SIMULATING MIXING PROCESSES WITH WATER ADDITION USING DEM – FROM BULK MATERIAL TO SUSPENSION

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Abstract. This paper introduces a model in the Discrete Element Method to simulate the mixing processes of dry materials with major water addition more realistically. The presented model covers the representation of liquid transfer from fluid particles or moist particles to dryer ones including increase in volume. Depending on the moisture content of the particles in contact, the adequate interaction model (friction, liquid bridge or suspension) and its parameters are applied.

1 INTRODUCTION

Optimising mixing processes of dry granular materials with major water addition (e.g. concrete mixing) is a challenging task. Reaching the main objective i.e. a homogeneous distribution of all constituents including the liquid phase is not a straightforward process since the material behaviour changes dramatically during the mixing. The mixer must handle first dry material and subsequently moist material and finally suspensions. In all stages, an adequate movement of the constituents has to be ensured to reach their homogeneous distribution; otherwise, as an extreme case, some dry materials may not be mixed properly and can remain in the mixer (Figure 1).

Figure 1). The experimental evaluation of the mixing quality is a time-consuming and complex task. The estimation of the dry materials’ distribution can only be performed by a combination of washing, sieving and weighing and is limited to the inherent components with bigger grain sizes. The distribution of the small size components and the liquid phase can only be tested indirectly by the comparison of the overall behaviour of the material. Therefore the optimization of the mixing equipment and the parameter setup is tedious and difficult, especially for new high viscous material mixes, for which no handling expertise exists.
An alternative analysis tool is numerical process simulation enabling a process-accompanying evaluation of the distribution of all components in all areas of the mixer. Such tools are already successfully applied for optimising mixing processes. Both fluids and bulk materials can be modelled using Computational Fluid Dynamics (CFD) or the Discrete Element Method (DEM). Currently, however, dry and fluid phases combined in a mixing process can be replicated only to a limited extent, particularly if both phases represent high volume fractions. The approach outlined in this paper aims to simulate this type of mixing process, reflecting the transition from dry to moist bulk material and eventually to a suspension whilst considering changes in material behaviour at each of the intermediate stages. A parametric contact model is necessary for each of the material states and the related state-transitions in order to represent the specific conditions in a process-oriented manner. Such a model was developed with focus on fresh concrete using the DEM approach. One of the key steps of this model replicates how moisture is transferred to and absorbed by, the individual solid particles.

At the moment of inter-particle contact, the contact model is selected depending on the moisture variables of the particles and the overlap. A friction model is used for dry particles, whereas additional liquid bridge forces are considered for moist particles. In the case of a high portion of liquid phase, a specific model is needed to adequately simulate the suspension behaviour. For this purpose, particles are represented by a two-layer model, and interact according to a Bingham model.

The targeted application of the model at hand is the analysis and optimization of complex wet-mixing processes within a wide range of consistencies, e.g. the concrete production process. The model shall enable the evaluation of the liquid distribution and the overall mixing quality with much less effort compared to the experimental approach to detect critical areas within the mixer and to reveal possible options for improvements.

2 APPROACH

During the mixing process of wet mixing processes like in concrete fabrication, the source bulk materials pass several phases, from dry, to wet, ending up as a suspension (Figure 2). To simulate the mixing process, each of these stages has to be represented in the model and especially the transition of the water causing the stage changes must be implemented. Therefore a user defined model has to be implemented, representing the transition from the
early dry state to the final suspension state. The modeling of the transition is based on the results of experimental investigations and known theoretical models.

![Figure 2: Different moisture states of bulk material during wet mixing and associated contact model](image)

The representation of these states for a single particle in the simulation is introduced by an additional moisture variable. Each particle therefore has its own moisture content. Also the kind of liquid, present at the particle is noted, whether it is water or an already mixed cement paste or mortar. Depending on the moisture variable of two contacting particles, the contact model is chosen at the time of the particle contact. For dry particles a friction model is used, while for wet particles additional liquid bridge forces are integrated. For the suspension state a complete new model has been developed at the IAB, on the base of the Bingham model. The transition between these stages in simulation is triggered by the adsorption and absorption of moisture by the solid particles. At the beginning water is added as particles. When they get into contact with dry material, a time and state dependent transfer of the moisture is calculated and the moisture content of the former dry particle and its volume increases over time, while the water particle loses volume. The process dependent implementation of the moisture content also enables simulating different stages of concrete mixing. Since various particles come in contact with water at various moments in time, also heterogeneity of the mixture and its transition to a homogenous one can be simulated.

