博士論文（要約）

Study on solid mixing phenomena in geometrically complex vessels by the discrete element method

(離散要素法を用いた複雑容器内の粉体混合現象に関する研究)

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論 文 の 内 容 の 要 約

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The mixing of powders is a critical step in ensuring the quality and performance of various products in food, pharmaceutical and chemical engineering industries. There are many different parameters that are important to mixing; e.g., particle sizes and densities, particle surface and air conditions, the mixer design and its fill, and the mixing speed and time. A wide variety of industrial mixers exist for different mixture types, and while mixing dynamics can be evaluated analytically for specific cases, experimental approaches are usually taken; e.g., particle sampling, visual tracking, particle image velocimetry, positron emission particle tracking and even magnetic resonance imaging. However, such approaches cannot track all particles, making it difficult to understand the granular flows and particle mixings.

The application of numerical simulations is desirable when investigating mixing because it allows for better control of physical properties and a faster analysis. In addition, numerical simulations based on the Discrete Element Method (DEM) allow for the tracking of all particles in the mixture. The DEM was firstly proposed by Cundall and Strack, and over the years, this method has been improved, modified and coupled with other methods to suit various applications and approaches. Solid–fluid interactions can be simulated using the DEM with smoothed particle hydrodynamics, the DEM with a moving particle semi-implicit method, DEM-computational fluid dynamics or direct numerical simulation coupled with the DEM. Effects such as agglomeration, breakage and inter-particle bonding can be investigated using the DEM with a more general contact model. Industrial large-scale systems can be simulated using

massively parallel DEM approaches or by introducing a coarse-grain model to simplify the system.

The DEM is also applied to mixing analysis because of its power and flexibility; e.g., the analysis of particle mixing induced by a flat blade. Through the analysis of particle positions, binary mixing can be observed and tracked. The effect of particle size or liquid bonding between particles on the powder mixing performance can also be explored using the DEM. Recently, numerical mixing index calculations were performed to analyze solid particle mixing in a plowshare mixer, slant cone mixers, an industrial twin-screw kneader and a ribbon mixer. These studies demonstrated the applicability of the DEM in analyzing the effects of initial loadings, powder amounts and mixing speeds on the mixing performance.

Mixing phenomena is also important for nuclear engineering. For example, large-scale mixing processes in advanced passive reactors can be analyzed using DEM approaches. Radiochemical and nuclear facilities use mixing to prepare materials for treatment, heat transfer, reaction, and sampling. Mixing of multiple phases (including fast settling solids in Newtonian and non-Newtonian fluids) poses significant challenges to the engineering design and prediction of process and degree of mixing. Overall, there is a huge potential of the DEM application in the nuclear engineering.

The mixing phenomena have been already widely tackled using various simulation approaches. However, most cases are simple and only with few hundreds or thousands of particles. More relative cases with complex vessels and hundreds of thousands of particles are needed to be analyzed in order the simulations to be an important practice in the mixing industry. Therefore, this study explores these possibilities.

The main objective of this study is to analyze solid mixing phenomena in complex vessels by the discrete element method. The understanding of such phenomena is important and relevant for the mixing industry; however, no analysis has been performed before due to the complex vessels and the huge number of particles. While some approaches analyze the complex boundaries and other approaches are considering the huge number of particles, there are no appropriate approach for the huge number of particles in complex vessels. Therefore, in the current study the simulations of the mixing will be performed using a novel approach based on DEM with a wall boundary model based on a signed distance function (SDF).

The current study on the mixing phenomena will be focused on several different things. First of all, the validation and the sensitivity analysis of the simulation parameters of the new DEM/SDF approach are needed to be performed. As was shown by the literature analysis there are a lot of different areas, which have not been analyzed yet. To have a good understanding of mixing, different mixers with different observable phenomena should be analyzed. Therefore, in this study three complex mixers were chosen. Mixing and transportation will be analyzed in a complex twin screw kneader. The convection mixing will be analyzed in a ribbon mixer, while the diffusive mixing will be analyzed in a batch mixer with double-axial movement.

