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Back-calculation of mechanical parameters of shell and balls materials from DEM simulations

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Abstract
Discrete Element Method (DEM) is extensively used for mathematical modeling and simulation of behavior of discrete discs and discrete spheres in two and three dimensional space, respectively. Prediction of particles flow regime, power draw and kinetic energy for a laboratory or an industrial mill is possible by DEM simulation. In this article, a new approach was used to assess the main parameters of a transparent ball mill constructed in mineral processing laboratory of University of Tehran. The mill shell and crushing balls are made of Plexiglas® and compressed glass, respectively. The true values of mechanical parameters for these materials, required for DEM modeling, were unknown. The authors back-calculated the best values of mechanical properties of Plexiglas and compressed glass materials based on a large number of DEM simulations. Back-calculation procedure was mainly based on the comparison between electrical power draw measured in real mill and mechanical power draw calculated by DEM model while trying to accurately simulate particle flow regime inside the real mill. The results showed that the optimal number and design of lifters can be adequately determined by improving torque and kinetic energy in crushing elements through DEM simulation trials based on the back-calculated mechanical parameters.

Keywords: *DEM model calibration, lifter design optimization, modeling and simulation, DEM simulation validation*.

1. Introduction

In mineral processing plants, tumbling mills of various kinds are used for size reduction. This process consumes energy in high levels [1]. For economical matters, experts in the field focus more on modeling of tumbling mills in a short period of time and approaching to most optimized mill with extensive level of utilization. For this reason, almost from twenty years ago, discrete element method (DEM) has been used as a practical modeling method of industrial equipment. DEM models the behavior of assemblies of disks and balls realistically [2].
For the first time, two dimensional numerical methods were used for improving the deficiency of ball mills during 1990’s [3]. After that, discrete element method was used extensively in modeling of ball and AG/SAG mills. Also, this method was used adequately in prediction of charge motion, power draw and segregation in ball mills [4]. Furthermore, other investigations such as comparison between numerical modeling and experimental measurements in a pilot SAG mill were done in recent years [5].
Optimization of the power draw has a drastic effect on the overall economic performance and environmental effect of a mineral processing plant [6]. In past decades, DEM has been established as a useful and powerful tool in simulation and

optimization of various kinds of mills at laboratory or industrial scales. In many cases, power draw has been calculated as one of the inferences that can be made by DEM simulation. In this research, the authors have used mill power draw in experimental and numerical studies for a new purpose, i.e., back-calculation of materials mechanical properties. The numerical simulations was performed using PFC3D (Particle Flow Code in 3 Dimensions) software.

In geotechnical engineering, researchers define many parameters for various kinds of materials to explain the behavior of materials and having tangible explanations for many different responses of materials against natural effects. Values of parameters such as normal and shear stiffnesses, cohesion, Young modules, Poisson's ratio, frictional angle and coefficient are necessary for the physical equations that are used in DEM numerical modeling. Therefore, to achieve adequate correspondence between reality and numerical modeling, these parameters should be defined accurately in numerical equations. In laboratory or industrial cases, when there is no geotechnical laboratory equipment for measuring the values of parameters, or in cases where laboratory tests are either inaccurate or uneconomical, a back-calculation method based on comparison between net power draws to assess the best estimates of materials' parameters can be used as describe by authors. The details of the back-calculation method are presented in this paper.

A transparent ball mill was built at mineral processing laboratory of University of Tehran which can be used to demonstrate the movement regime of crushing elements inside the mill. The shell of the tumbling mill is Plexiglas® with 5 mm thickness and its inner wall is protected by diaphanous plastic liner with 2 mm thickness. Also, the lifters have been made of diaphanous plastic. The mill is filled with balls made of compressed glass as crushing elements. As there was no available information about the values of mechanical parameters for Plexiglas, plastic liner and compressed glass, DEM model calibration was done to obtain the optimal values of the required parameters. This was performed by comparisons made between observed and predicted values of parameters. Balls movement regimes and net power draws are criteria for this comparison. Electrical net power draws in experimental cases and mechanical net power draws in numerical simulations have been compared. The optimal values of parameters will be found when an adequate agreement between experimental observations and numerical predictions is achieved. On the other hand, the shape and conFigure uration of the lifters are considered as important design parameters which affect mill load behavior, the amount of power draw, kinetic energy and consequently the efficiency of grinding. In this study, the shape and conFigure uration of lifters are considered as design search variables for mill performance optimization.

