MODELING OF COAL COMPACTION WITHIN STAMP-CHARGED COKE MAKING BY MEANS OF COMPUTATIONAL PHYSICS

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ABSTRACT

Within stamp-charged coke making a large volume of coal is compacted to one single coal cake before entering the coke oven chamber. This is done by means of several falling stampers in a stamping machine having a mold nearly of the oven's dimensions. Producing a high quality coke also from inferior coals requires a cake density of approximately 80% of the coal density. Besides that the industrial stamp-charging process demands a minimum mechanical strength of the coal cake to move it from the stamping mold into the oven chamber without failure.

Densification and the build-up of cake strength were investigated earlier in stamping tests using a micro-stamping device. The quantities derived from these tests (as e.g. cake density or porosity) represent average values for the entire cake. Statements describing the local compaction state at different heights are difficult to achieve without destructing the cake.

In order to gain better insight into the densification process and the inner structure of the coal cake a computational model based on the discrete element method (DEM) has been set up using 2 and also 3-dimensional simulation software. The stamper's position and velocity as well as the force acting on the stamper were monitored and the model's response was compared against measurement data from laboratory stamping tests.

It was possible to reproduce the force and displacement pattern of the stamper in response to the viscoelastic properties of the cake using standard DEM bonding and contact models. Furthermore, the rearrangement of particles in response to the compaction by the stamper was tracked by calculating their displacement at the point the stamper hit the coal surface. The latter can also be used as indicators of particle deformation or breakage. By defining control points at different heights the particle displacement, stress and strain rates, porosity could be studied at different heights.

Keywords: coke making, coal stamping, compaction, agglomeration, DEM, simulation

INTRODUCTION

Coking of coal blends using high volatile coals with poor caking properties and other blendable components to still produce a high quality blast furnace coke can be achieved by compacting the whole oven charge prior to the carbonization. This is achieved in the so-called stamp-charge operation (Kuyumcu, 1990). The compaction of the oven charge to a single huge coal cake of up to 50 tons at industrial scale involves a stamping machine consisting of a mold of slightly smaller dimensions than the coke oven. The machine is equipped with a row of stampers that are periodically lifted up and dropped on the coal charge.

The objectives of the stamping process are to obtain a homogenous cake density of approximately 80% of the coal density and at the same time a sufficiently high mechanical strength. Mechanical stability is necessary to prevent the cake from failure while it is moved into the oven chamber. Cake density and cake strength are depending on several material-related parameters, as coal type and rank, the particle shape and size distribution,

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moisture content, and on the stamping energy applied (Abel et al, 2009 a, b). These objectives together with demands on increasing productivity, i.e. corresponding to short stamping times, are subject to optimization.

In the systematics of agglomeration processes the stamping process falls into the category of pressure agglomeration with binder addition. i.e. the wet agglomerate strength is determined by liquid bridges and capillary forces. To investigate the two sub processes of densification and strengthening during stamping, theoretical and experimental work has been done earlier. For this purpose a micro-stamping test unit in combination with a strength tester suited to the dimensions of the stamped cake was developed (Abel et al, 2009 a, b). The physical quantities derived from these tests (as eg cake density or porosity) allow to describe the densification but represent average values for the entire cake. Statements describing the local compaction state at different heights are difficult to achieve without destructing the cake. In order to gain better insight into the densification process and the inner structure of the coal cake, a computational model describing the particle system is to be recommended.

There are several examples of simulation studies of compaction processes carried out by continuum or discrete element methods. Finite element-type methods have been well represented (Marques and Martins, 1991; Khoei, 2002; Jonsén et al, 2007; Berg et al, 2010). Simulations utilizing continuum methods can offer insights into many aspects of particle or powder compaction. It is not possible, however, to gain in-depth understanding of particle interaction and displacement mechanisms, localized porosities, effect of particle size or size distribution, etc. Particle-based discrete simulation methods have traditionally been less common in this context. This is believed to be due to several factors; eg higher complexity of modeling and simulation setup, the typically large number of particles needed to represent a powder material, a small time step as well as difficulty in identifying and selecting appropriate parameters for use in simulations. Recent examples of particle system compaction or consolidation include compression studies by coupled Lattice-Boltzmann and DEM (Planet et al, 2008), 1D simulation of high velocity compaction by DEM (Shoaib et al, 2011) and substrate absorption and evaporation-driven consolidation of mineral suspensions (Sand et al, 2011).

The objective of this work is to gain insight into the densification process and a better understanding of the micro-processes within the stamp charge operation. This is in order to improve process efficiency and optimize the properties of the stamped coal cake. The particle simulation approach allows comparison with experimental investigations of the stamping process, while simultaneously enabling elucidation of micro-level phenomena not possible to study experimentally.