The characteristics of the liquid thereby influence the contact model parameters like viscosity and surface tension and therefore affect the contact model calculation e.g. for the liquid bridge force. Thus a smooth transition between all stages is provided.

### 3 SIMULATING WATER TRANSFER

One of the key issues of the suggested model is to replicate how moisture is transferred between individual particles. For this purpose additional moisture variables are assigned to each particle to simulate the moisture content, type of liquid, (i.e. water, cement paste or mortar) and its exact composition. Initially, water is added as spherical particles. A time- and
state-dependent transfer of moisture occurs upon contact between water and dry particles. The volume and moisture content of the initially dry particles increase over time, whereas the volume of the water particles is decreased (Figure 3). In the first step, the dry particles become wet and build up a two-layer particle with a solid core and an outer liquid film. When small particles absorb a sufficient amount of liquid, they will turn to a suspension and can also be considered as liquid particles. In the concrete mixing process this approach is used to create suspension particles that simulate mortar or cement paste, which can be adsorbed by the bigger aggregate particles. This results in new fluid transition regimes. A general overview of the transfer scenarios is displayed in Figure 4.

**Figure 3**: Contact of a water particle (top) and a dry particle (bottom), leading to a volume increase and a moisture transfer. The color of solid particles corresponds to the absolute water content

<table>
<thead>
<tr>
<th>Transfer Scenario</th>
<th>t0</th>
<th>t1</th>
<th>t2</th>
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<tbody>
<tr>
<td>Union with equalization (water and suspension particle)</td>
<td>![Image]</td>
<td>![Image]</td>
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<tr>
<td>Union with double layer creation (fluid and dry particle)</td>
<td>![Image]</td>
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<td>![Image]</td>
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<tr>
<td>Exchange with equalization (two suspension particles)</td>
<td>![Image]</td>
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**Figure 4**: Different water transfer scenarios depending on the contacting particles

The transfer is based on the models by Darcy used in [8] and Washburn [9], depending on the real particle size of the absorbing material and the constitution of the absorbed liquid.

\[
\nu_f = \frac{K}{\eta} \left( \frac{2\gamma}{\pi s(t)} - \frac{h}{l} \rho g \right)
\]

where \( K \) is the permeability, \( \eta \) the viscosity, \( \gamma \) the surface tension, \( \frac{h}{l} \) the ratio between the height difference and the distance of the particle centres, \( \rho \) the fluid density, \( g \) gravitational constant, \( s(t) \) the current penetration depth of the fluid. To keep \( s(t) \neq 0 \) fulfilled at all times the dry starting condition is set \( s(t_0) = s_0 = 5e^{-4m} \), accordingly to the initial wetting layer.
thickness defined in the model. The real particle size thereby has to be implemented as a particle attribute, because for fine materials like cement the particle size in the simulation is larger by several magnitudes in comparison to the real particle size. One simulation particle models a representative volume of cement.

If a liquid and a dry particle get in contact the first time, an additional amount of liquid is transferred to the dry particle. This models the fluid part that sticks to the surface of the dry particle no matter how long the particle contact was. This is essential for liquids with high viscosity, since they pass liquid by the described model very slowly. For the mixing process there exists also another aspect of. A faster relative movement of the particles leads to a stronger mixing and therefore a faster liquid exchange. To take this effect into account an additional liquid exchange volume was implemented in the simulation using a heuristic formula in the following form is used

\[
V_{\text{exchange}} = V_{\text{min}} \left( \frac{\dot{y}}{\dot{y}_{\text{ref}}} \right) \Delta t \times
\]

where \( V_{\text{min}} \) is the minimum volume of the interacting particles, \( \dot{y} \) is the local shear rate, \( \Delta t \) is the timestep and \( x \) is the percentual portion of the liquid exchange per second.

Besides the speed of the liquid exchange, also the maximum amount of liquid a single particle can adsorb is of interest. This depends mainly on the particle size, surface condition (roughness, wettability) and the type of liquid. A series of experimental tests were performed to estimate the maximum liquid amount for several dry material and liquid combinations. Figure 5 shows exemplarily the dependency of the maximum water adsorption by gravel depending on the grain size in a complex structure.

![Figure 5: Maximum volume of adsorbed water as a function of average grain radius in a complex structure](image)

\[ y = 0.7064x^{2.5603} \]

\[ R^2 = 0.9997 \]

4 CONTACT MODELS

At the moment of inter-particle contact, a contact model is selected depending on the moisture variables (Figure 2) of the particles and the degree of overlap (Figure 6). A friction
model is used for dry particles, whereas additional liquid bridging forces are considered for moist particles and a suspension model is used for the suspension state. The friction model is based on the standard models of the DEM and therefore is not presented in detail here.

