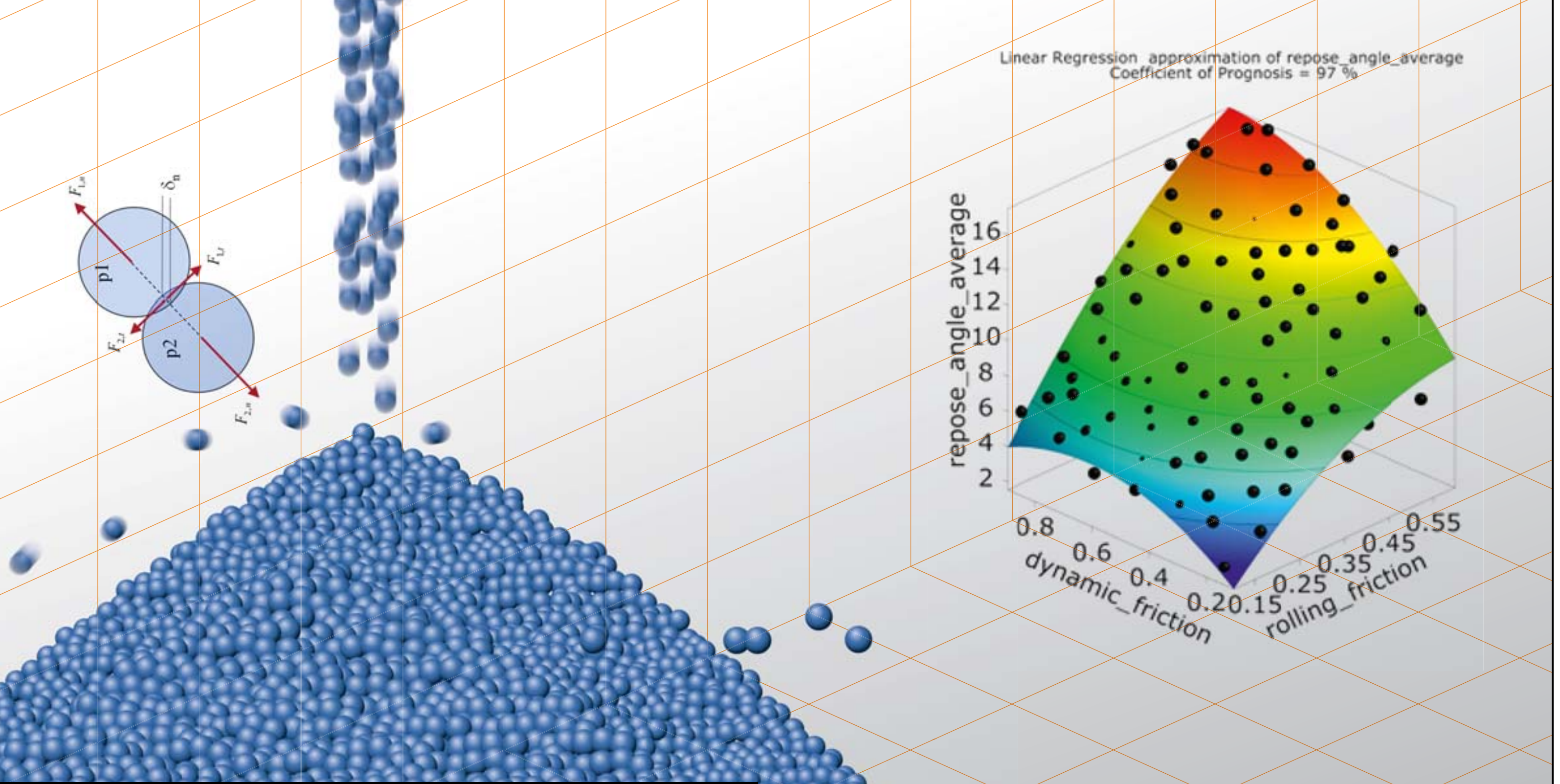

CALIBRATION OF ANGLE-OF-REPOSE AND DRAW-DOWN ANGLE USING A ROCKY-DEM SIMULATION

Rocky Discrete Element Method (DEM) and optiSLang were used to calibrate a model for the simulation of particle behavior in order to optimize the geometry of a bulk material funnel.

Motivation

The angle-of-repose and the draw-down angle are critical parameters for assessing the particle behavior, e.g. regarding bulk material. Prior to a particle simulation, the unknown properties and parameters of the numerical simulation should be determined by reproducing an experiment within a particle simulation.

Calibration represents the starting point of a parameter study, especially if uncertainties regarding the determination of material constants or the arrangement of constraints have to be considered in numerical simulation. Dealing with particle simulations, this is a constant challenge, because the individual properties depend not only on the material of the particle, but also on its shape and the environmental conditions. This results in a large amount of parameters, which make the identification of interactions significantly more difficult. A sensitivity study was first performed to generate the Metamodel of Optimal Prognosis (MOP) and to identify the important parameters. Such an approach is particularly important and challenging for the Discrete Element Method (DEM), because of the consideration of many parameters and the processing of quantities due to the noise of the numerical solution. These boundary conditions require a variant study with an efficient investigation of the parameter space. In the procedure, metamodel algorithms are used to not simply "fit" the data, but also take into account the influence of solver noise and, thus, illustrate global trends. These requirements can be fulfilled by using the MOP approach.

