DESIGN OPTIMIZATION OF HIGH ENERGY BALL MILLS BY DISCRETE EVENT SIMULATION

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ABSTRACT

High energy ball mills are used to grind powder material down to a particle size below one micron. Up to now, the detailed physical mechanisms of the grinding process inside the mill have not been fully understood. Hence, the design of these mills as well as their process parameters is based on empirical results.
The ball mill has been simulated by discrete event simulation (DES) using typical process parameters to monitor the balls motion and their collisions. The DES method – if applicable – strongly outperforms typical DEM methods.
Furthermore parameter variations of the main process parameters have been made and the distribution of the balls impact velocities in normal direction has been analyzed, which is responsible for the grinding effect.
Based on the new knowledge about the ball's motion inside the grinding chamber and the probability distribution of the impact's velocity, we developed a new grinding chamber. Its shape has been optimized by a computer simulation. The new design of the grinding chamber allows higher impact velocities and therefore finer powder of new mechanical alloyed powders.

DISCRETE EVENT SIMULATION

The grinding medium (about 4000 steel balls in a lab scale mill) is accelerated by rotor blades in a horizontal drum (Figure 1). The powder is grinded between two colliding balls. Hence, the collisions between balls as well as the grinding chamber are the important events to monitor. Due to the high number of objects, efficiency is a major goal of algorithm development.
In the case of the ball mill observations with typical process parameters in a transparent grinding chamber using a high speed camera have shown that only pair wise collisions occur [1]. Thus, collisions can be modeled as instantaneous and pair wise. Consequently, in this work, the high energy ball mill is described by an event driven particle simulation using collisions as basic events.

Figure 1: Transparent experimental grinding chamber of a high energy ball mill

Event driven molecular dynamics processes in general are modeled as a series of discrete instantaneous collision events. These events are stored in an event list ordered by time.

The Simulation Loop

Generally, the event processing in this paper is a iteration over the steps 1-4 below [1], [2]:

1. The simulation clock jumps from one collision event to the next. The simulation time is updated by handling the next event of the event list, e.g. a ball to ball collision.
2. The algorithm searches for the next possible collision time for each of the two balls involved. This is computed analytically. In a system of hard spheres, events refer to collisions, involving:
   - exactly two balls
   - one ball and the cylindrical walls of the drum
   - one ball and the flat side walls of the drum
   - ball and one of the rotor blades

The collision time is the flight time from the actual event to the new event.

3. The locations of the two new collisions are calculated using the flight time just computed to the collision point. The calculation of the collision response leads to the new flight direction at this point caused by the collision event.
4. These new events are inserted into the event list. Hereby, predicted collisions may become invalid as a result of another ball crossing a flight path. In this case, the event list handling routine must ensure

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consistency by deleting the invalid events and all events following.

Operations 1 and 4 are the event handling routines. Several approaches exist to speed up the access operations of the event list [6]. In [2], an efficient data structure to handle these operations was presented.

Steps 2 and 3 function quite differently than in continuous simulations, and are described in the immediately following sections.

Collision Detection

Air resistance can be neglected due to the fact that the process in evacuated, because many powders become extremely reactive when they are processed under a normal atmosphere.

Most of the computational time in continuous simulations is spent for the correct calculation of the ball positions. Assuming that a priori information about the evacuated grinding chamber, the absence of air resistance and Magnus forces are given. Thus, there is no need for numerical integrators, because the ODE for the trajectory has a well known analytical solution given by a parabolic flight path, equation (1).

$$\vec{s}(t) = \vec{r} + \vec{v}t + \frac{1}{2}\vec{g}t^2 \qquad (1)$$

Here, all the vectors are in three dimensional space, the gravity vector $\vec{g}$ is defined to be negative in the z-direction, and the initial position and velocity are given by $\vec{r}$ and $\vec{v}$ respectively.

The contact time of the collisions is assumed to be negligible. Hence, the probability of multiple contacts is zero. The balls are modeled as hard spheres undergoing binary inelastic momentum-conserving collisions [4].

Due to the fact that only pair wise collisions are allowed, the algorithm checks collisions from the viewpoint of one single ball against the other objects separately. Objects are members of a class (body shapes), namely about 4000 balls in the balls class, 5 rotor blades in the rotor class, one drum and two walls [4].

For each class, a time dependent distance function has to be defined, representing exactly the distance between the surface of the actually observed free flying ball (equation (1)) and the surface of a member of the other object class. The ball will collide with the other object when the distance of the surface is zero for the first time.

