9] However, as shown by Bertrand et al.[9] the computational cost is significant since the equation of motion for each particle must be solved at each time step which limits the applicability of DEM models. In order to overcome this limitation the particle morphology is approximated or the number of particles are reduced.[12,13]

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However, in many cases only a small area of the mixer has to be modeled using a detailed DEM simulation. This has been shown by Zhou et al.[8] that illustrated that for sufficient fill levels the physical actions of the impeller no longer affect the contents of the vessel within certain sections. The method proposed in this article takes advantage of this fact and combines the computational simplicity of compartment modeling with the detailed particle simulation of a mixing process achieved by DEM. Along the same lines, McCarthy and Ottino[14] proposed an approach based on the integration of geometric insight with particle dynamics to form a hybrid technique for a tumbler operating in the avalanching regime.

In the proposed approach, the areas that need better characterization in order to model the mixing process are solved with DEM whereas the rest of the system is captured with a compartment model. For example, in the case of a horizontal-stirred mixer, the impeller area is captured using DEM, and the surrounding area is simulated using compartment modeling. The compartment and DEM simulations are run in parallel, interchanging particles for the desired mixing time. The proposed framework results in a detailed description of the mixer with a substantial reduction of computational time compared with DEM simulation.

Following this introduction, the rest of the article is organized as follows. In the second and third sections, the main ideas of compartment modeling and discrete element method approaches are outlined, whereas the new hybrid approach is presented in the fourth section followed by hybrid parameters in the fifth section, and a number of case studies for a horizontal mixer in the sixth section. Finally, the last section presents a discussion of the results and future research directions.

Compartment Modeling

Compartment modeling has been effectively used to model the mixing of fluids in reactors in an attempt to incorporate micromixing effects. Correa[15]and Shah and Fox[17] have utilized this idea to model turbulence in chemical reactors. Specifically, the fluid is represented by a large number of particles, and at each time step a certain number of particles enter the reactor, while particles randomly selected from the ensemble, exit the reactor at the same mass flow rate. The interactions between particles are represented by random collisions, based on the mixing regime.

In our recent work,[5] compartment modeling is applied to granular mixing by spatially partitioning the system into a number of subsections that are assumed to be perfectly mixed, and contain a stipulated number of particles. Discretizing the time domain, a number of particles are allowed to flow from each compartment to the neighboring ones, at each time step. The number of particles transferred account for the mixing occurring throughout the vessel. Following the ideas of Fan et al.[17] who described powder mixing as a random process, the particles chosen to leave and enter each compartment are randomly selected following a probability distribution.

Compartment modeling can in principle be applied to any mixing process as long as there is information regarding fluxes to identify different mixing regimes, and define the number of compartments needed. This information can be obtained computationally using detailed particle simulations or experimentally by using particle tracking methods, such as positron emission particle tracking (PEPT),[18] or near infrared (NIR) spectroscopy.[19] PEPT uses radioactive tracer particles that are tracked by a scintillation camera as they move within a bed,[18] whereas NIR spectroscopy[19] measures the wavelength and intensity of the absorption of near-infrared light within a set of particles, which calculates the content within the sample. One advantage of PEPT is that it is a noninvasive method. However, the accuracy of the technique decreases as the particle velocities increase, because the laser cannot move at the same speed as the particles. When using NIR, the measurements could be intrusive when samples are physically removed from the mixer or noninvasive when placed on-line, however the chemical compound identification is not as informative as with other methods, such as Fourier transform infrared (FTIR) analysis that provides information about the chemical structure of the material.

Discrete Element Method (DEM)

Discrete element method (DEM) was developed by Cundall and Strack[20] and refined by Walton and Braun.[21] The method is based on a finite number of discrete, semi-rigid spherical shaped particles interacting deterministically by means of contact or noncontact forces. All the particles within the system have a known exact spatial position. The system is spatially discretized into a number of three-dimensional (3-D) grids, and each particle is contained within at least one grid. If a force is exerted on the particle, the particle will most likely collide with other particles that exist within its grid or neighboring grids. The force model between two particles considers that the collision or interaction between two particles occurs either in a single point or a finite area.[22] Walton and Braun's[21] partially latching spring model is utilized for elastic particle collisions. Once the collision takes place, the force on the particle is calculated using Newton's equations of motion and the particle trajectory is determined.

DEM models have been extended to account for the cases where a moving impeller is present in a mixing system. One strategy is based on discretization of the boundary surfaces by means of a finite-element mesh that can be determined using a mesh generator known as multi-wall method established by Kremmer and Favier.[23] Another approach is developed by Cleary et al.[7] that use a series of particles to represent a boundary domain. For the case of a rotating drum with a blade, the blade consists of an assemblage of particles with physical properties that mimic the interactions that the particles have with the impeller. Due to the increasing number of interactions and particles, the simulations become computationally cumbersome. As shown by Bertrand et al.[9] the computational complexity increases exponentially with the number of particles in the vessel, which limits the applicability of DEM (Table 1). Another alternative to reducing the computa-

Table 1. CPU time/Impeller Revolution with DEM from Bertrand[9]

Number of Particles	Serial Computer	32 procs (Speedup = 16)	64 procs (Speedup = 32)
10^3	3 h	10 min	5 min
10^4	1.25 days	2 h	1 h
10^6	4 months	1 week	3.5 days

tional time of a DEM simulation is parallelizing the model algorithms. Parallel programming takes advantage of parallel computing systems by separating tasks, allocating and synchronizing tasks to different processors. As shown in Table 1 increasing the number of processors linearly decreased the computational time.