The following example applies the fixed-funnel method to identify the parameters for describing the particles. The simulation process of this method is shown in Fig. 1. As soon as the cylinder is completely filled with particles, it is moved upwards creating the typical form of solid bulk. Here, both the angle-of-repose and the draw-down angle can be determined as a mean value along the bulk material heap.

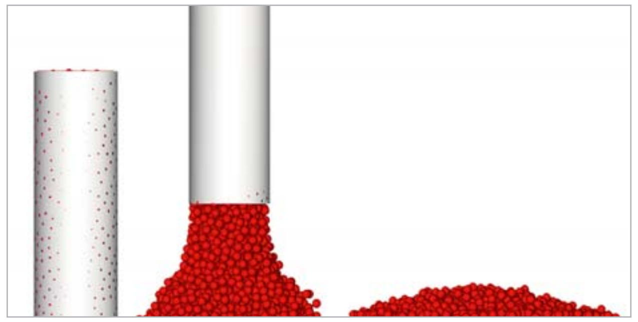

Fig. 1: Illustration of the transient simulation to determine the angle-of-repose and the draw-down angle of a bulk material

The angle-of-repose represents the outer angle of the bulk material and can be determined directly after such an experiment. The draw-down angle describes the inner angle after the bulk heap has dispersed from the middle. The mean value along the bulk material was then calculated for both angles and the results were used in the subsequent analyses.

	Name	Parameter type	Reference value	Constant	Operation	Value type	Resolution	Range		Range plot
1	particle_density	Opt.+Stoch.	2750	☐		REAL	Continuous	2700	2800	
2	static_friction	Dependent	0.6875	☐	scaling_factor_friction*dynamic_friction					
3	dynamic_friction	Opt.+Stoch.	0.55	☐		REAL	Continuous	0.4	0.6	
4	restitution	Opt.+Stoch.	0.55	☐		REAL	Continuous	0.1	0.6	
5	rolling_friction	Opt.+Stoch.	0.55	☐		REAL	Continuous	0.1	0.6	
6	mass_flow	Opt.+Stoch.	20	☐		REAL	Continuous	19	21	
7	particle_diameter	Opt.+Stoch.	10	☐		REAL	Continuous	9	11	
8	E_Modulus	Opt.+Stoch.	1e+07	☐		REAL	Continuous	8e+06	1.2e+07	
9	scaling_factor_friction	Opt.+Stoch.	1.25	☐		REAL	Continuous	1	1.5	

Fig. 2: Overview of the parameter and their corresponding ranges

Procedure

The process of solving this task is divided into two steps. First, the conduction of a sensitivity analysis and, second, the use of an optimizer to minimize the deviations between the simulation model and the experiment.

Calibration

The aim of a calibration is to match the results of a simulation to the measurements. This can only be obtained after an identification of the important parameters. Once they are detected, a variation can be conducted to minimize the deviation. In this study, the physical properties were used as parameters and varied in the ranges shown in Fig. 2. It should always be noted here that some parameters cannot be considered as independent. In this case, the static and dynamic friction is multiplied by a weighting factor that describes the ratio between them and is always less than one. This value also represents a physical constraint in the parameter study. In addition, the particle density, the particle diameter and the mass flow while entering the test tube were examined.

The general procedure for a calibration is shown in Fig. 3. First, the important parameters should be identified. Afterwards a calibration between simulation and experiment can be achieved with these important parameters by means of an optimization algorithm.

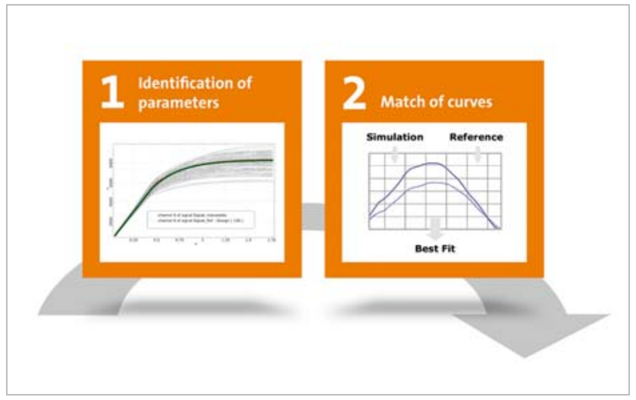

Fig. 3: General workflow of a calibration with, first, the identification and, second, the optimization of these found parameters to fit the simulation with the reference data

Workflow

Based on the obtained parameters, 100 simulations were generated arranged in a Latin Hypercube as part of a Design-of-Experiment. The parameters were transferred to Rocky DEM using the custom integration that is pre-installed in optiSLang. Then the model was updated and numerically solved. Fig. 4 (see next page) illustrates the workflow.

