Simulation of Mixing and Segregation Phenomena in Industrial Material Flows with Discrete Element Methods

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Abstract

This paper presents the theoretical basis of a mixing index methodology that can be used to quantitatively predict the degree of mixing or segregation in a discrete element analysis of a system of particles with non-uniform properties. The non-uniformity in the particle system may be of a general nature. For example, the system of particles may have a non-uniform size distribution or different material properties such as density, friction, etc.

The overall concept in the development of the mixing index methodology is to compute a quantitative measure of the difference between the evolutions of the states of the system of particles as predicted in a discrete element analysis with that of an ideally mixed system. A spatial grid is used to bin the particles into a system of grid cells. This data is then analyzed with a squared difference approach that determines a normalized mixing index value such that a perfectly mixed particle system has a mixing index value of 1, and a perfectly segregated particle system has a mixing index value of 0.

The application of the mixing index methodology is illustrated by analyzing the particle system position data generated from a three-dimensional discrete element analysis. A case study of industrial significance with complex geometries have been analyzed. Four datasets of particle system data were generated from three-dimensional discrete element analyses of a rotating cylindrical kiln with baffles and without baffles. These analyses show that this mixing index methodology can be readily applied to quantitatively determine mixing or segregation rates for a wide range of industrial mixing systems used in bulk solids handling.

Introduction

The design of efficient industrial mixing and segregation systems for bulk materials is an important concern since the energy consumption these systems is a significant cost. A major consideration in the design methodology requires the accurate determination of mixing or segregation rates. The traditional design process usually requires the fabrication and the exhaustive testing of many scale model prototype systems which is a laborious and expensive endeavor.

During the last decade or so with the advent development of sophisticated discrete element numerical simulations for granular materials for predicting the flow characteristics, see Walton 1993, Dury and Ristow 1997, it is now possible to use these simulation technologies as part of the design methodology.

The use of these simulation technologies can be used in conjunction with the traditional design approach to improve the overall efficiency and quality of the final design. This may be achieved by analyzing a number of prototype designs and rating them in terms of predicted mixing rates prior to the physical testing of scale models. In this way the number of prototypes that are fabricated and physically tested can be significantly be reduced. An example of a simulation-based mixing study is a comprehensive analysis of mixing of grains in rotating drums with the discrete element method and using the entropy of mixing methodology by

Schutyser (Schutyser 2003) described in his PhD thesis. Note, that this work also included experiments using video and image analysis techniques. Similar work is also detailed in Gupta et al 2010, where a large-scale industrial Lindor mixer was analyzed using DEM with in-line and on-line mixing quality indices determined by three different approaches: particle numbers, the number of contacts between different particle-types, and the generalized mean mixing index (GMMI).

The simulation methodology in this paper is a two-step procedure using DEM and a mixing index based on a squared difference approach. Firstly a discrete element analysis of a system is modeled and analyzed. The results of the DEM analysis consist of a detailed description of the motion of all the particles of the bulk material throughout the duration of the simulation. This data is defined with a series of digital snapshots which contains the coordinate locations and the velocity components for all the particles within the system at a series of time values throughout the simulation. The second step in the procedure is to compute various mixing index values for each digital snapshot in time throughout the DEM simulation.

Mixing Methodology

A summary of the non-dimensional mixing index theory based on a squared difference approach is described below. Consider a system of particles located within an arbitrary three-dimensional volume in which the system consists of particles that can be defined in terms of a set of different particle types. For example, a system consisting of particles with two different radii may be defined as a system with two different types of particles, see Figure 1 a). Another definition of a particle type could be defined by the initial location of the particles before the oscillatory excitation of the particle system. For example, a volume of settled particulate material could be defined by three types, where each type is a horizontal volume layer of particles. In this system type 1, type 2 and type 3 particles are the particles in the lower, middle and upper layers, see Figure 1 b).