Compartment Modeling and DEM Comparison

A comparison between compartment and DEM modeling is performed in this section to illustrate the advantages and limitations of each method. A discrete element model was used by Wightman and coworkers[24] to describe a horizontal cylindrical vessel undergoing rotational motion. The study consisted of modeling the motion of identical particles, red and blue. The vessel was initially loaded with side-by-side loading, one half of the cylinder filled with red particles and the other half with blue particles. The granular mixing vessel was subjected to pure rotation, meaning the cylinder rotates along the horizontal axis. Wightman and coworkers[24] compared the results of the DEM simulation with experimental data[25] obtained from solidifying the powder mixture at a moment in time. Once solidification occurred, slices of the mixture were taken and analyzed under image analysis. The fraction of red particles throughout the vessel showed good agreement with the experimental study and DEM simulation. To compare with this study a 16-compartment-model, is used to simulate the horizontal cylindrical vessel (Figure 1). The fraction of red particles is determined as a function of axial length at four different time points. The graph in Figure 2 shows that the compartment model can very well capture the particle compositional behavior as a function of axial length.

The main advantage of compartment modeling is its computational speed. For this case, the compartment simulation required 2,084 CPU sec on a Sun Sparc 900 MHz Processor 2GB, whereas the DEM simulation performed by Wightman and coworkers[24] required about 48 h of CPU time for every second of real time simulated on a Sun Sparc 20.6 workstation, thus, revealing huge computational savings. However, it should be pointed out that the DEM simulation results in the detailed characterization of particle behavior including particle position and trajectory, which is not obtained using compartment modeling.

Hybrid Compartment-DEM Modeling Approach

As described in the previous section, DEM calculates the spatial trajectory of every particle under the effects of convective, shear, dispersive, and gravitational forces. The main drawback, however, is that DEM simulations can be computationally very expensive, especially when complex geometries are considered. Thus, the main objective of this work is to reduce the computational expense of powder mixing simulations by partitioning the mixing system into regions of higher complexity, to be modeled by DEM and regions of lower complexity to be simulated using compartment modeling.

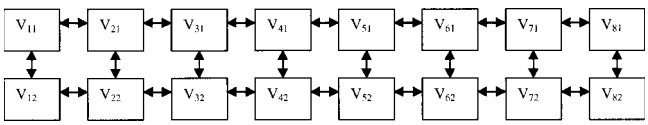

Figure 1. Compartment model representing a horizontal tumbling blender.

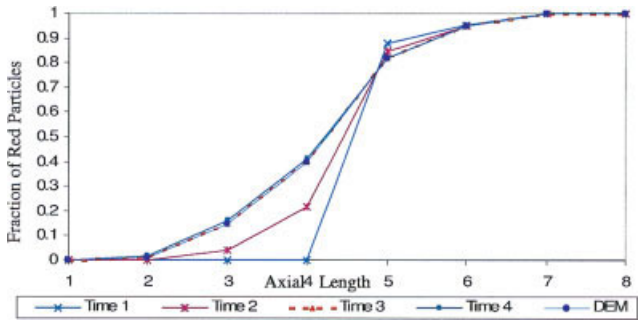

Figure 2. Compartment model results for the red particle fraction at time points 1 through 4 in comparison with a DEM simulation at one time point for a horizontal tumbling cylinder.

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

Proposed Framework

The steps of the proposed approach, which are shown in the flow chart depicted in Figure 3 are as follows:

Step 1. First, the mixing system is partitioned into different mixing regions depending on the level of complexity. Complexity is defined as the degree of variability within particle circulations that exists within that mixing region. Regions of

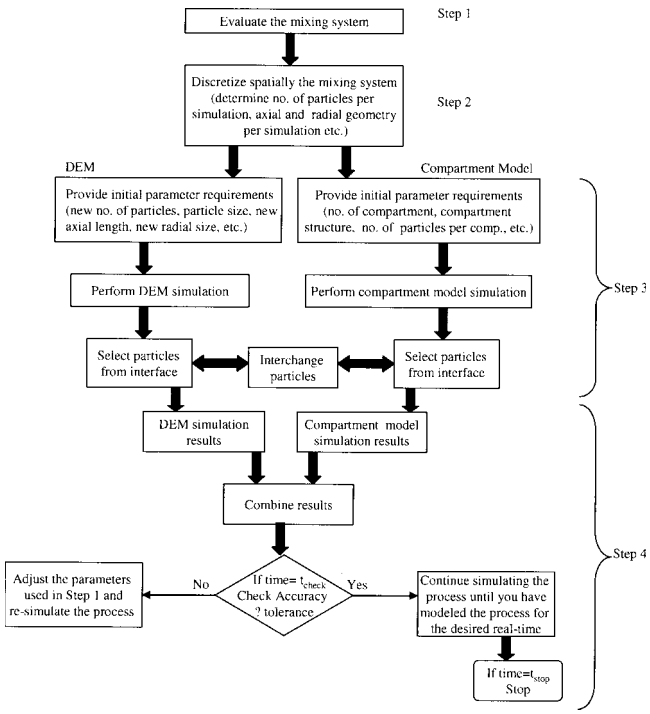

Figure 3. Proposed new hybrid algorithm.

