

The new granular simulation software Granuleworks enables theoretical evaluation for the degree of mixing concerning powder and granular material, which was relied mainly on empirical engineering.

*Granuleworks is the simulation software specialized for powder and granular materials, which has been developing by improving the existing DEM (Discrete Element Method) capability in Particleworks. The official product release is scheduled in 2017.

Tsukishima Kikai has consistently responded to the demands of society and the people living there by providing with the technologies including systems and plant facilities which serve as a foundation for the industry, water and wastewater facilities which are essential to our daily lives, as well as environment conservation facilities, for about one century since our establishment in 1905. In accordance with the company policy “Dedicating to the industry development and environmental protection by taking advantage of our leading edge technology to make contributions to society”, Tsukishima Kikai has been improving existing environment and energy technologies for global warming prevention which is a worldwide trend, and actively promoting overseas businesses mainly for emerging countries. We have had the pleasure to interview Mr. Yoichi Nakata of the Process Design Department, Industrial Business Division in Tsukishima Kikai, to hear the consideration of the evaluation method for degree of mixing concerning powder and granular materials using DEM simulation.

Please introduce your business and your role in the process design department?

One of the missions of the Process Design Department is the basic design of plants and equipment for the processes including distillation, crystallization, filtration, separation, drying, measurement, and transportation mainly for the chemical, steel, and food industries. In this department, I'm in charge of design for the drying process. The materials that we are handling cover a broad range from ore to chemical, for example coal used for steel and terephthalic acid which is the in-process material for polyester fiber and Polyethyleneterephthalate. As those materials are different and there is a wide range of variations in the material properties, we consider not only the drying process but also early and post processes completely to provide the best drying equipment to our customers. Regarding CAD/CAE tools for such products, we have used FEA software for mechanical structural design and CFD software for fluid process design for the past 15 years ago.

When and for what reasons did you start using Granuleworks for powder and granular simulation?

Most of the dryers handle powder and granular materials, and we have been relied on the empirical rule of the veteran engineers as such

powder and granular materials are very difficult to deal with and to predict behaviors theoretically. It was the trigger to start discussing possibilities of the new developing technologies of computers simulation software as tool to improve the situation and change the way into a more theoretical approach. Then we met Prometech and entered an agreement for joint research. It was lucky that Prometech was working on the development of the new granular simulation tool, Granuleworks, during the same period, and that leads us to good results through the joint research. Thereafter, we have been seeking the theme of how to redefine empirical engineering of powder and granular materials, and how to establish the theory and evaluate the behavior quantitatively to realize the mechanical design which we hadn't been able to do.



Steam tube dryer

Could you please tell us about your research in detail?

We have studied the evaluation method of the degree of mixing for powder and granular materials quantitatively. At first, please



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let me explain the operation of mixing. The mixing operation in the process influences the product quality. Therefore, it is considered very important in different industries producing batteries, foods, resins, ores, and organic/inorganic materials, and it should be evaluated properly. The mixing operation is not just mixing, but it is required to mix enough and sometimes it is required not to mix too much. In order to show

the mixing states numerically, the degree of mixing has been used, and it's not easy to measure. There are 3 points that we should pay attention to when evaluating the degree of mixing. The first point is to evaluate multi-component systems. This means that the real powder and granular materials which will be mixed include many types of components including different particle sizes and ingredients. The second point is to mix materials accurately. It can be evaluated that the materials are mixed accurately if the degree of mixing for a very small portion taken out from the entirety is homogeneous after mixing. It's better to understand the nonhomogeneous mixing in detail to sample a small portion than a large portion. So it's demanded to take a method with less error, even if the number of samples is small. The third point is to quantify the non-homogeneity. The local non-homogeneity of mixing state is commonly observed in powder materials and there exist simultaneously different conditions that some portions are mixed well and others are not. Therefore, it is necessary to numerically evaluate those conditions in some way.