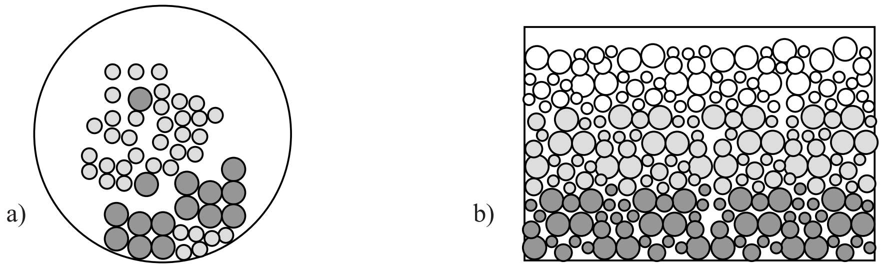

Figure 1: Particle system types– a) defined by two different particle radii, b) defined by spatial locations of three layers

The arbitrary three-dimensional volume is divided into a uniform rectangular cubic system of volume grid cells. Note, the grid spacing is defined so that the size of a volume grid cell is large enough to obtain an accurate estimate of a mixing measure within each volume cell.

Within a typical volume cell which can be defined as the $(j,k,l)^{th}$ volume grid ‘cell’ a squared difference measure of mixing can be determined by computing SD_{jkl} :

$$SD_{jkl} = \frac{1}{N_{jkl}^2}\left\{\sum_{i=1}^{m}\left[(n_{ijkl} - n'_{ijkl})^2\right]\right\},$$

where n'_{ijkl} is the number of type i particles in the $(j,k,l)^{th}$ volume grid 'cell' in a perfectly mixed system, N_{jkl} is the total number of particles within the $(j,k,l)^{th}$ volume 'cell', and n_{ijkl} is the number of type i particles in the $(j,k,l)^{th}$ volume 'cell' predicted in the system by the DEM simulation at an arbitrary time t.

Note, SD_{jkl} should be interpreted as a non-dimensional quantity which quantifies the degree of mixing within the $(j,k,l)^{th}$ volume grid 'cell'. For example, if the particles in the volume cell are in a perfectly mixed state then $SD_{jkl} = 0.0$. Note, as the degree of mixing in the volume cell decreases the value of SD_{jkl} will approach a maximum value.

A measure of the degree of mixing within the whole system of particles can be determined by computing a combined or total SD at time t for the whole particle system is defined by:

$$SD = \frac{1}{N_{tot}^2}\left\{\sum_{l=1}^{N}\sum_{k=1}^{N}\sum_{j=1}^{N}\sum_{i=1}^{m}\left[(n_{ijkl} - n'_{ijkl})^2\right]\right\},$$

where N_{tot} is the total number of particles in the system, and N is the number of volume grid cells in each of the three spatial directions.

The above global mixing measure SD can be normalized by defining GMI as

$$GMI = (SD_{\max} - SD)/SD_{\max}$$

where SD_{max} is the maximum value of SD which is attained when the particle system is in a perfectly segregated state.

We define GMI as the global grid mixing index which is a normalized mixing index, such that GMI = 0 indicates a perfectly mixed particle system and GMI = 1 indicates a perfectly segregated particle system.

Using the above methodology we can also define a local grid mixing index for each volume cell that can be used to determine the degree of mixing in a spatial sense throughout the particle system. Another generalization of the above method can be realized by using grid systems based on different shapes of volume cells, such as a system of annuli cell volumes or x-section sector volume cells as shown in Figure 2.