**METHOD**

In the first the stamping process is simulated using a commercial discrete element simulation software, Particle Flow Code in 2 dimensions (PFC2D 4.00-123) developed by Itasca Consultants, Minneapolis, MN. The model setup for studying the stamping process includes the following steps:

1. Representation of the stationary walls of the mold.
2. Representation of stamper as a moving wall in the vertical direction and decryption of its motion in the gravity field.
3. Generation of the coal particle collective as a polydisperse size distribution with a size range obtained from experiments.
4. Selection and calibration of DEM models, including adjustment of micro-level parameters within the mechanistic model to experimentally obtained macroscopic values.
5. Description of the filling process, including random placement of particles followed by deposition and gravity-driven consolidation in the stamping mold.
6. Simulation of the compaction process.

To model the particle-particle and particle-wall interactions, the mechanistic model parameters describing particle contacts and bonds need to be adjusted. This calibration procedure is a critical step in the model setup. It takes place by an iterative procedure, where some initial DEM model parameters are first selected and simulations carried out. Simulation results are then compared with experimental input, by selecting a number of control parameters. The experimental input in this case comes from stamping tests, but can also include particle analysis, shear tests, etc. Based on the results of the comparison, model parameters are adjusted and the procedure repeated until agreement between simulations and experiments is obtained with acceptable accuracy.
The comparison between experimental and simulation data for multiple control variables, in this case first impact rebound amplitude, attenuation and peak force, often takes place only in a qualitative way. A more satisfying approach to quantify the agreement is given by a multiple objective optimization strategy that uses the deviations in the individual control variables as the criteria to be minimized. The initially unknown model parameters are defined as the optimization variables and the best fitting set of parameters is identified within a numerical directed or non-directed search. For determining the “best fit” the multiple criteria first need to be aggregated in one single objective function, e.g. in a weighted sum of least squares. The following sub-sections describe the laboratory-scale tests used to obtain experimental data as well as the model and simulation setup based on the calibration procedure described above.

**Laboratory-scale stamping tests**

The laboratory-scale stamping device consists of a mold of base dimensions 100 mm × 100 mm and a height of 150 mm. The mold was filled with 1 kg of coal sample plus varying amounts of water as binder. A metal weight of 40 kg was used as stamper, with a drop height varying between 0.25 and 0.55 m above the surface of the coal sample. This setup is designed to give a similar specific energy input as in the industrial scale. A displacement transducer and a load cell are mounted on the equipment to enable tracking of stamper movement and forces acting on it during stamping. The equipment setup and an example of measurement output are given in Figure 1.

![Laboratory micro-stamping device (left) and example of instrumentation output (right), from Abel, Rosenkranz and Kuyumcu (2009 a, b). Control parameters for the calibration are enclosed; rebound amplitude and coefficient of restitution](image)

Data points are collected at a rate of 4800 s\(^{-1}\). The test equipment setup is described in detail elsewhere (Kuyumcu and Rosenkranz, 2006). Typically after impact, the stamper makes a series of characteristic bounces before settling on the coal cake. This behavior can be observed when tracking the displacement of the stamper. A series of force peaks signifies each bounce by the stamper. From tests such as bulk shear tests and angle of friction, additional information can be obtained for input in simulations. These parameters include coal solid and bulk density (which can be translated into initial porosity before stamping), as well as friction coefficients. The moisture content can be used as input in more sophisticated cohesion models, which include physical effects such as capillary forces and liquid bridging. The parameters derived from the experimental work included a coal solid density of 1430 kg/m\(^3\) and a bulk density of 667 kg/m\(^3\), a moisture content of 10\%, angles of friction for the coal bulk material of 35° and for the stamped coal cake of 50-60°, as well as a stamper coefficient of restitution of 0.27.
Model and simulation setup

Simulation domain and boundary conditions

The simulation domain is constructed with mold confinements represented by stationary walls. The stamper is defined as a servo-controlled movable wall, added in the upper part of the simulation domain. It translates in the vertical direction, with its motion being described by the gravity field. The fall height was defined in the same way as in experiments, thus being dropped from a height of 0.55 m above the top surface of the coal cake. The response of the coal cake to the impact of the stamper can be monitored in terms of stamper displacement and velocity over time, which in turn is related to the viscoelastic properties of the cake.

A number of control points are defined at different heights in the stamping mold model. This enables time or compaction state-dependent tracking of various properties such as cake porosity, stresses inside the cake, coordination number, etc. These properties are not possible to obtain by experiments, but can be used as indicators for eg particle migration and interaction mechanisms. Simulations also allow calculation and visualization of interparticle contact forces, and tracking of particle motion by the use of displacement vectors.