2. Transparent laboratory ball mill

The main purpose of constructing a transparent ball mill was to make it possible to view the charge motion inside the mill and capturing necessary images by a high-resolution camera. The properties of the transparent mill are as follows in Table 1.

Table 1. Mill specifications

Property	Value
Mill diameter (cm)	25
Mill length (cm)	30
Effective mill length (cm)	20
Diameter of small balls (cm)	1.6
Diameter of big balls (cm)	2.5
Number of small balls	500
Number of big balls	90

The properties are also shown in Figure 1. The mill filling is equal to 18% of mill's total volume.

Figure 1. A view of the transparent ball mill with main geometrical dimensions.

There are some unknown mechanical properties such as the normal and shear stiffness of mill's shell and balls (K_{nwall}, K_{swall}, K_{nball} and K_{sball}) and also the friction coefficient (μ) of shell and balls which are needed in order to apply DEM simulations.

3. DEM model calibration

In discrete element method, assembly of discs in two dimensional or balls in three dimensional modeling are influenced by stresses. Therefore, displacements and contact forces are found through a series of calculations. These calculations trace the movements of the individual particles [2]. To perform these calculations, some physical parameters for mill shell and balls are necessary. Normal stiffness (K_n), shear stiffness (K_s) and friction coefficient (μ) for mill shell and balls should be used in numerical modeling.

During preliminary laboratory work, the mill was put in rotation with just one ball (large or small).The rotational speed was set to 71 rpm. All experimental conditions in laboratory; such as mill and its charge specifications and rotational speed were used to set variables in numerical modeling. In DEM modeling procedure, unknown values of mechanical properties are some of the main sources of discrepancies between observed measurements and simulation predictions. To back-calculate the mechanical parameters, the initial values of stiffness and frictional coefficients for Plexiglas and glass were considered the same as the values of these parameters published in rock mechanics literature. In this part, the visual results from numerical modeling are qualitatively compared with images that were taken from the rotating transparent ball mill. Changing mentioned parameters in numerical modeling and simultaneously comparison between experimental and numerical visual results, made it possible to approach to the proper properties. It should be mentioned that only comparison between images is not a suitable approach for achieving the best parameters for DEM modeling. Comparison between measured power draw in laboratory and numerical modeling helped in approaching to the best values for mechanical properties.

The best approximate values of normal and shear stiffness and frictional coefficient for making proper agreement between experimental and numerical modeling are displayed in Table 2

Comparing measured and predicted net power draws from experimental and DEM modeling is elaborated in this section. If an acceptable correlation exists, then a calibration coefficient can be assessed by a linear regression between measured and predicted net power draw.

Table 2. Initial values of mechanical properties for various parts of the mill

	Mechanical Properties		
	K_n (N/m)	K_s (N/m)	μ
Wall	400000	400000	0.85
Lids of Mill	400000	400000	0.85
Lifters	1500	1500	0.85
Big ball	600000	8000000	0.25
Small ball	600000	8000000	0.45

In laboratory work and DEM modeling, seven mill conFigure urations were considered as basic designs for assessing calibration coefficient. These conFigure urations are presented in Table 3. The net power draw was measured by a highly sensitive wattmeter that was connected in series with the mill electrical circuit. Therefore, the first row of Table 3 demonstrates electrical net power draws that have measured during laboratory work**.**

In the present numerical modeling, mechanical net power draw was calculated and compared with the electrical net power draw. The calculations of net power draw in numerical modeling are as follows:

$$W_{\mathrm{net\,(new)}} = W_{\mathrm{net\,(old)}} - \sum_{N_w} F_i \Delta U_i + M_i \Delta\theta_i \qquad (1)$$

where N_w is the number of walls, F_i and M_i are the resultant force and moment acting on the wall at the start of the current time step; and ΔU_i and $\Delta\theta_i$ are the applied displacement and rotation occurring during the current time step. It should be noted that this is an approximation as it assumes that F_i and M_i remain constant throughout the time step [7].Total cumulative work, W, is the work done by all walls on the crushing elements which can be calculated by Eq. (2):

$$\mathrm{W} = \frac{\Delta \mathrm{W}}{\Delta \mathrm{t}} \qquad (2)$$

The net power draw calculated based on Eqs. 1 and 2 have been presented in second row of Table 3. To fit the mechanical parameters, their values were changed until an acceptable agreement between experimental and numerical net power draws is achieved. The final parameters that were considered for DEM modeling are presented in Table 4.