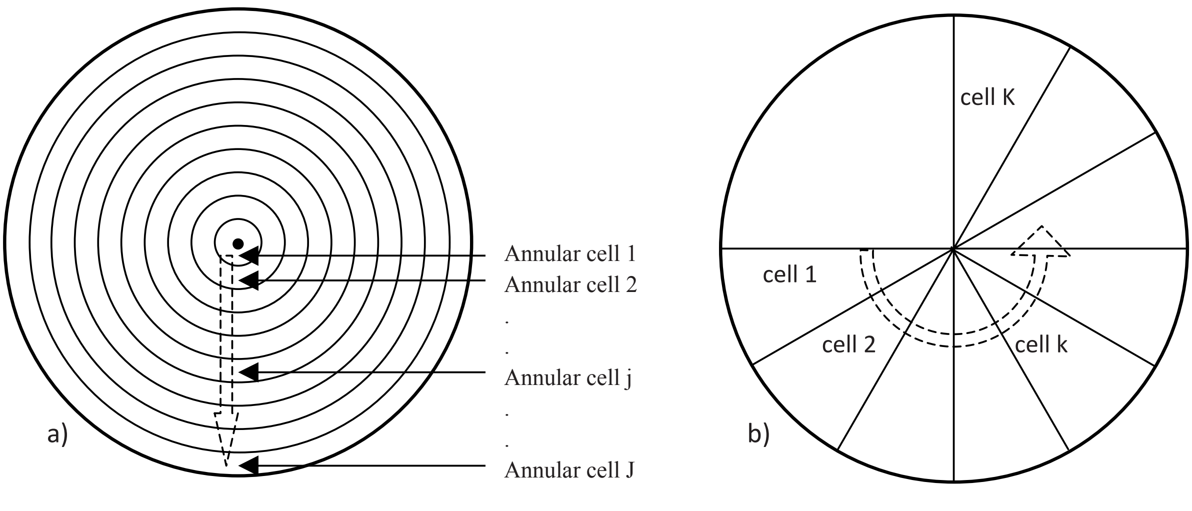

Figure 2: Generalized geometry of volume cells for a rotating cylinder - a) Annular volume cells to determine mixing in the radial direction, and b) Sector volume cells to determine mixing in the circumferential direction.

Note, the annular volume cells can be used to determine the mixing rate in the radial direction (or through the bed depth) and the sector volume cells can be used to determine the mixing rate in the circumferential direction (or around the circumference of the cylinder).

Application

This example is a generic rotating cylindrical mixing system with a continuous feed of bulk material as shown in Figure 3. Note, the axis of the rotating cylinder is tilted at 5 degrees with respect to the horizontal direction so that the elevation of the exit section is slightly lower than the upstream feeder section. A schematic of the actual mixing system geometry is shown in Figure 3 a). Because the cylinder is very long in the axial direction and the geometrical arrangement of mixing baffles repeats along the axial direction the DEM model simulates the flow within a short section of the physical problem which employs periodic boundary conditions, see Figure 3 b). Note, these periodic boundaries allow the material to flow freely out of the downstream boundary of the model and flow back into the upstream boundary of the model.