Table 2. Simulation Parameters for the DEM Simulations of a Horizontal Cylinder with a Blade

Number of Red Particles	700
Diameter of Red Particle	.01 m
Number of Blue Particles	700
Diameter of Blue Particle	.01 m
Radial Length of Vessel–D	.1 m
Axial Length of Vessel–L	.5 m
Length of Impeller Rod–Lr	.45 m
Diameter of Impeller–Dr	.1 m
Impeller thickness	.05 m

high complexity are modeled using DEM (or any other detailed simulation approach), and lower complexity regions are simulated using compartment modeling (or any other statistical model). In the next section, two approaches are presented for partitioning the mixing system.

Step 2. In this step, the parameters needed to perform the numerical simulations are determined. For the areas described by DEM, the number of particles, particle diameter, and vessel geometry corresponding to each chemical or physical group within the vessel must be specified. For the compartment model, the number of compartments, the number of different particles within each compartment, and the particle fluxes must be defined. The particle flux is defined as the number of particles exchanged, between compartments per time step. The particle flux is calculated based on the difference between the number of particles (N) that are within the region (i) at time ($t + \Delta t$), and the number of particles at the same region at time (t) divided by the elapsed time (Δt): $\frac{N(i,t+\Delta t)-N(i,t)}{\Delta t}$.

Step 3. Once the system parameters are defined in the previous step, the DEM and compartment simulations are run in parallel. The trajectory of particles leaving one mixing regime and entering another are captured as particle exchanges between the compartment and DEM simulations. Thus, at selected time points, a designated number of particles located at the interface between DEM and compartment modeling are randomly exchanged. The approach used to model the particle exchanges is described in the Exchanging Particles between Model section.

Step 4. The simulations continue to run until the check point time is reached t_{check}. At this point, we check the hybrid results to those obtained from well-established methods (described in the Quantifying Model Accuracy and Validation section). If the difference is within an acceptable tolerance level, which is prepostulated by the user, the simulation continues to run and stops when the desired real-time has been modeled t_{stop}, otherwise parameters are adjusted and the simulations are repeated.

Mixing Process Partition

As mentioned in the previous section, the first step in the proposed hybrid approach is to determine the degree of complexity in each section in order to treat each section with the appropriate modeling tool. In this section, two methods are described that can be used to partition the mixing system. The first approach is based on heuristics and geometric arguments, whereas the second approach is centered on estimation of particle velocities.

Partition Method I

The first method involves the spatial discretization of the mixer given prior knowledge of the different mixing regimes. Once the vessel is divided into regions, the particle flux defined as the slope of the number of particles at different time intervals (j) is denoted as m_j. This is determined for each section computationally or experimentally. Since the particle fluxes at each region vary as a function of time, the particle fluxes are evaluated at different time intervals. The standard deviation is evaluated based on the difference between the average particle fluxes with one region at different time points. If the particle fluxes exhibit high variability in terms of the standard deviations (σ), a detailed model is used to account for the mixing behavior in that region. On the other hand, if the particle fluxes show a small degree of variability at different time intervals, then a less expensive model, such as a compartment model can be used to simulate this region.

Partition Method 1 — Illustrative Example

An illustrating example is used here to demonstrate the previously described approach. The system studied is a horizontal cylinder with an impeller with the parameters shown in Table 2. The vessel is loaded with two types of particles distinguished by their color (red or blue). The horizontal cylinder within an impeller attached to a rod, shown in Figure 4a, is divided into five regions all with the same diameter, d, and axial length L/5, as shown in Figure 4b. Once the vessel is divided into the preselected number of regions, the particle flux (that is, the number of particles exchanged within each region j, at each time step) is determined. The fluxes denoted as m_1, m_2, and m_3, for three different time intervals, and all the regions, are displayed