The sensitivity analysis and validation of the simulation approach was performed on a laboratory sized twin screw kneader. Granular distributions and mixing torques at different powder amounts and different mixing speeds were analyzed and compared with the experimental data. Using the validated DEM/SDF simulation approach mixing and transportation in an industrial twin screw kneader was simulated. The effects of the screw speed were analyzed using the visual distribution of the powder and mixing index of the mono-sized powder. These simulations showcased the power of the DEM/SDF approach.

To clarify the convective mixing mechanism, dense granular flow in a complex ribbon mixer was simulated by the DEM using the signed distance function (SDF)-based wall boundary model. All analyses were carried out in a mono-dispersed system. Simulations of the DEM/SDF approach were validated using experimental granular flows observed with a high-speed camera and extracted using the PIV method. The different degree of mixings were evaluated using the mixing index of a binary mixture, while the different granular behaviors were differentiated using the granular temperatures. In the evaluations, the effects of amount of powder, blade speed and initial powder loading on the degree of mixing in the ribbon mixer were investigated.

To clarify the diffusive mixing mechanism, a cylindrical batch mixer with double axial movement and two interior blades was analyzed. The blades and secondary movement are applied to improve the mixing performance. However, the mixing mechanism in this type of batch mixer has not been fully resolved, owing to the complex double mixing. For example, the degree of mixing and effect of initial loading, powder amount, mixing speed, secondary mixing and granular parameters have not been evaluated in previous studies on such systems. Dense granular flow in a batch mixer with double axial movement was simulated using the DEM/SDF method. All analyses were carried out for a mono-dispersed system. Simulations of the DEM/SDF approach were validated using experimental granular distributions. The degree of mixings were evaluated using the mixing index of a binary mixture, while the granular behaviors were differentiated using the granular temperatures. In the evaluations, the effects of the powder amount, blade speed, initial powder loading and secondary mixing on the degree of mixing in the batch mixer were investigated.

Density effects of the powder mixing were analyzed only in the ribbon mixer. The density effects are also important for the nuclear engineering, for example, in nuclear waste quite heavy radioactive elements are mixed with lighter elements. The uniformity of the radioactivity in the waste product will ensure the safety and the longevity of the containment. Therefore, a large range of the densities was analyzed in the current study to close the knowledge gaps of the density effects in the ribbon mixer.

The current linear adhesive models and their applications will be discussed, before the development of the new model. There are several widely used adhesive contact models: like JKR or DMT. Both theories are highly successful in the field of small particle attraction: JKR model for softer sphere and DMT model for harder sphere. Due to DEM soft sphere approach, the new linear adhesive contact force model was based on a specific linearization of the JKR model. Therefore, deep and informative JKR model presentation will be also made. The special formulation of the JKR model was used to derive the new model. Some other derivations of the model are also possible and will be presented. The connection to the DEM/SFD approach was done using the usual simulation parameters. The importance of the rolling resistance to the adhesive behavior was also analyzed. At the end, the validation of the new model was performed.

Finally, several originalities of this work should be mentioned. For the first time, the novel DEM/SDF approach was applied and validated for the simulation of powder flows in complex vessels. Different mixing mechanisms in complex mixing devises were investigated and analyzed, which gives novel and insightful knowledge of the mixing phenomena. And finally, the new adhesive linear contact force model for adhesive mixing was developed and validated. Several conclusions can be drawn:

- Based on the extensive experimental validations, the current DEM/SDF approach and its parameters are appropriate for the powder simulations in complex vessels.
- The mixing performance changes to the increasing powder amount differ in the ribbon and the batch mixers. In the ribbon mixer the mixing performance increases, while in the batch mixer the mixing performance decreases.
- In these two mixers, the mixing in the rotational direction is much slower that in the other directions, while the mixing performance increases when the mixing speed is increased. However, this increase is much stronger in the batch mixer.
- In the ribbon mixer the dominant mixing is convective, while in the batch mixer the dominant mixing is diffusive.
- Different granular temperatures can be used to reflect different mixing mechanism and to compare the different mixing performances across them.
- The increase in the powder density differences will reduce the mixing performance in the ribbon mixer; however, the increase of the powder amount can reduce this effect.
- The current adhesive powder simulation using straightforward van der Walls incorporation into DEM or its corrections is not fully correct.
- The new linear, adhesive energy conserved contact force model can simulate adhesive powder behavior more accurately.