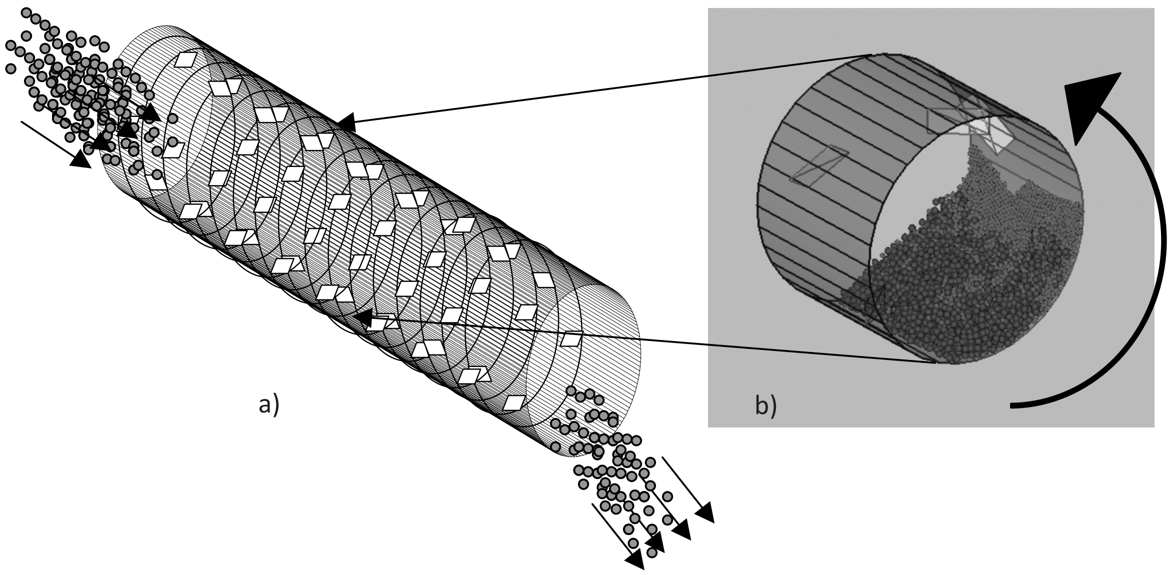

Figure 3: Cylindrical Rotating Mixing Problem - a) Schematic of the physical geometry of the mixing system, and b) An illustration of the DEM model which consists of a short section of the mixing system with periodic boundaries.

This system is analyzed under a range of different conditions defined as follows:

a) The bulk material is comprised of two different sized radius with a size ratio of 1.5: 1.0.

b) There are two mixer geometries - a cylinder lined with baffles and a cylinder with no baffles

c) The initial material is segregated by radius in two layers (called bed segregated).

d) The initial material is segregated by radius in two regions (called vertically segregated).

Figures 4 and 5 show snapshots of the DEM analyses with material that was initially bed segregated into two horizontal layers with the larger particles on the bottom layer and the smaller particles in the overlying layer. Figure 4 shows the evolution of the particle motion in a cylindrical mixer with baffles at three instants: initially after zero rotations, after 3 rotations and after 7 rotations respectively. Similarly, Figure 5 shows the evolution of the particle motion in a cylindrical mixer with no baffles at three instants: initially after zero rotations, after 3 rotations and after 7 rotations respectively. The effect of the baffles on the mixing of the material is clearly illustrated in Figures 4 and 5. Figure 4 shows a significant mixing takes place in the system with baffles during the first 7 revolutions. This figure indicates mixing in most of the material volume except near the right hand surface of the material where there is an excess of smaller radius particles. Figure 5 shows much less mixing is taking place in the system with no baffles during the first 7 revolutions when compared with the system with baffles. Figure 5 shows that the larger particles that were initially in the lower layer have not moved significantly upward after 8 revolutions.

Figures 6 and 7 show snapshots of the DEM analyses with material that was initially vertical segregated (or axially segregated) into an upstream region of large particles and a downstream region of small particles. Figure 6 shows the evolution of the particle motion in a cylindrical mixer with baffles at three instants: initially after zero rotations, after 1 rotation and after 3 rotations respectively. Similarly, Figure 7 shows the evolution of the particle motion in a cylindrical mixer with no baffles at three instants: initially after zero rotations, after 1 rotation and after 3 rotations respectively. The effect of the baffles on the mixing of the material is clearly illustrated in Figures 6 and 7. Figure 6 shows significant mixing takes place in the system with baffles during the first 3 revolutions. This figure indicates mixing in most of the material volume except near the right hand surface of the material where there is an excess of smaller radius particles. Figure 7 shows essentially no mixing takes place in the system with no baffles during the first 3 revolutions when compared with the system with baffles.