The conventional method to evaluate the degree of mixing is, for example, to take out a portion of the powder materials including A and B particles, which are dispersed in the system. Then, evaluate the ratio of its composition. If the number ratio of A to B is 1.0 in the whole system and the ratio of the sample taken out for the study is also the same, the materials are mixed perfectly. This is called dispersion or standard deviation in statistics engineering. However, we noticed that there are many cases in which the degrees of mixing is not presented properly if using the method based on statistics. This means that the Lacey mixing index, one of the method based on statistics, is used for the degree of mixing conventionally, but for the systems, which have a biased number of particles for A and B which will be mixed, the mixing index value doesn't fall within 0-1 range and it is evaluated as unstable, if using Lacey index. In addition, as Lacey method uses the equation based on statistics, if the number of samples is small, the reliability of the data will decrease. Therefore, in the case of evaluating the degree of mixing for a local area, the credibility of the data cannot be assured due to lack of samples, bringing a serious effect on results for precise mixing. In addition, it can't deal with multicomponent systems in an integrated way, and it's needed to organize the mixing index for each component. It is not

reasonable because it can't evaluate the mixed many-component system as a single index. So it would be helpful if there is an index which can evaluate the mixing state of spatially local area of a multi-component system with enough stability. To realize this, we discussed if Shannon mixing index can be applied on powder and granular systems, which had been researched for evaluating the mixing state of polymeric systems. Results are introduced below.

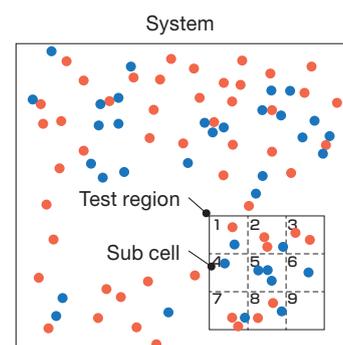


Fig1, Shannon test method

Shannon entropy shows the randomness of the system, which is applied to evaluate the degree of mixing, and it has characteristics that the more the granular system becomes homogeneous, the more entropy increases. The entropy of the system is calculated by dividing the test region into sub-cells with the same size, calculating the entropy of each sub-cell, and finally summing up each entropy of all the sub-cells. Here, the spatial segregation of particles and the degree of mixing of mixture of different species of powders, are described by the entropy associated with the overall spatial distribution of particles irrespective of species and the spatial average of the entropy of mixing of species conditional on location, respectively. In addition, by using the normalized entropy, absolute evaluation of the degree of mixing becomes possible. However, this method is not applicable to compare with experiments because experiments can't be performed in the same way. Therefore, the computing method of Shannon entropy was modified in order to become comparable between simulations and experiments. Next, we had to confirm if the improved Shannon entropy can be used for any kind of system, as powder systems used in the industry very often shows highly segregated. It suggests that we need to evaluate the degree of mixing state correctly even in extreme cases such as only a few particles are inserted, like flavoring. So we checked the cases from a ratio of 1 to 1, to a ratio of 99 to 1 shown in Fig.2 and found that it would be usable for cases that spatial distribution of the system is extremely bad.

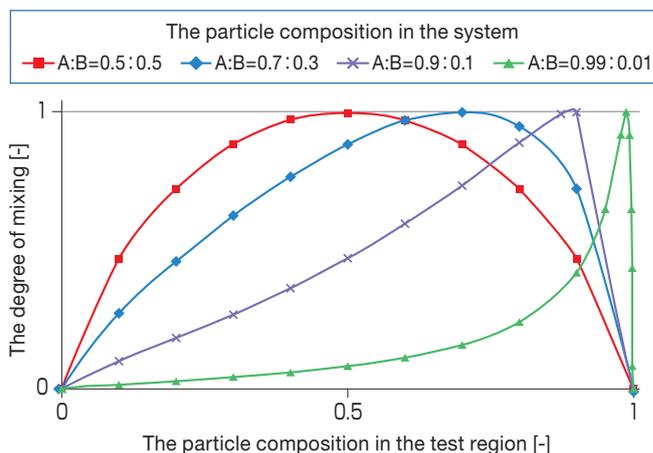


Fig2, Verification using improved Shannon entropy

Then it is discussed if the degree of mixing of powder system can be evaluated by both simulation and experiment with 2 different containers. One is a cylindrical container which is hollow, and another is a cylindrical container which is also hollow but including rotating rods. In those containers, 2 kinds of ceramic particles, of average diameter of 2mm colored in yellow and 3mm colored in black, are inserted longitudinally halved and rotated with the number of specific rotating rate. In case of the experiment, we can see the inside as the transparent plate is in front, and monitored how the yellow particles and black particles mixed using a video camera. In addition, the position, the number and the ratio of the particles were measured at 1 to 5 test regions defined for each rotating amount, and the normalized the spatial average of the entropy of mixing of species conditional on location was calculated to obtain the degree of mixing data. For simulation, the rolling resistance was considered for the subtle roughness and non-spherical properties of the ceramic particles, and the same particle size distribution as the particles obtained experimentally was applied.