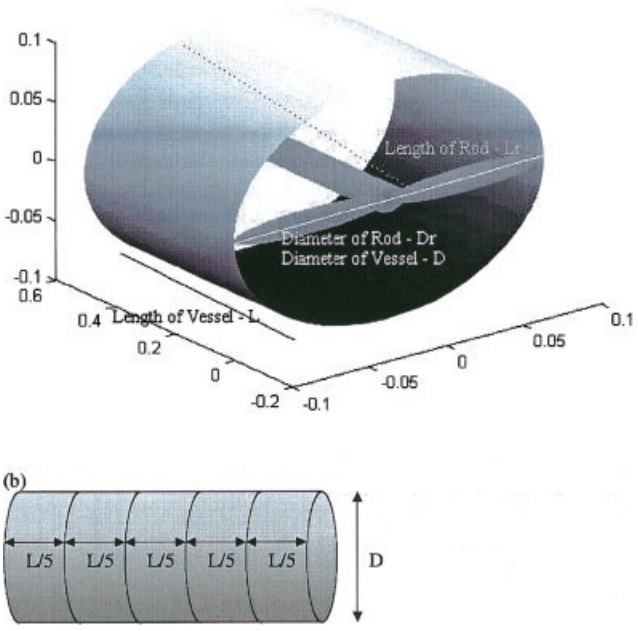

Figure 4. (a) A mixer modeled in the case studies, and (b) mixer partitioned into 5 regions with the same radial and axial distance.

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

Table 3. Particle Fluxes for Both Red and Blue Particles in Five Regions within the Horizontal Cylinder

	Blue Particles					Red Particles			
Region	$\|m_1\|$	$\|m_2\|$	$\|m_3\|$	σ	Region	$\|m_1\|$	$\|m_2\|$	$\|m_3\|$	σ
1	27.08	11.69	12.84	8.6	1	2.34	14.01	20.97	12.0
2	2.48	6.82	7.50	5.6	2	0.13	2.36	10.10	9.9
3	1.58	2.40	4.90	1.7	3	0.76	6.41	4.95	5.7
4	3.78	4.92	9.54	3.1	4	3.26	3.48	10.10	3.9
5	1.83	0.70	2.74	1.0	5	3.22	2.58	6.16	1.9

in Table 3. Regions 1 and 2 exhibit higher variability. This is expected since these regions are closer to the moving blade. Thus, using the first approach regions 1 and 2 will be modeled using a discrete element method, while regions, 3, 4, and 5, will be simulated using a compartment model.

Partition Method 2

The second approach partitions the mixer into separate regions depending on the particle velocities in comparison to the first approach that uses the variability in particle fluxes. For conditions where no experimental measurements exist, the velocity profiles can be determined using a computer simulation. In this case, in order to limit the computational requirements, the simulation time is reduced to the necessary time needed to characterize the system. To determine whether reducing the modeling time affects vessel partitioning, the particle velocities at succeeding time intervals are evaluated. For the system described in the previous section, the particle velocities as a function of axial length at different time intervals are obtained from a DEM simulation, and displayed in Figure 5. The figure illustrates that as time increases, the particle velocities exhibit the same behavior with respect to axial length. The average velocity variance as a function of local axial area is shown in Figure 6, which also illustrates that as time increases the variance does not pose significant changes, confirming that running the DEM simulations for a small period of time is sufficient to identify the areas of high complexity.

Partition Method 2 — Illustrative Example

This section focuses on illustrating the partitioning method that utilizes particle velocities obtained from a DEM simulation with the geometric specifications shown in Table 2. Using these parameters, the particles' radial velocity is obtained and plotted in Figure 7, with respect to axial length. As the figure shows, the mixer can be partitioned into two areas, a region with an axial position greater than .25 m which is modeled with a detailed DEM simulation, whereas the rest of the vessel is simulated using compartment modeling. Thus, the mixer was discretized into 10 regions, considering that the mixer length is .5 m, and the particle distribution at every .05 m needs to be monitored. Thus, five regions will be simulated using the DEM and the remaining five will be simulated using compartment modeling. Comparing the two partition methodologies, we observe that the second method resulted in a larger percent of the total volume modeled using DEM, 50% compared to 40% with the first method. This is mainly because the second partition method utilizes a more accurate description of the particle behavior based on particle velocities compared to the first method, which is based on system knowledge.

Exchanging Particles between Models

Particles are exchanged between the different model simulations in order to account for the realistic trajectory of particles moving throughout the mixer. The particles are randomly selected from the regions closer to the neighboring simulation boundaries. However, a problem arises when exchanging particles between a DEM simulation and statistical model, because the positions, velocities, and forces of the particles entering the DEM simulation are unknown. Defining these values is important since a detailed simulation like DEM requires the particles' present conditions in order to calculate the particle's future trajectory. To address this problem, we tag each of the particles entering the DEM simulation with the exact position, velocity, and force of a randomly chosen particle exiting the DEM simulation. For example, if particle l leaves the DEM simulation, whereas particle k enters, particle k will replace the position occupied by particle l as shown in Figure 8. It is important to point out that the physical identity of the particle does not change because the idea behind exchanging the particles is to account for the variation in composition.