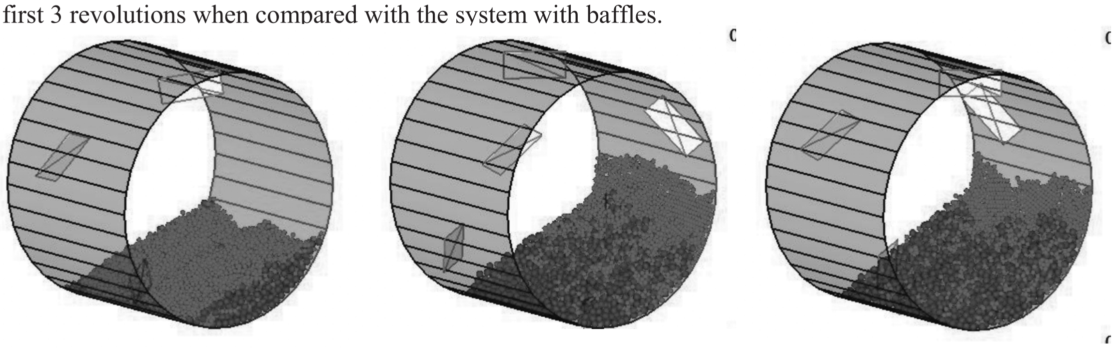

Figure 4: Mixing Problem with Baffles and Initial Bed Segregation - a) Initial segregated system, b) System after 3 revolutions, and c) System after 7 revolutions

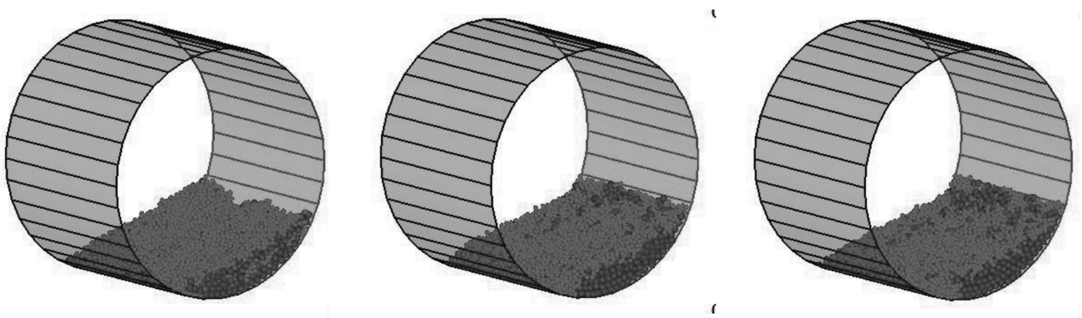

Figure 5: Mixing Problem with no Baffles and Initial Bed Segregation - a) Initial segregated system, b) System after 3 revolutions, and c) System after 7 revolutions

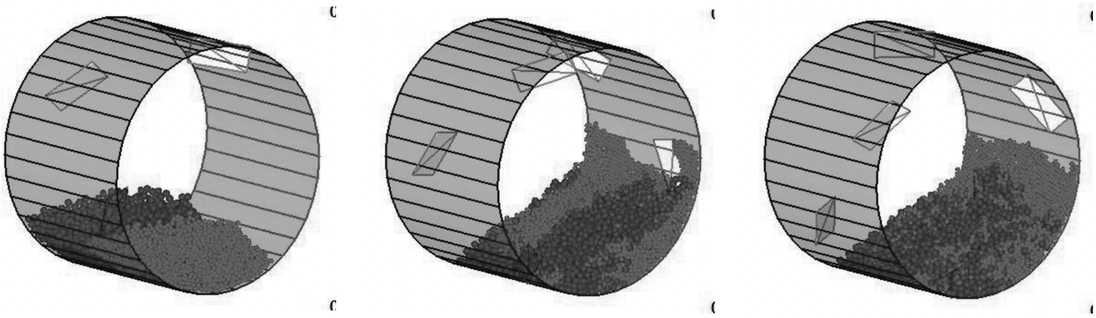

Figure 6: Mixing Problem with Baffles and Initial Vertical Segregation - a) Initial segregated system, b) System after 1 revolution, and c) System after 3 revolutions