In terms of realistic powder behaviors, the coefficients of spring and damper for the contact force were adjusted, to match how they splash and how they spatter, simply by dropping powders from on a height, as preliminary experiment. Fig.4 is the simulation result, from which, the trajectories of particles in black under the process of mixing seemed to be almost correct. In this situation, what we can empirically understand during the rolling motion of cylindrical container, called "kiln action" is the appearance of the accumulated region. This is because, the inertia force for each different granular material is not the same when they are mixed by the mechanical rotation, and the materials with larger inertial force gets close to the external side and the material with smaller inertial force getting close to the internal side. We, working at the field, know it from our experience, and were

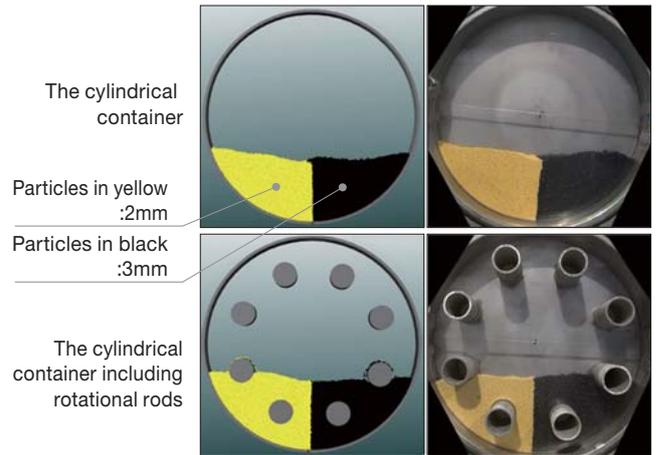


Fig3, The simulation model (left) and the experiment model (right)

impressed very much by the simulation results that could show the same behavior. In addition, we know that the materials are homogeneously mixed if some rods are placed inside the container, while the materials are segregated in the center and the outer side if using a hollow container. In fact, when comparing the situation in the hollow container and the container with rods, we could see that the materials in the container with rods were mixed better from the simulation result. The degree of mixing was compared to understand this quantitatively. A sample in each layer was taken by the sampler at the specific rotation amount in the experiment to evaluate the composition in the upper layer, in the middle layer and in the lower layer. On the other hand, composition in each layer was evaluated by the Granuleworks post-processing capability in the simulation. This procedure was repeated at the predefined rotation amount to measure correctly. Granuleworks prototype was used for the discussion and the results almost match the experimental result with the physical

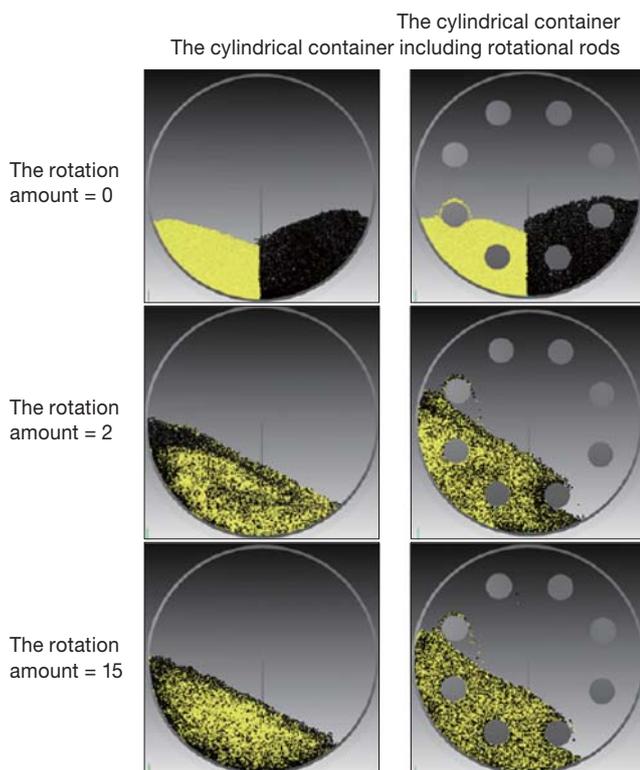
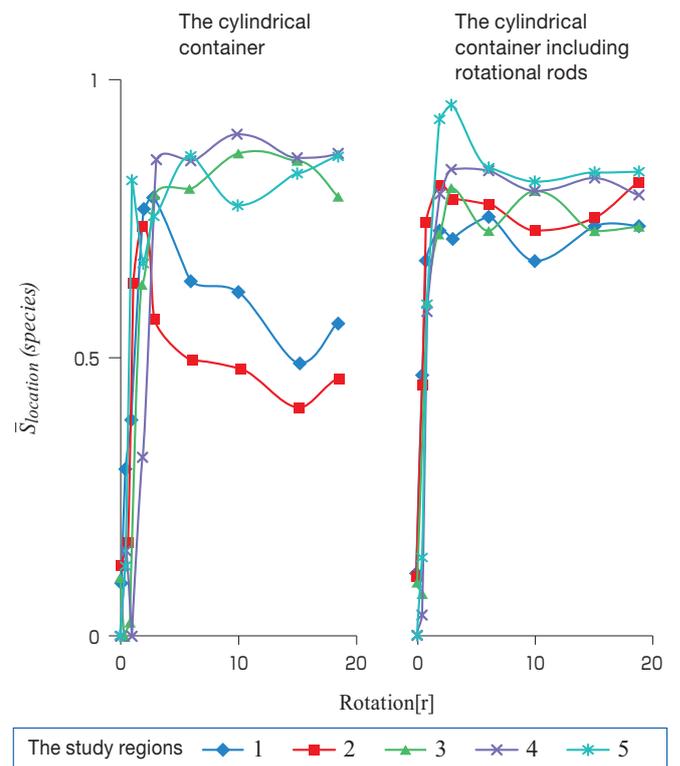