4.1 Liquid Bridge Model

The liquid bridge model is chosen when two particles are in contact and the liquid volume of the contact is in pendular or funicular state or a wet particle interacts with a wall of the mixer. In this case, an additional cohesion force acts on particles. The liquid bridge forces depend on the size of particles, liquid volume, surface tension of liquid, liquid type and the distance between the particles. The model is based on an approach suggested by Mikami [1]:

$$F = 2\pi r_{\text{harm}}\gamma F^*$$

The model was verified with experimental data (the experimental setup is shown in Figure 7) and showed a good agreement for low liquid volumes (Figure 9). Furthermore the model was tested on a simple angle of repose test as shown in Figure 8. Additional experiments were performed to get data for higher liquid volumes and various liquid viscosities to widen the range of the model.

![Diagram of contact types for the interactions of two double-layer particles](image)

**Figure 6:** Contact types for the interactions of two double-layer particles
Figure 7: Schematic view of the setup for measuring liquid bridge forces

Figure 8: Comparison of dry (left) and wet (right) angles of repose for gravel in the experiment (top) and in the simulation (bottom)

Figure 9: Comparison of the liquid bridge forces of glass spheres with various radii and water volumes computed by the theoretical model by Mikami and measured in the experiment
4.2 Suspension Model

In the case of a high liquid volume at the contact spot of two interacting particles, a specific model is needed to adequately simulate the suspension behaviour. Modeling suspensions like concrete in DEM is not trivial and this is not the typical field of application for this simulation method. Suspensions often have a non-Newtonian material behavior so has fresh concrete. It is usually abstracted by Bingham-Model or the more general Herschel Bulkley model [3]. In CFD simulations these models can be used directly neglecting the phenomena occurring by the direct influence of the granular phase [4]. In the DEM different approaches are needed due to the discrete manner of modelling heterogeneous matters like fresh concrete [6], [7]. Most of the existing DEM models developed for concrete use double layer models to represent the solid aggregates uniformly covered by an imaginary layer of fluid fine mortar. Figure 6 shows the schematic structure of a two-layer particle as used in the present approach.

The constitutive relations used in this paper are based on the Bingham model as described in [2]. Since Bingham model is valid for the continuum mechanics only, it must be adapted to the DEM approach by several heuristics, for example an approximated contact area and shear rates (see Figure 10) as well as transformations to extract the contact force from the shear stress. The basic idea is to approximate the local shear rates by the relative velocity of the particles and the liquid layer in between. From the consistency of the liquid in the contact region the rheological Bingham parameters yield stress and viscosity are derived and the shear stress can be calculated. The shear stress is approximated to a contact force based on equation (4) from [5]:

\[ \sigma = \frac{\phi k}{4\pi r^2} F \]  

Thereby k is the coordination number and \( \phi \) the solid volume concentration.

Figure 10: Schematic view of the compensational Bingham model in DEM

5 RESULTS

The developed model was tested on a two phase system of cement and water within a typical mortar mixer. After a mixing phase of one minute the liquid was mostly equally distributed within the mixer. There was a dry area at the lower bottom of the tank (Figure 11) where the mixing tool does not directly interact with the material. This observation is congruent with the experience from the experimental testing.
Figure 11: Moisture distribution in a DEM simulation of a cement-water mixing process after one minute of mixing. The color represents the moisture states from dry (white) to completely wetted (blue). The dry parts at the bottom are highlighted.

Furthermore, another mixing process was simulated using gravel as an additional third phase. After the water addition, the power consumption derived from the total torque showed the typical curve that can be observed during mixing of concrete (Figure 12). First, an increase of the power consumption occurs, caused by the additional cohesive forces from the liquid bridges. After some time the power consumption drops because of the starting liquefaction of the mixture.

Figure 12: Relative power consumption starting from a dry mix of cement and gravel adding water (time zero)
6 CONCLUSIONS

A new DEM model was suggested to simulate the mixing process of dry granular materials with a massive liquid addition. The model includes the transfer of liquid between particles as a function of their size, moisture state and the liquid’s properties. Depending on the particular moisture state adequate contact models are chosen using frictional, cohesive or Bingham-like behavior. The representation of the particles is based on a double layer approach and additional particle variables storing information related to the liquid. The general applicability of the model was demonstrated on two examples of mixing. This offers a basis for investigating more complex mixing processes.

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