In addition to checking closeness of net power draws, the real power draw measured by Wattmeter in laboratory experiments and predicted power draw calculated by using Eq. 2 (work and torque at a specified Δt) based on presented parameters in Table 4, were compared. The visual validation of DEM modeling has been illustrated in Figure 2.

By comparing (1) between photographs from laboratory rotating mill and prepared snap-shots in DEM simulation; and (2) between net power draws in experimental and numerical modeling that are presented in the Table 3, a calibration diagram to find an acceptable relationship between numerical and experimental results of net power draw has been demonstrated in Fig. 3. A correlation was found between measured and predicted net power draws of the mill with a linear regression coefficient equal to 0.442 with an R-squared value equal to 0.764 (the linear relationship can be seen in Fig. 3 with solid line). It is evident that one data point corresponding to DEM simulation No. 6 is off-the-curve. For this reason, the authors repeated the same simulation with no change in result. Therefore, the data point was included for calibration purpose. However, if this point is removed, while there is a little change in linear regression coefficient, the R-squared value increases to 0.900. The linear regression equation will be used in next step, to optimize mill performance by considering three criteria: ball mill net power draw, kinetic energy of crushing elements and movement regime of balls.

Table 3. Seven experimental setups to assess calibration coefficient of DEM model

Mill Property	**Mill Setups**						
	No Lifter-Big Balls	No Lifter-Small Balls	No Lifter-Big & Small Balls	2 Lifters (6 mm)- Big & Small Balls	4 Lifters (6 mm)- Big Balls	4 Lifters (6 mm)- Small Balls	4 Lifters (6 mm)- Big & Small Balls
Measured net power draw, Experimental (W)	5.000	10.000	15.000	17.500	10.000	15.000	25.000
Predicted net power draw, Numerical (W)	4.846	15.446	22.780	39.323	14.198	48.285	53.392

Table 4. Optimal mechanical parameters obtained for DEM simulations

	Mechanical Properties		
	K_n (N/m)	K_s (N/m)	μ
Wall	400000	400000	0.85
Lids of Mill	400000	400000	0.85
Lifters	1500	1500	0.85
Big ball	600000	8000000	0.25
Small ball	600000	8000000	0.45

4. Lifter profile optimization

DEM simulations with the best back-calculated values of parameters (Table 4) were carried out to find the optimal mill design.

At first, the number and height of lifters were changed. Three conFigure urations were considered based on the number of lifters: 4, 6 and 8. In all conFigure urations, the width of lifters was the same and equal to 2 cm and the length of lifters were exactly equal to effective length of the mill. The height of lifters was: 4, 6 and 8 mm. Figure 4 demonstrates changes in net power draw and kinetic energy by using various combinations of number and height of the lifters.

In Figure 4, average net power draws were calculated using Eqs.1 and 2 multiplied by calibration coefficient. As it is evident, the net power draw varies by changing the number of lifter used. This result is confirmed with the findings of other researchers, [6]. When the number of lifters increases, the power draw increases from a non-zero value to a constant value. After a specified number of lifters, a further increase has no effect on net power draw of the mill.

On the other hand, by increasing the height of lifters, net power draws will increase too. This result could be different by changing the rotational speed of the mill [6].

The second row of each table in Figure 4 illustrates average kinetic energy during steady state of rotating mill. The average kinetic energy has been calculated by Eq. 3 as follows:

$$K = \frac{1}{2}\sum_{N_{\mathrm{p}}}\sum_{i=1}^{6} M_i V_i^2 \quad (3)$$

where K is the total kinetic energy of all particles accounting for both translational and rotational motions. In Eq.3, kinetic energy is expressed in terms of the generalized mass and velocity of each of the N_{P} particles. Generalized mass and velocity are described as follow equations:

$$F_i + F_i^d = M_i A_i \; ; i = 1, \dots, 6 \quad (4)$$

$$M_i A_i = \begin{cases} m\ddot{x}_i & \text{for } i = 1, \dots, 3 \\ I\dot{\omega}_{(i-3)} & \text{for } i = 4, \dots, 6 \end{cases} \quad (5)$$