When using DES, time-space collision coordinates are computed by finding the minimum positive real root of the distance function of each object. These different collision times are calculated separately, ignoring the presence of other objects. Hence, for each class, a minimal collision time will be calculated. Only the first of these is valid, because the ball will change its direction after this collision.

If, in one class, no collision can be found, e.g. no ball to ball collision, its value is set to infinity. A collision with the system's boundary will take place in any case.

Collision Response

Energy will be dissipated when a collision takes place, resulting in a lower kinetic energy after the collision. Theoretical investigations commonly use the inelastic hard spheres model, which has proven very useful, despite the simplicity of its definition: hard spheres undergo binary inelastic momentum-conserving collisions, thereby losing a fraction of their relative normal velocity during the collision (and therefore losing energy). The ratio of the (relative) velocity in the normal direction before $\vec{v}_n$ and after $\vec{v}_n'$ the collision is the normal restitution coefficient, ε_n [3, 4, 5, 6]:

$$\vec{v}_n' = -\varepsilon_n \vec{v}_n \qquad (0 \le \varepsilon_n \le 1) \qquad (2)$$

A fully elastic collision, without any energy dissipation, is represented by $\varepsilon_n = 1$, whereas a fully plastic collision is represented by $\varepsilon_n = 0$. Physically, the loss of kinetic energy in the normal direction will cause the ball to bounce back at a lower angle α' (Figure 2).

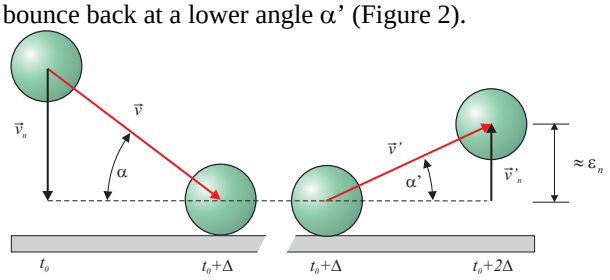

Figure 2: The loss of kinetic energy in normal direction causes the ball to bounce back in a lower angle.

The collision response of two balls with the same mass can be calculated using equation (3). Here, $\vec{e}$ is the unit vector through the balls' centres during the collision. The normal velocity component $\vec{v}_n$ in equation (3) is calculated by $(\vec{v}_{rel}\ \vec{e})\ \vec{e}$

$$\vec{v}' = \vec{v} \pm \frac{1}{2}(\varepsilon_n + 1)(\vec{v}_{rel}\ \vec{e})\ \vec{e} \qquad (3)$$

SIMULATOR VERIFICATION

The accuracy of the numerical calculations in general, and the validity of the molecular dynamic model in particular, can be conveniently checked by performing a molecular dynamic simulation of an ideal gas with the simulation program. For a system of elastic hard spheres, abbreviated below as "ideal gas", the molecules are modelled as hard spheres undergoing fully elastic collisions. In the absence of gravity, only kinetic energy is present, and the sum of all kinetic energies must be constant over time. Any deviation from this constant value must be caused by numerical or algorithmic errors.

In the experiment, *n* = 4000 balls are homogeneously positioned in a cylinder. The initial direction of each velocity vector is equally distributed in space, but every ball has the same initial absolute velocity. Every 0.03 seconds, the *n* absolute velocities and the *n(n-1)/2* relative velocities are measured. Furthermore, the

normal components (important for the milling process) of the velocity of the *m* collisions during the time interval are measured. In theory, the empirical distribution of the absolute and relative velocity of the balls should perfectly fit a Maxwell distribution. The empirical distribution of the normal components should fit a Rayleigh distribution [6]. In [7] similar distributions have been computed for the generalized case of non-Maxwellian distributions.
As an example, the histogram of the normal components during 0.06 and 0.09 seconds of simulated time is shown in Figure 3. Additionally, the theoretical Rayleigh distribution and the corresponding Maxwell distribution are shown for comparison.