Quantifying Model Accuracy and Validation

For many industrial products, processes need to be strictly characterized throughout the processing stages in order to guarantee product quality. Typically the homogeneity of a powder mixture is measured via sampling within the actual

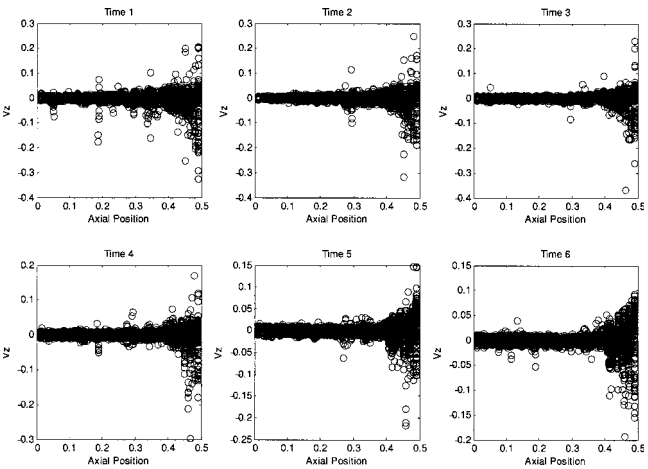

Figure 5. Velocity component profile at increasing time intervals (a) (.5s–.75s), (b) (.75s–1s), (c) (1s–1.25s), (d) (1.25s–1.5 s), (e) (1.5s–1.75s), and (f) (1.75s-2s).

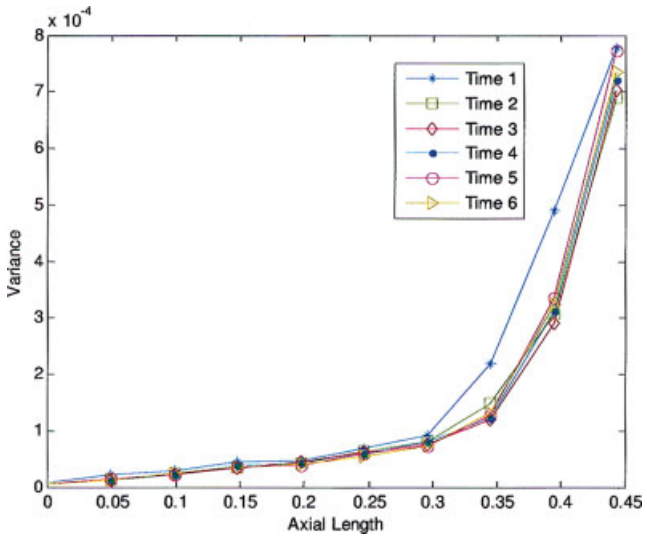

Figure 6. Velocity variability as a function of axial position for the following time intervals: Time 1 (.5s–.75s), Time 2 (.75s–1s), Time 3 (1s–1.25s), Time 4 (1.25s–1.5s), Time 5 (1.5s–1.75s), and Time 6 (1.75s–2s).

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

process or model. The variability within the samples must comply with guidelines that require that the variance does not exceed a certain limit. There are several factors that contribute to the variability of the mixture that are not a result of mixture in-homogeneities, but other inaccuracies, such as the sampling parameters, and the uncertainty due to the method used to retrieve samples. In order to minimize the error introduced due to modeling approximations, the variance is measured and bounded by a prespecified tolerance as follows.

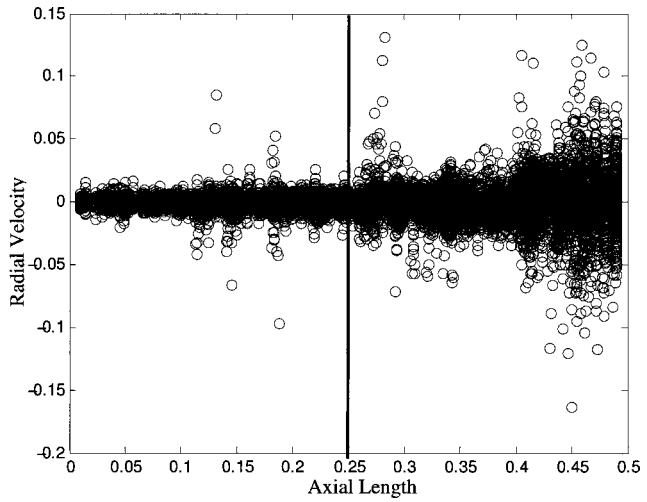

Figure 7. Radial velocity of particles with respect to their axial position within the cylinder.

The solid line represents the point where we differentiate between two simulations.

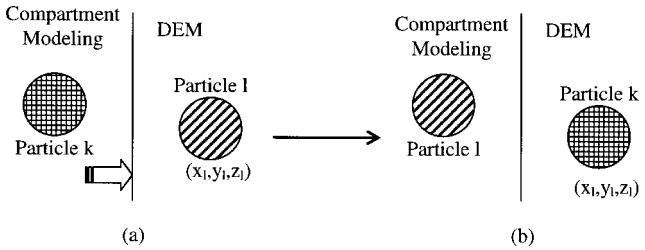

Figure 8. Simulation interface exchanging particles between compartments (a) before an exchange, and (b) after an exchange.

