CHAPTER 6  SIMULATION WORK

6.1  Introduction

The simulation work involved three major tasks; firstly, to adapt the general purpose Particle Flow Code (PFC) from Itasca (1993) to produce a mill simulator, secondly, to establish suitable parameters for the simulator and thirdly, to do simulations corresponding to milling experiments discussed in the previous chapter.

6.2  Design of the mill simulator

6.2.1  Introduction to the PFC Software

The development of efficient DEM code as discussed in the literature review is a considerable task that requires long man-hours to do. Itasca developed the PFC software that can be adapted to model many industrial applications with less programming effort. An indication of the versatility of this package can be seen from the number of papers presented at the 1st symposium on PFC (2002).

The program is controlled by commands that can be typed at the command line or by using its Fish programming language to write structured code with functions, using any text editor. The program script is saved with the extension “Dat” in the same folder as the PFC program. To run the program, the command “call” is typed followed by the script name. All the functions and variables are loaded and compiled before running. It is possible to load many scripts in one session as long as these are not conflicting. For example, it is possible to run one script and then load the next to use the data generated by the previous script.
6.3 Development of the PFC based mill program

It was decided to use two scripts for mill simulations, a variable script that would be generated according to user input and a permanent script to read the data from the variable script and perform the simulation accordingly.

6.3.1 The Variable Script

A windows Graphical User Interface (GUI) program was developed to allow users to draw the mill internal geometry and specify the number of balls of various sizes. Other required inputs are listed below. Once the data has been entered the file is saved using the name specified by the user.

List of Parameters specified by user:

- ball and wall property parameters
  - Ball and wall stiffness in both the normal and shear direction
  - Ball and wall coefficient of restitution
  - Ball and wall coefficient of friction

- Simulation parameters
  - Mill speed
  - Number of revolutions before any data sampling is effected
  - Number of data sampling revolutions
  - Total number of frames to be collected for visualisation of the simulation
  - Scale for classifying the energy spectra
6.3.2 The mill Simulator (permanent script)

When the variable script is loaded, it automatically loads the mill simulator. The mill simulator performs a series of procedures that are best summarised by the chart shown below.

![Chart showing sequence of tasks](image)

1. Variable script file loaded.
3. Data arrays created.
4. Time step calculated, and simulation steps and intervals for sampling particular events calculated.
5. Particles generated and allowed to settle before mill starts to rotate.
6. Mill rotates without any data sampling for revolutions specified by user.
7. Mill rotates for specified number of revolutions while data is sampled.
8. Simulation ends and the requested reports are generated.

Figure 6-1 Sequence of tasks accomplished by the simulation program
A few comments are in order to clarify the figure.

6.3.2.1 Array creation (3)
The purpose of this procedure is to allocate adequate data storage space for anticipated events. For the purpose of this research work, the arrays focused on capturing energy conversions at the points of contact between the various interacting elements. The consequence of this procedure was memory expense, thus the data structure which is beyond the scope of this discussion was given due attention to optimise memory usage.

6.3.2.2 Time step calculation(4)
The simulation time step was chosen to ensure that any contact event involved at least twenty time steps. The maximum time steps that can be used without creating unstable simulation can be derived by treating the interacting elements as having springs at points of contact. The maximum time step that can be tolerated when using numerical integration is given by the equation below (Blithe and Wilson 1976):

\[ \delta t = 2\pi \sqrt{\frac{m}{K}} \]  

(6.1)

where \( \delta t \) is the time step, \( m \) and \( K \) are the mass and stiffness of the particle respectively.

To get more accurate integration of the energy during contact this number is further divided by some constant. For all the simulations discussed later, the time step used was calculated using the equation below.

\[ \delta t = 0.1 \sqrt{\frac{m}{K}} \]  

(6.2)

where \( m \) is the mass of the lightest particle in the simulation.
6.3.2.3 Simulation and interval sampling steps (4)
The cycles (time steps) required for the simulation are calculated by dividing the real time represented by the mill revolutions with the calculated time step. The number of cycles for sampling intervals of some of the data items such as power, particle position frames etc. were also calculated by dividing their real time intervals with the simulation time step.