After completion of the simulation, the results were transferred back to optiSLang and used for the evaluation. Using these 100 simulations from the sensitivity study, the MOP could be created for the two result values draw-down angle and angle-of-repose. The MOP was then used for an optimization to minimize the deviations between simulation and experiment. The aim of the optimization was defined as

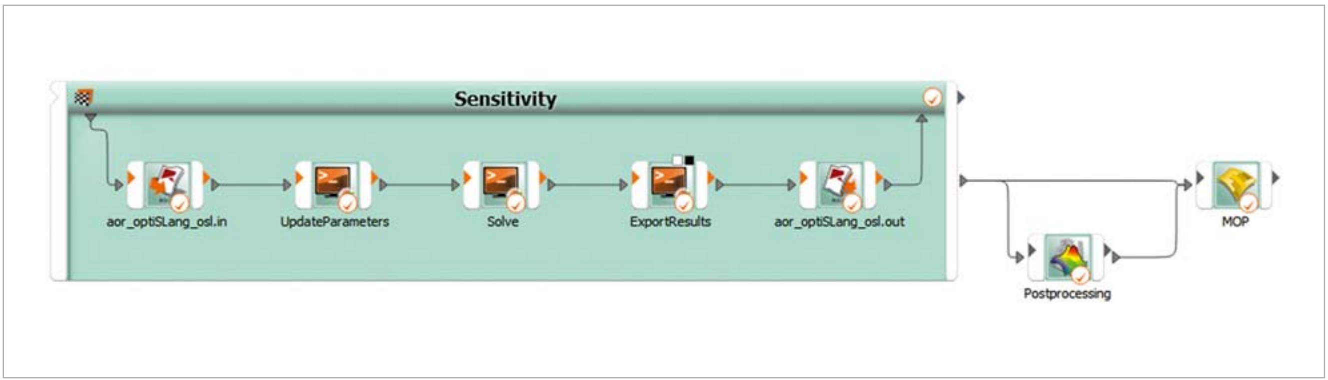

Fig. 4: optiSLang workflow of an automized sensitivity study for a Rocky DEM simulation

the sum of the squared differences between simulation and experiment. Here, a Non-Linear Programming by Quadratic Lagrangian (NLPQL) proved to be a suitable method. This procedure yielded a sufficient calibration without using another numerical simulation run.

Results

Based on the results of the sensitivity study, first, the range of values of the result variables could be compared with the experimental data. The results and the associated experimental data are comparatively shown in Fig. 5. The experimental values are positioned in the middle of the result space surrounded by the simulation results. This indicates that the parameter space is sufficiently chosen and a calibration is possible. At this point, however, the optimum in the parameter space cannot yet be located. For this purpose, a reduction of the parameters and a subsequent optimization is required.

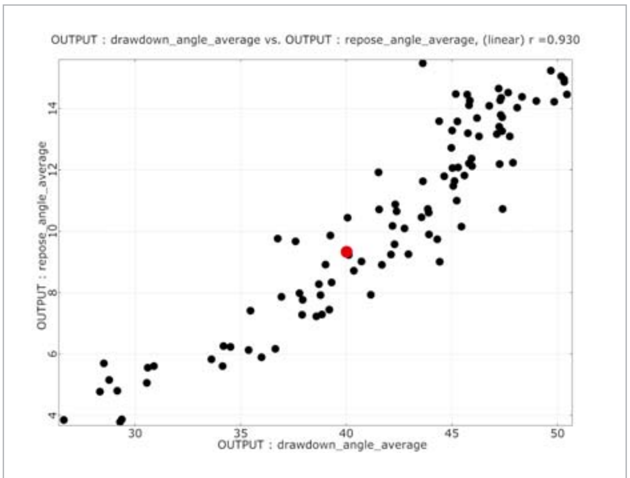

Fig. 5: Illustration of the experimental values (red), which are the calibration target and the results of the performed simualtions

The reduction of the important parameters could be reached by using the MOP. Beside the identification of important parameters, the MOP also enables the elimination of the strong solver noise as a typical phenomenon in a DEM simulation.

For the data set examined here, the rolling friction is of importance, because it only describes the two result variables. With the help of the subsequent optimization based on the MOP, the rolling friction could be identified. Here, the deviation between simulation and experiment was minimal. Thus, both values were accurately determined, the angle-of-repose differs 0.21° from the experiment and the draw-down angle with 0.1°. This small remaining deviation can be seen exemplarily for the noise of the Rocky simulation in this example.

Conclusion

Using the created workflow, Rocky DEM simulations can be coupled with other platforms via optiSLang and optimizations can also be carried out. The procedure is fully automated and, thus, less prone to errors. The workflow was used to determine the numerical input variables based on experimental data for the simulation of the angle-of-repose and the draw-down angle. The identification of the rolling friction as an important parameter as well as a sufficient plausibility check including a physical test would not have been possible without an automated parameter study using the MOP. Those parameters identified as not important cannot be calibrated by the experiment. Such values have to be considered in other experiments.

By means of optimization, the suitable rolling friction could be determined. For this purpose, not only the values of the MOP but also the values of the numerical model were calculated. The deviation between them is just a few percent, thus, this value of rolling friction could be used for further simulations.

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