In order to determine how well the hybrid approach captures the overall flow in the mixing vessel we compare our results with a detailed particle dynamic model, such as DEM. The accuracy of the hybrid approach is quantified by calculating the difference between the compositional profiles determined in each iteration of the hybrid approach to ones obtained either from experimental data obtained using NIR or PEPT as described in the Compartment Modeling section, or through another computer simulation as a DEM model. The results are used to validate the proposed hybrid approach; ideally the hybrid approach distributes the particles as closely to the realistic distribution in the mixing system examined. In a given spatial domain (i), the number of particles of component (j) found using the hybrid approach is defined as H_{ij}, and the expected number of particles is denoted as E_{ij}, using an experimental analysis or computer simulation. Thus, the percentage error is defined as $e_{ij} = \frac{(E_{ij}-H_{ij})}{E_{ij}} \times 100$. Alternatively, the sum of squares of deviations of different measurements $\sigma_j^2 = \frac{1}{\eta}\sum_{i=1}^{\eta}(E_{ij} - H_{ij})^2$, can be used to evaluate the accuracy of the proposed model where η are the total number of regions.

A smaller time-point is used to prognosticate the behavior of the system denoted as t_{check}. The longer the time period modeled, the greater the computational requirement. As shown in the Partition Method 2 section, the behavior does not change as time progresses, leading us to believe varying the check time point will not necessarily improve the validation of the results. The metrics used to quantify the differences between the composition profiles obtained from the simulation, and the results obtained either from experimental evidence, or from simplified simulations are discussed in the previous section. At t_{check}, if the hybrid model obtains similar outcome to that of the substantiate results, the simulation continues until completion. Otherwise, the number of particles interchanged between simulations, the number of particles within each simulation, and the area modeled with the detailed simulation approach are adjusted and the simulation is repeated using the new parameters.

Case Study

In this section the hybrid approach is applied to model a horizontal agitated mixer, which is the same as the one depicted in Figure 4a. A similar horizontal mixing system was simulated by Müller and Rumph,[26] they demonstrated that the inclination of the blades promotes axial convection, likely by improving the flow of the material in the space above the

Table 4. Simulation Parameters

Number of Red Particles	5000
Diameter of Red Particle	.055 m
Number of Blue Particles	5000
Diameter of Blue Particle	.055 m
Radial Length of Vessel–D	.1 m
Axial Length of Vessel–L	.5 m
Length of Impeller Rod–Lr	.45 m
Diameter of Impeller–Dr	.1 m
Impeller thickness	.1 m

blades. Moreover, Laurent and Bridgwater[27] showed by using PEPT with two different tracers that the mixing of a horizontal mixer has two zones in the transaxial plane, one immediately above the agitator shaft, and the other beneath it.

The geometric specifications of the horizontal mixer studied in this section are shown in Table 4. The vessel was loaded with two types of particles distinguished by their color (red or blue). The mixer was discretized into 10 regions in order to track the particle distribution axially at every .05 m. The vessel is partitioned using the method discussed in the Partition Method 1 section. As a result, the variability that existed within the particle fluxes, showed that four regions should be modeled using DEM (Figure 9a, nonshaded area), and the remaining six (Figure 9a, shaded) can be simulated using compartment modeling as shown in Figure 9b. The results were analyzed using the metrics discussed in the Quantifying Model Accuracy and Validation section by comparing the compositional distribution of the different types of particles with the results of a simulation, which is based entirely on DEM.

The compositional distribution of the blue particles as a function of time for 3 regions (2, 3, and 4) is shown in Figure 10a, and as a function of time for 2 regions (9 and 10) 10b. It is important to point out that the compositional distribution behavior determined using a DEM simulation is accurately captured by the hybrid approach. The percentage errors for both the red and blue particles in all 10 regions are shown in Table 5. The average error for all regions and components is 7.96%. Notably, DEM simulations randomly distribute particles throughout the vessel, and as the particles collide at different positions on the impeller, the particles are deflected to

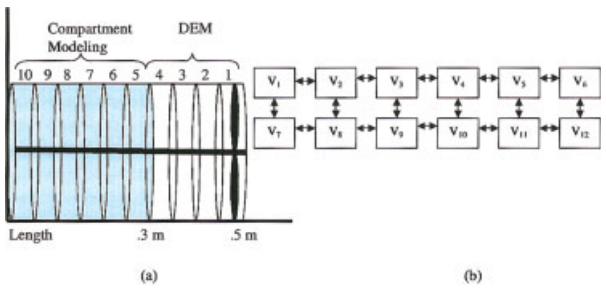

Figure 9. (a) Horizontal cylinder partitioned into regions tagged with a numerical representation shown on the top of the vessel, and (b) compartment model using the partitioning strategy described in Partition Method 1 section.