6.3.2.4 Particle generation (5)
In the experimental mill, all the particles are initially settled at the bottom at the beginning of each run. For the simulator, the balls were generated in a box bound space within the mill and allowed to settle by gravity. Settling was accelerated by initially using lower stiffness before gradually raising it to the normal value.

6.3.2.5 Simulation without any data sampling (6)
It takes four to six revolutions for the mill to reach steady state (see Appendix I); it was thus decided to omit data sampling for the first four revolutions of the simulations. In Figures I2 and I3 (Appendix I), it is seen from the power behaviour that no two revolutions are identical even after stabilisation and thus time permitting, a high number of sampling revolutions is recommended.

6.3.2.6 Simulation with sampling (7)
All the required information is collected during this period. The process involves searching for all the existing inter-element contacts at every time step and carrying out required computations as shown in the chart below and thus at this stage the simulation becomes 2 to 8 times slower.
Figure 6-2 The Simulator routine computation scheme

Most of the tasks in the chart are straightforward and only the tasks requiring clarification are discussed. The emphasis is on calculations performed at every time step on each existing contact.
6.4 The simulation computational scheme

6.4.1 Overlap calculation

The calculation of overlap ($\Delta$) between Ball-Ball and Ball-Wall elements has already been discussed in Chapter 2.

6.4.2 Strain energy

From the contact forces given by PFC, the strain energy absorbed by a particle at time interval $i$ is calculated by numerical integration as follows:

$$E_i = \frac{1}{2} (F_i + F_{i-1})(\Delta_i - \Delta_{i-1})$$  \hspace{1cm} (6.3)

where $E$ is the energy, $F$ is the force and $\Delta$ is the overlap distance between the contacting elements. Further compounding issues are discussed in Appendix J. The energy is continuously accumulated each time overlap increases and only when it does. The maximum strain energy attained at the end of the contact event is recorded and classified in accordance with its energy level. A spectral distribution of energy such as shown in Figure 6.14 is thus obtained for the sampled simulation interval.

6.4.3 Dissipation energy

The energy dissipated at a contact at time step $i$ is calculated using the equation below (Itasca 1993)

$$E_i = \frac{2D(\Delta_i - \Delta_{i-1})}{\delta t} \sqrt{Km}$$  \hspace{1cm} (6.4)

where $D$ is the damping ratio and the other terms are as discussed before. The energy is continuously accumulated till the end of the contact event. A similar energy level spectrum as that obtained for strain energy is also obtained for energy dissipated in each contact event and similarly recorded at the end of the simulation.
To improve the computational accuracy care had to be taken both at the beginning and at end of a contact to compensate for the uncertainty in the exact times when contact ended or began as illustrated in the figure below.

![Figure 6-3 Analysis of issues that may affect calculation of Contact relative velocity when using data from PFC](image)

6.4.4 Frictional energy

The frictional energy loss at a contact point for the current time step is available directly from the PFC program (Equation 2.21) and is simply accumulated until the end of a contact event. The energy is classified as discussed above to produce the corresponding friction energy spectra.

6.4.5 Sampling of data items

The mill simulator allows the user to decide what information to collect, though caution should be exercised as excessive information slows down the simulation. For the purpose of this research, other than the standard spectral energy data discussed above, there was a need to capture frames of ball positions for post-
simulation animation. From these frames it was also possible to plot the different positions occupied by each ball during the sampled period of the simulation. These plots are referred to as the Position Density Plots (PDPs).

The instantaneous input power was continuously calculated using the torque due to the balls directly in contact with the mill wall. At the end of each time period representing 1 second, the average input power was recorded along with the energy dissipated in the same period (higher time resolutions can also be set). The discrepancy between the two totals at the end, with net energy of the system taken into account, never exceeded 4% in all the simulations except for one involving large 126mm spheres and 8mm spheres.

### 6.4.6 Simulation report

At the end of each simulation a report is generated and a sample of these reports is given in Appendix H. Other reports such as a log of forces acting on lifters can also be generated when requested at the beginning of a simulation.

### 6.5 Discussion of criteria for choice of contact models and parameters

The need to be as close as possible to reality and the need to minimize computation demand were the two conflicting factors that affected the choice of parameters and the models.