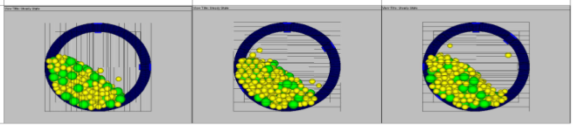
where F_i, M_i and A_i are the generalized force, mass and acceleration components, respectively and F_i^{d} is known as damping force. Generalized mass in three directions of x, y and z and in two forms of linear and angular accelerations are calculated using Eqs. 4 and 5. These data are used in Eq.3 to calculate average kinetic energy. Also, generalized velocity in Eq.3 can be calculated using Eq. 6:

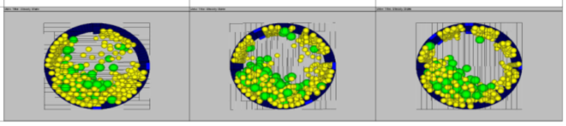
$$V_i = \begin{cases} \dot{x}_i & \text{for } i = 1, \dots, 3 \\ \omega_{(i-3)} & \text{for } i = 4, \dots, 6 \end{cases} \quad (6)$$

As it is observed, in all mill setups, by increasing either number or height of lifters; net power draw will increase which in turn causes a significant increase in average kinetic energy.

In optimization studies, conventional opinion is focused on obtaining maximum kinetic energy at contact between particles or crushing elements. Accordingly, considering the increasing trend in Figure 4, the mill with 6 or 8 lifters of 8 millimeter height might be selected as the most optimized setup. However, considering the corresponding balls movement regimes as can be seen in third rows of tables in Figure 4, the choice of optimized mill setup will be different. In this case, a mill setup with a medium net power draw and a high kinetic energy is considered as optimal. Figure 5 shows a large view of the mill setup including 8 lifters with 8 mm height to explain why this mill setup is not the optimal one. The best balls movement regime has been defined when balls are lifted under applying force and torque, approaching to zero degree position of mill and release from top of the mill by using gravity force to 180 degree position of the mill. The mentioned movement regime is satisfying for cataracting of balls and extensive contacts instead of abrasion between particles. Yang et al. [8] referred to six movement regimes in a rotating mill, including slipping, slumping, rolling, cascading, and cataracting and centrifuging regimes depending on operational condition. As it can be seen in Figure 5, most of balls are lifted from the base position and are returned to the base without significant contacts between balls or balls-walls. In this case, net power draw is high but does not have a satisfactory effect on making contacts and great kinetic energy. The reason why the power is drawn ineffectively can be explained by the fact that most of the work and torque is wasted for returning balls (right side of the mill) from top of the mill to the base position, without using gravity force instead. Subsequently, kinetic energy will be wasted during small contacts and abrasion between balls.

Therefore, an innovative geometrical design for lifters was devised (Figure 6) to obtain an acceptable net power draw, a high level of kinetic energy and a desirable balls movement regime for the rotating mill at steady state. Hence, to solve the problem of right side of the mill, lifters with a combination of quadratic cubic shapes as the base positions and two tilted parts in the shape of pyramid laid down on the base position, were designed.

Kind Of Mills / Mills Property	4 lifters;4mm	6 lifters;4mm	8 lifters;4mm
Ave Net Power Draw (W)	15.87	18.20	19.61
Ave Kinetic Energy (J)	0.054	0.066	0.072
Example for Mill Regime in Steady State			

Kind Of Mills / Mills Property	4 lifters;8mm	6 lifters;8mm	8 lifters;8mm
Ave Net Power Draw (W)	42.15	42.74	42.35
Ave Kinetic Energy (J)	0.71	0.80	0.78
Example for Mill Regime in Steady State			

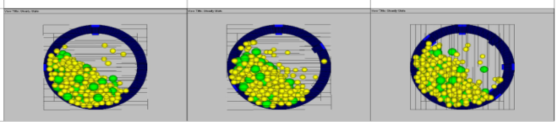
Kind Of Mills / Mills Property	4 lifters;6mm	6 lifters;6mm	8 lifters;6mm
Ave Net Power Draw (W)	23.60	28.00	30.94
Ave Kinetic Energy (J)	0.13	0.16	0.20
Example for Mill Regime in Steady State			

Figure 4. Changes in net power draw and kinetic energy due to changing number and height of the lifters