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

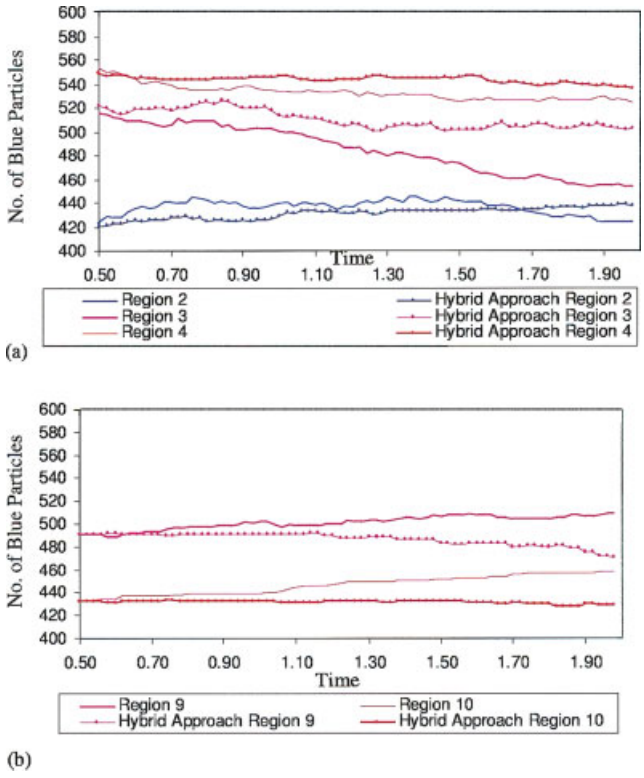

Figure 10. Results from the case study using the partitioning strategy described in the Partition Method 1 section.

The compositional distribution of a region detained from using an entirely based DEM simulation and the hybrid approach. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

neighboring regions. Thus, it is expected that region 2, the region closest to the impeller, exhibits the largest error in comparison to other regions.

The hybrid approach required 2603 CPU sec to run, whereas a simulation entirely based on DEM took 16625 CPU sec using a Sun Sparc 900 MHz Processor 2GB. Although there is an approximation error introduced in the system description utilizing the hybrid approach compared with the DEM simulation, the computational requirement is significantly reduced which allows the simulation of more realistic mixing systems.

Table 5. Average Percentage Error for Using the Partitioning Strategy Described in Partition Method 1 Section

Region	Red Particles Avg. % Error	Blue Particles Avg. % Error
1	1.60	3.47
2	26.69	20.45
3	2.42	10.89
4	7.39	2.11
5	12.87	9.60
6	11.39	9.38
7	10.60	11.24
8	1.18	9.90
9	1.32	2.95
10	0.29	3.49

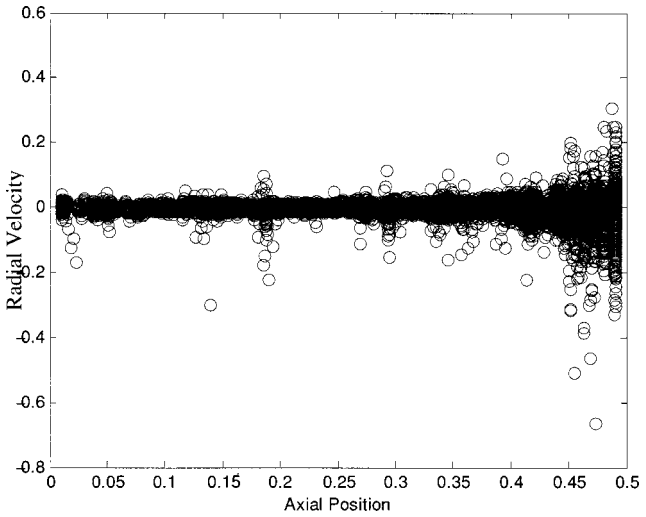

Figure 11. Radial velocities as a function of axial length using the partitioning strategy described in the Partition Method 2 section.

The second partition strategy as described in the Partition Method 2 section uses particle velocities in order to partition the mixing system. The particle velocities shown in Figure 11 are determined with a DEM simulation modeled for a short time period as discussed in the Partition Method 2 section. The velocity profile illustrates that the greatest particle velocity variability occurs for the particles that have an axial length greater than .4 m. As a result, the particles with an axial length greater than .4 m are solved with DEM, and a 16-compartment model is used for the remaining area. Using the second partitioning strategy the system is simulated in 2,540 s of CPU time, in comparison to an entirely based DEM simulation that took 16625 s of computational time. [The computational time decrease arises because this partition method predicts that a smaller volume of the mixer be modeled with DEM.] The vessel was partitioned into 10 regions in order to partition the mixing system as described in the Partition Method 2 section. Table 6 lists the percentage error for each region. The average percentage error for all regions is 5.46%, which is considered marginal given the inherent errors that exist within DEM modeling. DEM models assume several assumptions, such as spherical-particle morphology, large-particle dimensions, and vessels filled with small-particle quantities, given all these postulations the existing DEM model

Table 6. Percentages Error Results using the Partitioning Strategy Described in Partition Method 2 Section

Region	Blue Particles Avg. % Error	Red Particles Avg. % Error
1	3.99	7.35
2	5.17	3.95
3	15.79	10.60
4	2.29	5.13
5	11.83	3.26
6	8.15	5.31
7	9.45	3.38
8	1.60	1.09
9	1.46	2.02
10	3.86	3.43