Time discretization and particle system

Due to the high velocity of the stamper in relation to the size of the particles, a very small time step is needed. It was found that a time step as low as $10^{-9}$ to $10^{-10}$ s should preferably be used. However, for the particle size distribution defined in the simulation, a maximum time step of $10^{-8}$ s was found acceptable. Nevertheless, this makes simulations computationally costly and already a simulation consisting of 1000 particles translates to a wall-clock simulation time of nine to ten hours on a desktop computer. The only means of significantly influencing the simulation time consumption is to limit the number of particles or possibly by simplifying the particle interactions. Adjustment of domain properties or the procedure for initial particle deposition is deemed to have only limited influence in this context. Plotting and data collection intervals in simulations were adjusted to correspond to the experimental sampling rate.

Due to the limitation in number of particles in simulations, a completely accurate particle size distribution and stamping mold filling degree is not possible. Consequently, the coal particle collective consisting of 1000 particles were generated based on a Gaussian size distribution with a mean particle size of $\mu_d = 0.9$ mm and a standard deviation of $\sigma_d = 0.6$ mm, illustrated in Figure 2.

![Particle Size Distribution](image.png)

**Figure 2.** Particle size distribution in simulations compared with the experimental distribution.
As can be seen, the particle size distribution used in simulation deviates from the experimental counterpart by overestimating the number for large particles and underestimating small ones. These modifications limit the number of particles in simulations, while still maintaining a realistic particle size range. In this sense, the simulated particles can be considered as scaled DEM-particles, which thus is a means for discretizing the coal cake. This enables appropriate bulk cake mechanical behavior simultaneously as allowing study of micro-scale mechanisms taking place in the cake during stamping.

**Interaction models and parameterization**

Built-in contact and bonding models are used in this study. PFC2D contains two bonding models; contact bonds and parallel bonds. The contact bond defines interparticle adhesion at the infinitely small area at the contact point. The parallel bond can be used to represent the cohesion between two particles over a longer distance, resulting from the presence of an interstitial binder. This distance is referred to as the bond radius. The contact bond represents the case of the parallel bond radius being zero. However, both the contact and parallel bonding mechanisms can be applied simultaneously. As the Hertz contact model is not defined for tensile forces, it is incompatible with bonding and a contact bond can thus not be defined. Instead, the linear contact model in conjunction with the viscous damping component is utilized in this study. For producing particle cohesion, both the contact and parallel bonding models were used.

The linear contact model is defined by normal and shear stiffness, while the viscous damping model is described by a normal and shear damping component. Viscous damping is applied to dissipate energy from the impacts of the stamper, thus being analogous to internal friction and wave scattering mechanisms as observed in real material samples (Potyondy and Cundall, 2004). The parameters that describe a contact bond are normal and shear strength, $\phi_n$ and $\phi_s$. A parallel bond, on the other hand, is characterized by five parameters; normal and shear stiffness, $k_n$ and $k_s$, normal and shear strength, and bond radius $R$. More information on bonding models can be found in the PFC2D user’s guide.

A challenge in DEM simulation is the determination of the micro-level parameters discussed above. Some parameters can be estimated based on empirical studies or obtained from the literature, as is the case with eg friction coefficients, solid and bulk density. Other parameters should be considered as case or even simulation specific, although some initial input can be found from literature. This is the case for instance with stiffness values, which need to be estimated by calibration using physically determinable control parameters. Finally, some parameters can be tuned to offset errors induced by idealizations used in simulation. In DEM simulation, the most typical example is when complex-shape particles of a real material are being approximated as being spherical. This approach can be acceptable if adjusting the friction coefficient in simulations, either by assigning a higher friction than what is observed in experiments or assigning a separate rolling friction as in the case of the Hertz contact model. In this case all three approaches are applied in one way or another. In this study, the model parameters were defined as follows:

- **Linear contact model with viscous damping**
  - Particle stiffness (normal/shear) subject to calibration.
  - Particle-particle and particle-wall friction coefficient $\mu = 1.0$.
  - Viscous damping (normal/shear) of 0.2, close to PFC2D default recommendation.
  - Wall stiffness (normal/shear) of $5.2 \times 10^9$ N/m, as often used for steel.

- **Parallel bond model**
  - Bond strength (normal/shear), $1.0 \times 1018$ N.
  - Bond stiffness (normal/shear), $1.0 \times 1018$ N/m.
  - Bond radius, 0.10m.