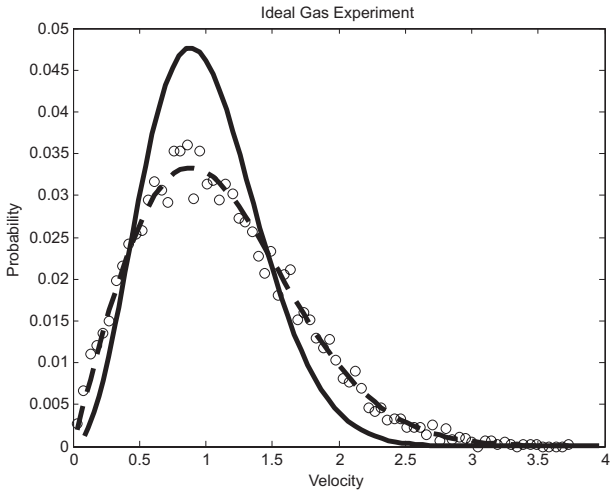

Figure 3: Circles: Measured normal component of the collision velocity between 0.06s and 0.09s. Line: Maxwell probability distribution. Dashed Line: Rayleigh probability distribution

All samples created by the various experiments repeatedly passed a chi square test with a probability of 0.9. Furthermore, it could be measured that the balls' positions are equally distributed per volume element, and that each velocity component has a normal distribution, which further proves the ideal gas behavior and the correctness of this simulation algorithm.
For visual observations, the ball's positions have been rendered using POWRAY 3.6 (Figure 4, right). The velocities are color coded. This visual aid turned out to be a powerful tool for code debugging because an irregular ball behavior (as e.g. incontinency) immediately becomes visible.
Furthermore the videos of the simulations and the videos of the high speed video camera have been combined. It is possible to compare both and to verify the quality of the simulation results (Figure 4).
The computing time for 1 second real time is about 6 minutes on a standard computer (2 GHz CPU).

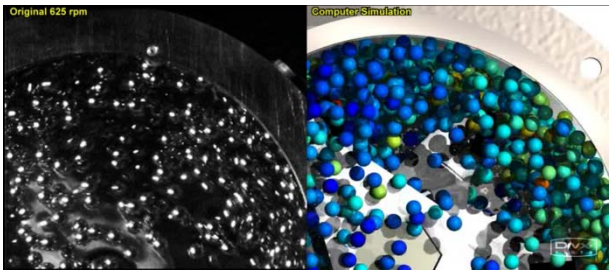

Figure 4: Snapshot of a rendered video (right) and the high speed video (left). The velocity of the balls is color coded (right).

OPTIMIZATION OF THE GRINDING CHAMBER

A statistical analysis of the collisions in space has shown that most collisions (> 50%) take place at the border of the grinding chamber (Figure 5, left). But the collisions with the highest energy transfer take place in the domain of the rotor blades (Figure 5, right). The maximum of the velocity distribution is equal to the velocity of a ball which falls from a height of 1.5 mm to the ground. I other words: Efficient collisions take place very rarely.

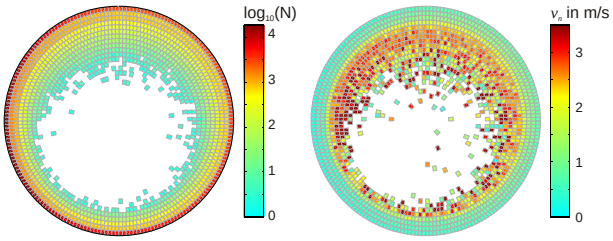

Figure 5: Axial cut. Left: Color coded number of collisions. Right: Color coded collision velocity.

Mathematical Model of the improved shape

Based on the knowledge of the grinding media motion inside the grinding chamber, three patents have been filed. The basic concept is to move the balls away from their circular path. One idea is to add concave parts inside the grinding chamber, e.g. a wavy shape.
These buckles have two parameters, namely the number of the buckles *n* and the height of the buckles *h*.
The wavy shape is assembled by alternating convex and concave parts of circles (Figure 6, green and blue circles). The bending of the curve switches at the contact point of the circles. The height *h* is the alternating minimal and maximal distance relative to the original circle – Figure 6, red line.
Depending on the position of the midpoint of a circle, a ball collides with its inner or outer surface. If the midpoint of a circle is located outside of the original shape (Figure 6, green circles), the ball will collide its outside. If the midpoint of a circle is located inside of the original shape (Figure 6, blue circles), then the ball will collide inside.