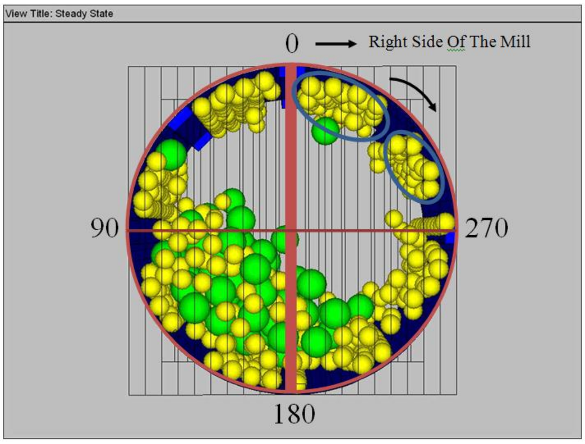


Figure 5. An example for balls movement regime in the mill including 8 lifters with 8 mm height

Therefore, an innovative geometrical design for lifters was devised (Figure 6) to obtain an acceptable net power draw, a high level of kinetic energy and a desirable balls movement regime for the rotating mill at steady state. Hence, to solve the problem of right side of the mill, lifters with a combination of quadratic cubic shapes as the base positions and two tilted parts in the shape of pyramid laid down on the base position, were designed.

In this study, as it is shown in Figure 6 (A), the total height of lifter is 8 mm; but, lifters have two parts: base part with 4 mm height and two tilted parts with 4 mm height. This approach has been applied on mill with lifters which have 12 mm height. If lifters with 12 mm height used as conventional, a high net power draw would be consumed for returning particles in the right side of the mill without using gravity effect. In mentioned approach, as it is displayed in Figure 6

(B), the half height of lifter has been designed in tilted forms.
The advantage of this approach has been demonstrated in Figure 7 and the results of this approach that has been applied on laboratory mill are shown in Figure 8.
As it can be observed in Figure 7, in rolling action, crushing elements are lifted from base position and approaches to the zero degree position in the left side of the mill, and then particles will roll on tilted parts and by using gravity effect fall on the based walls or balls. In this procedure, force and torque have been only produced for lifting particles in the mill.

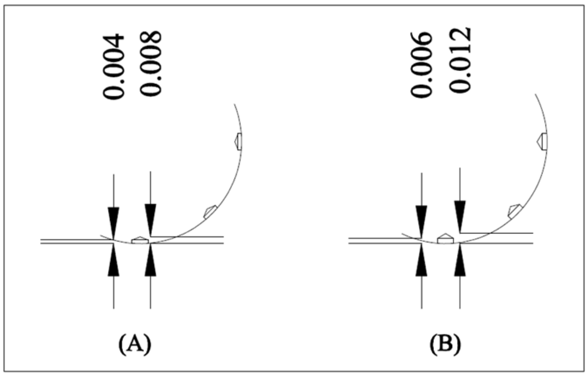


Figure 6. (A) Combination of lifters with 4 and 8 m height; (B) Combination of lifters with 6 and 12 mm height

Therefore, a medium net power draw and kinetic energy has been consumed during rolling action.
Figure 8 clarifies the advantages of using this sort of lifter geometry in a milling system. For example, in Figure 8 a mill setup with 8 lifters which have 8 mm height (height of cubic part= 4 mm and height of tilted parts= 4 mm) consumes a power equal to 23.60 W, this value is between net power draws of mills with 8 lifters which have 4 mm (19.61 W) and 8 mm (42.35 W) height. Therefore, this approach makes medium value of net power draw, kinetic energy and most important part of using this sort of lifter is acceptable balls flow regime in the mill.
Consequently, the optimal setup for the explained laboratory mill is the one with 8 lifters and 12 mm lifter's height (the base with 6 mm height and the two tilted parts in the shape of pyramid with 6 mm height). The mill with optimal setup consumes a power equal to 32.28 W as net power draw and produces a kinetic energy equal to 0.26 J. It should be mentioned that most of the kinetic energy is produced from big and significant contacts.

5. Conclusions

The following conclusions can be derived from DEM modeling and simulations:

- The unknown mechanical parameters required for DEM-based simulation and optimization can be back-calculated by qualitative comparison.
- To obtain the best estimates of mechanical parameters, values given for the same or similar materials in rock mechanics' tables can be considered as default and initial guesses to start search process. The best estimates of parameters can be found by changing default parameters, until approaching an acceptable agreement between experimental and numerical modeling for both net power draws and balls flow regimes in the mill.