- **Contact bond strength**
  - Bond strength (normal/shear), $1.0 \times 1018$ N.

The built-in particle bonding models in PFC2D are not well suited for producing interparticle cohesion resulting from liquid bridging, capillary forces and other liquid-solid related phenomena. Input values were in this case based on similar studies in the literature (Xie and Zhao, 2009; Yoon, 2007).
RESULTS AND DISCUSSION

Model calibration

Firstly, the model was calibrated by adjusting particle normal and shear stiffness according to three control parameters obtained from the laboratory-scale stamping device; stamper rebound amplitude at first impact, attenuation and force. The attenuation, or coefficient of restitution, is normally calculated as the velocity ratio before and after impact. An alternative method is to calculate from the rebound amplitudes of two consecutive impacts between the stamper and coal cake. In this case, the coefficient of restitution can be calculated as

\[ k_{COR} = \sqrt{\frac{A_n}{A_{n-1}}} \]  

Where \( A_n \) is the n:th rebound amplitude and \( A_{n-1} \) is the rebound amplitude of the preceding impact. Due to changes in cake structure and densification state at each impact by the stamper, it is important to use comparable peaks for the calibration. It is likely that the coefficient of restitution will change over the course of a full stamping cycle. In this study, the calculation is always based on the first and second impact.

Initial stiffness input values for the calibration were taken from Xie and Zhao (2009). Simulations were then performed for a range of stiffnesses and results compared with the control parameters, obtained from laboratory tests as described by Kuyumcu and Rosenkranz (2006). For a drop height of 55 cm, the experimental parameters were a coefficient of restitution of 0.27, a rebound amplitude after first impact of 3.24 cm and a peak force of 18.0 kN. By this approach, it was possible to identify the mechanistic model parameters that yielded a coal cake behavior in agreement with experiments.

The deviations between experimental and simulation results for all the three control parameters are summarized in Figure 3. The model parameters best fitting the prerequisites were a coal particle normal and shear stiffness of 4 to 6 \( \times 10^6 \) N/m. Using these settings, the average deviation is less than 10%, with the error in coefficient of restitution, rebound amplitude and peak force of 13.3%, 5.3% and 17.9%, respectively. The standard deviation between simulations with equal parameters was typically less than 1%. The average deviation does not, however, take into account that the relative importance of the various control parameters is not equivalent. Related to the discussion on multiple objective optimization, it was for instance found that the rebound amplitude is more critical than the coefficient of restitution. A good parameter fit in terms of reproducing accurate rebound amplitude should therefore take precedence over fitting the attenuation. The measured peak force deviates between simulations and experiments due to several factors.

For instance, the more uneven coal surface in simulations gives a longer contact time between the stamper and the cake at impact and thus broadens the force curve and reduces the peak force. Furthermore, there are other factors such as shape and shape distribution that are not taken into consideration in simulations. Figure 4 shows the best overall fit in terms of stamper trajectory, with the corresponding force comparison enclosed. This fit was obtained using the particle stiffness 6 \( \times 10^6 \) N/m.
Figure 3. Deviation between experimental and simulated values for stamper coefficient of restitution, first-impact rebound amplitude and peak force. The average deviation can be used to identify where the criteria are best satisfied (aggregation using equal weights).

Figure 4. Comparison between simulation using calibrated model and experimentally measured stamper trajectory. Enclosed is also the comparison between simulated and experimental force at the first stamper impact.

Structure analysis of the coal cake

Vertical porosity profile
By defining control points within the coal cake, local porosities can be monitored in simulations eg at various heights in vertical direction or as function of time during stamping. Furthermore, the bulk porosity over the full thickness of the cake can be calculated and compared with experimental data. Such an exercise is shown in Figure 5, where the porosity development in time and at different coal cake positions is studied during stamping. Each impact by the stamper is indicated by a sharp drop in porosity with a partial rebound as the stamper retracts.

The porosity in the simulation gradually decreases from around 45% to 18%, at the point the stamper settles on top of the cake. Such detailed information is not available from the empirical results, but it is known that the initial bulk porosity starts at about 50% and is then reduced to 25% after completed compaction.

**Figure 5.** Porosity development in time, shown for three separate coal cake positions in the horizontal direction as well as an average over the entire cake

Differences between simulations and experiments could partially be explained by the lack of particle aspect ratio. Spherical particles increase the probability of reaching a denser packing. This could partly explain the lower initial and end porosities in simulations, as compared to the experimental data. Also the friction coefficient in simulations is defined as a single value and particles are not allowed to deform or break as result of the stamping, as is not the case in reality. Additionally, the comparison between 2D and 3D porosities is not strait-forward.