Fig4, Simulation result



model implemented in Granuleworks. Comparing it to the result which was gained by using the physical model of the former version, it is found that qualitative trend of the result obtained by the latest model is much better and had a good impression that the newly developing Granuleworks is very useful.

The real powder material mixed in the dryer, that I've designed, is not in ideal conditions, like the ceramic particles used in the verification this time. Its surface flow is not constant always, and the landslide-like phenomenon occurs after accumulating at some level. We just began to verify how such real powder materials behave. The machine for the experiment is smaller than the real machine. To verify the powder behavior correctly, we use 2 types of machines, a small machine and a middle-sized machine with 2m in diameter. The experiment could show the powder-like behavior and we could confirm that the real powder material was lifted up by the rods and dropped curling up like a curtain. Such a real powder material behavior is very complicated and it's difficult to predict theoretically. However, we could obtain the same result by the simulation. From a series of this research, we have been recognizing that DEM is useful for real powder material simulation.

Could you please tell us the future vision about your research and the simulation activities using DEM solution?

As I explained in the case study, the phenomena of powder and granular materials are difficult to predict theoretically. So, experimental measurement of the powder behaviors are necessary for designing powder apparatus and devices, and it requires a lot of people, goods, and capital. On the other hand, simulation is an

extremely cost saving evaluation way compared to experimentation. We have a positive outlook of an innovation regarding design lead time reduction, cost saving and device improvement, by multiple evaluation using experimentation and simulation if DEM will grow as a practical design method. I think it is necessary for us to be positively involved in the software development, and I would like to continue our joint research as before.

How about your expectations of Granuleworks and Prometech?

I've heard that the current Granuleworks is still under development, and we have already obtained good results which accurately correspond to the real phenomena of the basic systems of powder mixing. We are impressed by the results and have great expectations of future progress. Although DEM has some advanced problems such as a variety of interacting forces, extension to the thermal and mass transfer phenomena, and handling of multi-phase problems, DEM research has been progressing rapidly today. I expect Prometech to quickly provide useful products for the industry from such advanced research results and to be a front runner to connect the leading technology to industry.

Thank you very much for your valuable input. We are really honored to hear that you have been taking advantage of Granuleworks, which is still under development. Prometech will continue to provide further support for your better research and product development. Again thanks a lot for taking the time in your busy schedule to introduce your case studies.

Reference

Prometech Simulation Conference 2015 paper

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Founded: In 1905

Activities: Industrial business (Engineering, Process equipment),

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Granuleworks®
Advanced Simulator for Granular Materials

Granuleworks is a *DEM based granular dynamics simulation software. It can be applied to various powder/granular manufacturing processes, and design and improvement of powder/granular devices in food, medication, chemical, transportation, and electronic materials industries. Powder/granular flow phenomena including mixing, conveying, filling, and powder compacting can be simulated easily by Granuleworks.

*DEM: Discrete Element Method is the most representative granular dynamics simulation method.

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