Table 7. Computational and Accuracy Effect as a Function of Time-Steps

Time Step, ∇t (s)	DEM CPU Time (s)	Hybrid Approach CPU Time (s)	% of Computational Reduction	Average % of Error
1.8×10^{-5}	38280	17340	55	5
2.7×10^{-5}	16620	8880	47	6.3
4.0×10^{-5}	10980	6480	41	8.04

results in errors that make the hybrid approach's 5.46% error seem marginal. The hybrid approach clearly reduces the computational time, but it is important to consider the trade-offs between model accuracy and computational efficiency. Using the first partition method the hybrid approach required 2,603 CPU sec (computational savings were 84% compared to DEM simulation), and the error of the solution is 7.96%. [Whereas the second partition method required a little less time 2,540 s for CPU time (87% computational savings) since in the first method an additional volume of the mixer is modeled with DEM, but the error in the second method is reduced to 5.46%.]

Effects of Space and Time Partitions

In this section we examine the effects of time steps and number of partitions on the performance and computational time of the hybrid approach. The cases examined use a similar vessel to the one mentioned in the previous sections, which is horizontal cylinder (.5 m) with a horizontal blade (.05 m thick) held up by a rod (.01 in dia. and .5 in length), which is located at one end of the vessel as shown in Figure 4a. The results shown in Tables 7 and 8 consider 40% of the vessel using a DEM simulation, and 60% using compartment modeling.

As shown in Table 7, increasing the time steps does reduce the computational requirements, however, within particle-dynamic simulations the barrier that exists is that larger time steps result in imprecise particle trajectory predictions. Which is a result of inaccurate calculations of the forces acting on the particles that leads to smaller accuracy. Also, as shown in Table 7, as the time step decreases the computational time required to run the DEM simulation increases due to the additional number of calculations, although the computational cost decreases for the hybrid approach is not as large since only 40% of the system is simulated using DEM. The computational cost increase in a DEM simulation is due to the fact that DEM simulations calculate particle positions and velocities as a first-order differential system, under the assumptions that the forces remain constant at each time step, particle positions are then calculated at each time step. Due to the constant

Table 8. Computational and Accuracy Effect as a Function of Partitions

Number of Partitions	DEM CPU Time (s)	Hybrid Approach CPU Time (s)	% of Computational Reduction	Average % of Error
10	16620	6240	63	6
12	16620	7620	56	3
16	16620	7500	55	1.1

force assumption during integration, the time step is kept small in order to achieve reasonable precision and conserve numerical stability.[24]

As mentioned in the previous paragraph, since 60% of the mixer is modeled using the compartment modeling, another important parameter of the system simulation is the number of compartments considered. As the number of partitions increases the spatial area of each compartment decreases, which means that, there is a better tracking of the particle behavior within each region. However, additional particle fluxes are required between each compartment. The computational efforts caused by increasing the number of compartments given that a constant number of particles exist is negligible in comparison to computational requirements of the spatial section modeled with DEM, as shown in Table 8. Increasing the number of compartments improved the accuracy of the method at the expense of a slight computational increase.

Discussion and Future Work

Although DEM modeling is well developed, the computational efficiency of DEM makes the applicability of this approach rather limiting. As described in the Discrete Element Method section, Bertrand and coworkers[9] showed that as the number of particles in the system increase, the computational intensity of a DEM simulation becomes prohibitive. Moreover, modeling the mixing effects of a large number of particles under the influence of a moving boundary increases exponentially the computational burden since convective, dispersive, and shear mechanisms should be considered. In response, DEM models are solved by embellishing the particle morphology,[12,13] and reducing the number of particles in the system in order to trim down calculations,[7,8] inarguably trading one type of model error for another.

In order to overcome computational complexity without sacrificing the accuracy of the calculations, a new approach is presented in this article to model powder mixing. The main idea behind the proposed approach is to identify areas that can be solved using a statistical model, and the areas that require a detailed particle dynamic model. As a result the computational time is reduced by an order of magnitude, while capturing the mixing behavior of the system. However, it is also important to note the limitations in the applicability of our model. For example, Alexander and Muzzio[28] showed that in a horizontal mixer the particle velocities are dependent on their axial position. As a result, decreasing the axial length of the vessel examined under DEM will result in dramatically different velocity values. Thus, if the exact velocity value for each particle is required, a detailed DEM should be used for the entire vessel. However, it should be noticed that based on a recent comparison to experimental measurements performed by Kuo et al.[29] it has been illustrated that even DEM simulations can overpredict the particle velocities. Particle-velocity calculations are affected using large-time steps. As a result, reducing the computational complexity, implores the possibility of trimming down the time steps. As a result, the hybrid approach can be utilized to reduce some of the computational complexity of the discrete element mixing models in order to improve the determination of particle velocities.

To our knowledge, no work has been published utilizing such a hybrid framework, but rather the common approach is to reduce the number of particles considerably. The work presented in this article illustrates that the computational savings are very significant, and no restrictions exist that hinder adapting this approach to other convective or tumbling mixers. As a result the algorithm developed shows enormous potential to improve performance of powder mixing models. Work is underway to utilize the hybrid approach for other applications.

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