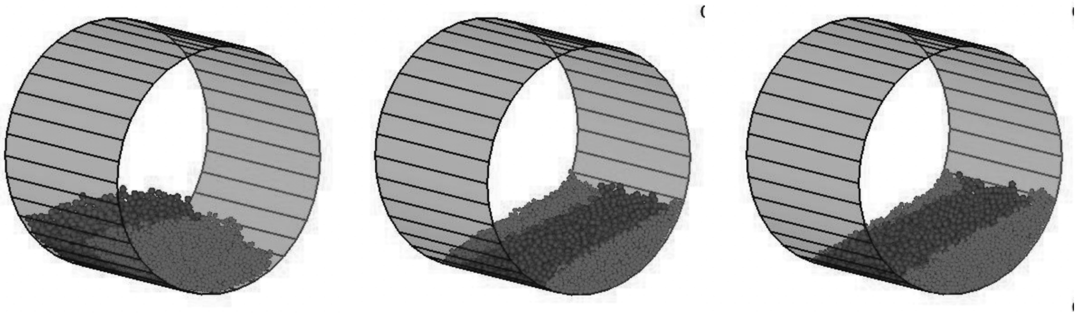

Figure 7: Mixing Problem with no Baffles and Initial Vertical Segregation - a) Initial segregated system, b) System after 1 revolution, and c) System after 3 revolutions

Quantitative Mixing Analyses

Bed Segregated Systems

In the bed segregated systems two measures of mixing rates have been computed based on: a) the global mixing measure (GMI) which is a Cartesian grid based mixing index that defines the average rate of mixing throughout the complete volume of the material at a specific time or after a specified amount of revolutions, and b) the radial mixing measure (RMI) which is a annulus grid (see Figure 2 a)) based mixing index that defines the average rate of mixing in the radial direction throughout the complete volume of the material at a specific time or after a specified amount of revolutions,

The results of the GMI analysis is shown as a time history of a quantitative measure of the average mixing within the whole region of material throughout the duration of the DEM simulation (8 revolutions) in Figure 8. In this figure the mixing rates are shown for the system with baffles and with no baffles. The GMI values for the system with no baffles indicates that no significant mixing takes place during 8 revolutions. In contrast the GMI values for the system with baffles indicates that mixing occurs within the first 2 revolutions and increases in oscillatory manner toward a steady value of approximately 0.75 after 8 revolutions.

Similar data for the RMI values for the two systems with baffles and with no baffles are shown Figure 9. Significant mixing occurs rapidly in the system with baffles as indicated by the time history of RMI values which increase and oscillate toward a steady value of approximately 1.0 after 8 revolutions. Partial mixing in the radial direction for the system with no baffles is indicated by a steady increase of the RMI to a value of 0.45 after 8 revolutions.