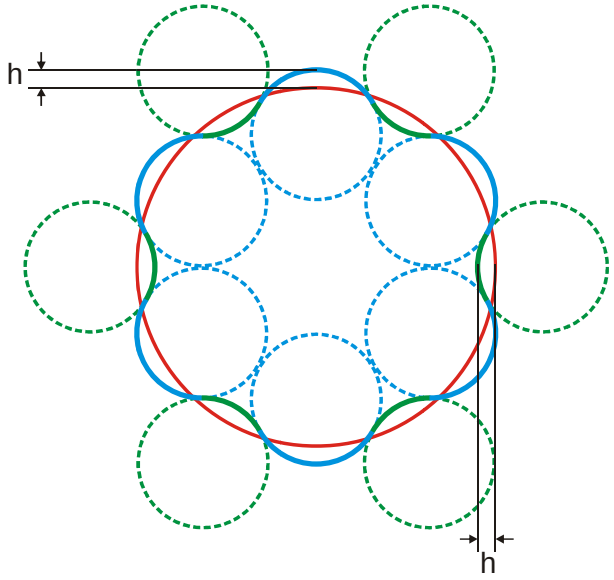

Figure 6: Model for the wavy shape. Red line: Original shape: Green circles for the concave parts. Blue circles for the convex parts.

Parameter variations

The aim of the optimization is to maximize the collision velocity in normal direction. Beside the shape should be producible and the parameters should be chosen with respect to the expected abrasion during the milling process.
The number of buckles has been varied between 2 and 20 (step size 1) and the height of the buckles has been varied from 0 mm to 10 mm (step size 0.01 mm).
Figure 7 shows a contour plot of the median of the collision velocity in normal direction. The surface has one single stable flat maximum. Obviously the original grinding chamber (height of buckles = 0 mm) is the global minimum. Any change of the shape of the grinding chamber improves the efficiency of the high energy ball mill.

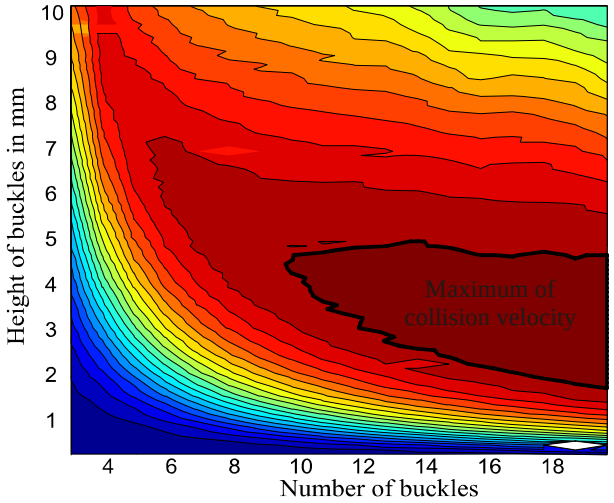

Figure 7: Contour plot of the optimization. The region of the maximum collision velocity is flat and stable.

CONCLUSIONS

A new simulation approach for the simulation of high energy ball mills has been presented, namely, the discrete event simulation. The basic concept of this approach has been pointed out. Improvements in the collision detection algorithm have been derived and the collision response routines have been explained, too. The statistical analysis of the time space coordinates of the collisions has shown the disadvantage of the traditional design of the mill.
The concept of a wavy grinding chamber has been explained and its mathematical representation has been derived. Several parameter variations of the design have been performed to choose the optimal design.

REFERENCES

[1] Reichardt, R.; Wiechert, W.: Simulating High Energy Ball Mills using Discrete Events, Simulation News Europe, Issue 38/39, December 2003, pp. 3-9
[2] J. Dahl, M. Chetlur, .P.A. Wilsey: Event List Management In Distributed Simulation, European Parallel Computing Conference (Euro-Par '01), August 2001.
[3] Kuwabara and Kono, Jpn. J. Appl. Phys. 26, 1987, p. 1230
[4] Pöschel, T. and Schwager, T., Computational Granular Dynamics, Springer, Berlin, 2005
[5] Brilliantov, N.V.; and Pöschel, Th.: Kinetic Theory of Granular Gases, Oxford Univerity Press, 2004, pp. 21-35.
[6] Reichardt, R.: Ereignisdiskrete Simulation einer Hochenergie-Kugelmühle, Dissertation, 2005, urn:nbn:de:hbz:467-1914
[7] I. Pagonabarraga, E. Trizac, P. C. van Noije and M. H. Ernst: Randomly driven granular fluids: Collisional statistics and short scale structure, Phys. Rev. E 65, 011303 (2002)

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ROLAND REICHARDT studied mechanical engineering at the University of Siegen, Germany. He worked from 1997 to 2001 for a mechanical process engineering company of ball mills in the company management. In 2002, he returned to the University of Siegen and obtained his doctoral degree in 2005. Since 2006, he is additionally lecturer at the Niederrhein University of Applied Sciences.

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