**Visualization of particle movement and acting forces**

Discrete element simulation can offer a level of detail in results that is not possible to obtain neither in continuum simulation approaches nor by laboratory trials. In the case of coal stamping, examples can include particle motion and rearrangement mechanisms during compaction and contact forces arising within the cake structure. Such detailed information on the particle level can provide valuable understanding on how the stamping operation influences the structures, cohesion and therefore the mechanical properties of the coal cake. Using built-in PFC2D functionality, contact forces can be monitored in terms of compressive and tensile forces. In addition to providing information on densification behavior during stamping, contact forces can also be used in studying the risk of cake cracks or failure. Problems of this type can cause operational problems in the real process, resulting in production downtime and costly cleanup procedures. Figure 6 shows some examples of visual output; particle movement illustrated as a vector map and contact forces between particles during stamping.
The simulation problem was extended to the third dimension using the discrete element tool EDEM by DEM-Solutions, Edinburgh, UK. This exercise was performed to qualitatively evaluate the feasibility of studying the process in 3D in terms of computational efficiency and visualizing the spatial movement of particles. Standard contact and cohesion models were used. These included the no-slip Hertz-Mindlin contact model in conjunction with a linear cohesion model. The parameters used in the Hertz-Mindlin model are Poisson's ratio and the shear modulus. The coefficients of restitution, static and rolling frictions were defined between each type of material of the system, i.e., particle-particle and particle-wall. Linear cohesion is defined by an energy density parameter. First orienting test runs comprised 3000 particles of monodisperse size distribution (d=8 mm). Issues related to the requirement of increased number of particles, particle size distributions and higher complexity of interaction models put greater strain on the computational resources. However, for getting a sufficiently good description of particle displacement and rearrangement during stamping, a 3D approach is most likely needed.

CONCLUSIONS

The results of simulations show that DEM is a feasible option in describing the stamp charge operation. Additionally, the simulation approach also offers complementary information to laboratory-scale empirical studies. To name but a few, particle displacement and rearrangement mechanisms in the coal cake, contact forces and local differences in porosity or cake density can be dynamically tracked during the stamping process. This tracking comes within the context of having a coal cake in simulations with mechanical properties calibrated to give a realistic bulk cake behavior in comparison with experiments. Currently, this calibration takes place by tracking of rebound amplitude, attenuation (coefficient of restitution) as well as peak force.

This work is based on standard PFC2D and EDEM particle interaction models in terms of contact and bonding behavior. Especially the bonding mechanisms need to be further developed, as the built-in models are unable to describe cohesion resulting from liquid bridging and capillary force-based interactions with sufficient level of detail. Ideally, increased predictive significance could result from inclusion of physics-based models that are better able of describing the properties of moist particle systems rather than tuning of existing mechanistic models for cohesion behavior. Mechanistic model parameters required for particle contacts, e.g., friction and stiffness, are known to be affected by the densification process and it should therefore be considered to define them in a dynamic way. Better predictivity could be reached by describing these parameters as functions rather than assigning static values for the full length of a simulation. Studying changes in model properties or parameters as function of time or densification state thus remain an interesting topic for further model development.

A general task that is not restricted particularly to the stamping process is how to formalize the model calibration step using multiple parameters simultaneously. The solution must couple the iterative procedure of parameter tuning with a directed numerical search to find the best-fitting parameters based on quantitative multi-criteria evaluation. Due to the quite high computing times for simulation, highly efficient numerical routines are necessary in this case.

Within the context of parameter tuning, a hierarchical modeling and simulation approach could be useful. Results obtained at one level of detail can be utilized as input parameters for simulations by another method and on another level of detail. This is especially so in the description of large-scale processes where information of interest can lie on several different size scales. Stamping of coal cakes is an example of such a process. The problem size and number of particles will in that case determine which methods are most feasible to use. Consequently, if interest lies on the macro-scale properties of a large coal cake, the finite element method (FEM) is the recommended approach. With interest in meso-scale behavior of a system, the problem needs to be scaled down compared to the macro-level approach. Suitable simulation methods in this range could be particle-based continuum approaches such as smoothed particle methods (SPH) or the particle finite element method (PFEM). On the smallest size scale and with interest in interactions between individual elements of a material, DEM is the feasible option. Thus, the hierarchical approach should be the preferred route if detailed information on a process is required on several levels of detail.
Figure 6. Particle system including measurement circles (top left), with same system drawn as particle displacement vectors (top right). Contact forces between particles can also be monitored. Compressive forces arising due to gravity (bottom left) and as the stamper impacts the coal cake (bottom right).

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REFERENCES