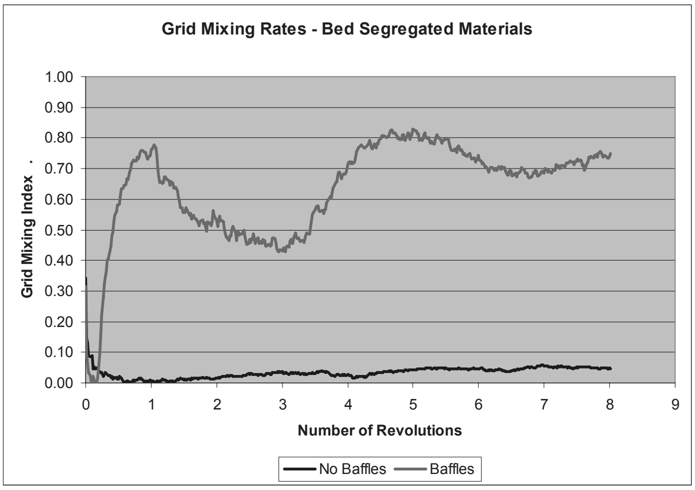

Figure 8: GMI Mixing Time History: Mixing Systems With and Without Baffles

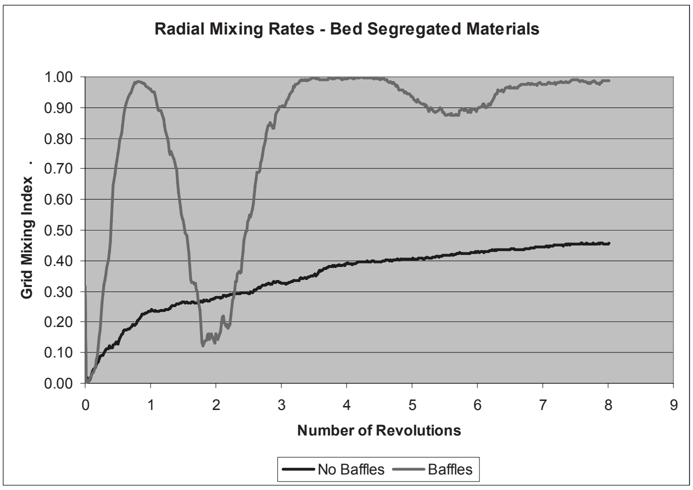

Figure 9: RMI Mixing Time History: Mixing Systems With and Without Baffles

<u>Vertically Segregated Systems</u>

In the vertically segregated systems a measure of mixing rates has been computed based on the axial mixing measure (AMI) which is a grid based mixing index that defines the average rate of mixing in the axial direction throughout the complete volume of the material at a specific time or after a specified amount of revolutions.

The results of the AMI analysis is shown as a time history of a quantitative measure of the average mixing in the axial direction within the whole region of material throughout the duration of the DEM simulation (8 revolutions) in Figure 10. In this figure the mixing rates are shown for the system with baffles and with no baffles. The AMI values for the system with no baffles increase slowly and reaches a steady value of approximately 0.35. This indicates that a steady partial mixed state has been reached during 8 revolutions. In contrast the AMI values for the system with baffles increase rapidly and reaches a steady value of approximately 1.0 after 7 revolutions. This indicates that axial mixing occurs very quickly and is well mixed in the axial direction after 7 revolutions.

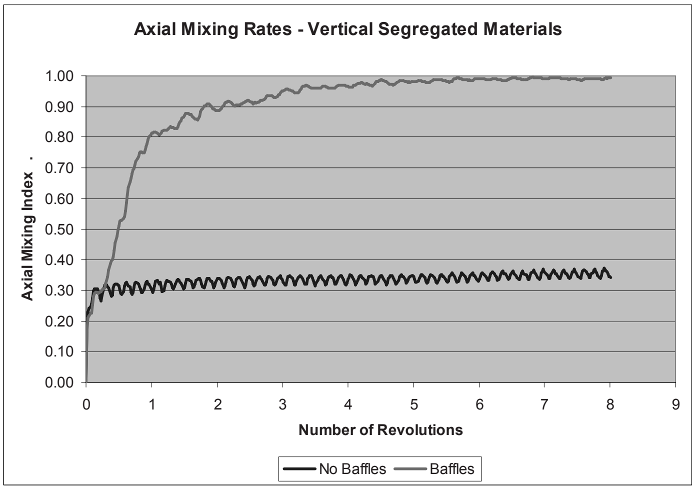

Figure 10: AMI Mixing Time History: Mixing Systems With and Without Baffles

Concluding Remarks

The DEM simulation and quantitative mixing analysis performed show the applicable of this computational methodology to predict the overall mixing rate throughout the volume of the bulk material and the mixing rate in specified directions such as the radial and axial direction in the rotating cylindrical mixing system. Note, in a design setting this methodology can be applied to rank the relative mixing rates of a number of prototype mixing systems and be part of the overall design process.

Some additional remarks regarding the comparison of the GMI, RMI and AMI mixing indices with other quantitative mixing measures are as follows:

a) The GMI, RMI and AMI mixing indices are somewhat similar to the entropy of mixing as used by Schutyser 2003.

b) The GMI, RMI and AMI mixing indices have a major advantage of the GMMI methodology employed Gupta et al 2010 which requires a problem dependent user-specified datum coordinate value.

Acknowledgements

The first author would like to thank Overland Conveyor Company Incorporated for making their discrete element computer software Bulk Flow Analyst (BFA) available for this work.

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