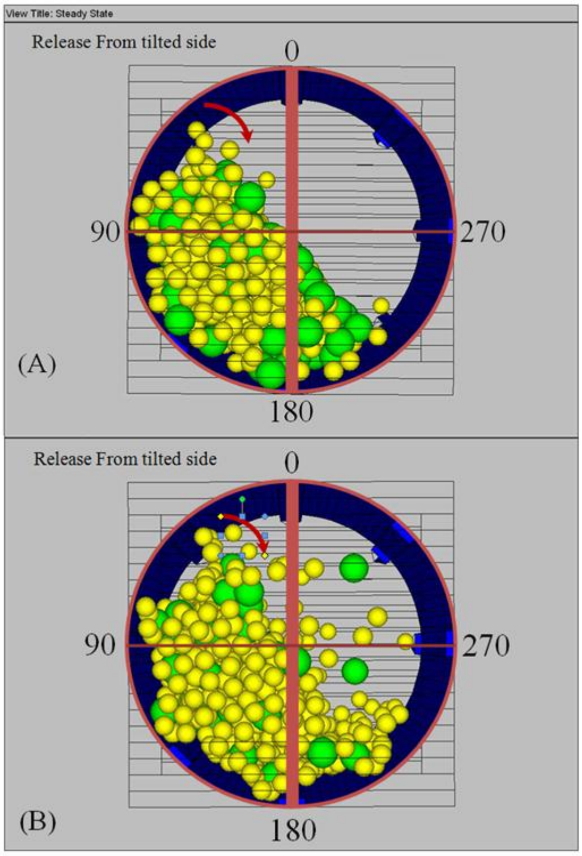
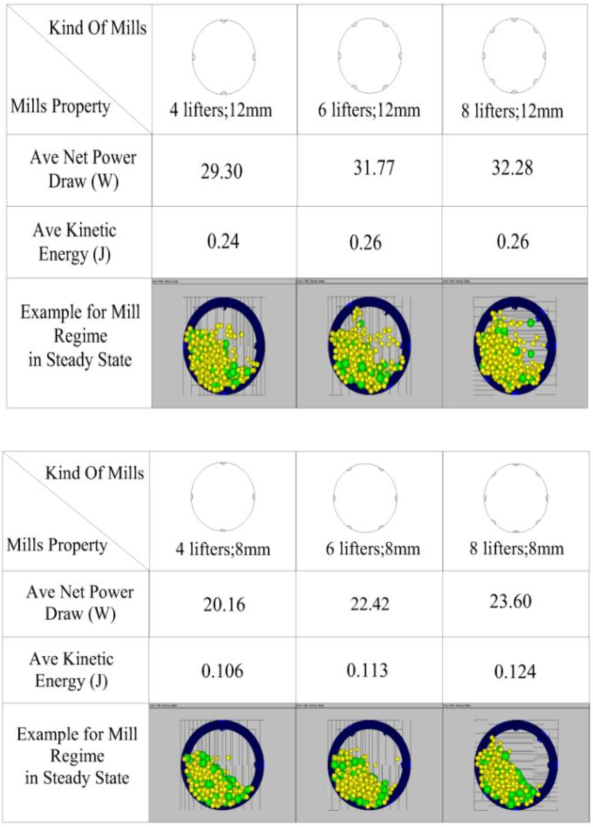


Figure 7. (A) Cascading flow in mill with 8 lifters which have 8 mm height; (B) Cataracting flow in mill with 8 lifters which have 12 mm height.

- Determination of calibration coefficient for DEM model can be done by modeling of mill at various conFigure urations using the best estimates of mechanical parameters.
- DEM simulations showed that by increasing the number of lifters and their height, net power draw and kinetic energy will be increased.

- The net power draw of a mill and consumed kinetic energy are not sufficient as optimization criteria, balls movement regime must also be considered as an important criterion in mill optimization studies.
- New lifter designs were devised based on considering all three criteria including net power draw, kinetic energy and balls movement regime to optimize the mill performance.



Kind Of Mills / Mills Property	4 lifters;12mm	6 lifters;12mm	8 lifters;12mm
Ave Net Power Draw (W)	29.30	31.77	32.28
Ave Kinetic Energy (J)	0.24	0.26	0.26
Example for Mill Regime in Steady State			

Kind Of Mills / Mills Property	4 lifters;8mm	6 lifters;8mm	8 lifters;8mm
Ave Net Power Draw (W)	20.16	22.42	23.60
Ave Kinetic Energy (J)	0.106	0.113	0.124
Example for Mill Regime in Steady State			

Figure 8. Net power draw, kinetic energy and visual results in mills with quadratic cubic base and two tilted parts

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