#### 6.5.1 The spring and dashpot model

The dynamic movement of particles was described by classical Newtonian equations discussed in Chapter 2, while the collision contact between elements was modelled using a simple linear spring-dashpot model (also discussed in Chapter 2) to minimise computation expense.
The disadvantage of this model is, as a direct consequence of the equation (see Equation 2.20), the model always produces a large instantaneous force at the beginning and a negative force before the colliding elements separate (see Figure 6.7). This behaviour is illustrated in a simulation that involves bouncing a 0.2m radius ball with an initial speed of -5ms$^{-1}$ against a flat wall in a gravity-free environment. In one case the ball is damped and in the other undamped (perfectly elastic). Various aspects of the behaviour of the two cases are compared in the following figures.

Figure 6-4 A Comparison of the collision velocities for a damped and undamped ball
Figure 6-5 A Comparison of the collision overlap distances for a damped and undamped ball.

Note that the overlap in both cases does not come back to zero because the time when contact ceases does not necessarily correspond with the time step interval i.e. the exact time when particles separate is never detected but is determined by extrapolation. This factor is also observed in the figure below where the relationship between force and overlap distance is shown.
Figure 6-6 The behaviour of force with respect to overlap distance for both undamped and damped ball.

Figure 6-7 Comparison of Force at a contact point for a damped and un-damped system

The large initial force observed at the beginning can be avoided and the negative force occurring at the end more or less eliminated if the following modification proposed by Crosley (1975) is implemented.

\[ F = K\Delta + C'V\Delta \]  \hspace{1cm} (6.5)
Where $C'$ is a modified damping constant.

It can be seen that in this equation the damping term is also dependent on the overlap and thus the behaviour of forces at the beginning and end of contact are better-behaved.

Zhang and Whiten (1996, 1999) suggest more robust ways of handling contact response during overlap. However since ball collision simulations showed that both energy and momentum were conserved provided the recommended time step is used, use of a more physically-correct model could not be justified. Further more, the energy conservation discrepancy in the mill simulation results discussed later was normally within 4%. Thus in all simulations discussed throughout this thesis, the simple linear spring and dashpot model was used.

### 6.6 Effect of contact parameters on the simulation

The initial parameter estimates used to model contact in the simulation of grinding experiments discussed earlier are given in section 6.8. Due to lack of adequate experimental data to guide the choice of parameters, a brief parameter sensitivity analysis was conducted on stiffness, coefficients of restitution and friction.

#### 6.6.1 Material stiffness

The real stiffness of rock and steel material is in the order of $10^9$ and $10^{10}$ which if applied to a 5g steel particle in a simulation, according to Equation 6.2 would require a time-step of about $10^{-7}$ seconds which is very slow. Cleary (2001) recommends a stiffness which limits overlap to 1% of the particle diameter. This guideline doesn’t however show the effect of varying stiffness. To study this, stiffness was varied while the rest of the conditions remained the same in simulations involving 100 large balls (0.2m diameter and 7800kg/m³ density) in a 4m diameter mill. Large and heavy balls were deliberately used to accomplish this exercise in a short time.
The operating conditions are summarised below:

**Figure 6-8 Geometry of the mill used to test contact parameters**

Mill: Diameter 4m, Length 1m, Speed 17.5 rpm (81% of critical speed), % Filling 15.

Contact Parameters: Stiffness; 40 000 Kn normal and 30 000 Kn shear, friction coefficient 0.3, Restitution coefficient 0.6 for both shear and normal.

Sampling: 4 Revs prior to sampling, 10 revs of sampling.

Power estimate using Morrell E-model is 114 000 watts (114Kw).

The table and the graph below show the change in the frequency of three energy levels as stiffness is increased. It is also seen in the table that the overall mill power remains the same.

**Table 6-1 Results of varying the Ball and wall stiffness on contact events and mill power**

<table>
<thead>
<tr>
<th>Energy range of Event (J)</th>
<th>Ball and wall Stiffness raised to the indicated power</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>5</td>
</tr>
<tr>
<td>0-50</td>
<td>24183</td>
</tr>
<tr>
<td>50-800</td>
<td>15188</td>
</tr>
<tr>
<td>&gt;800 *</td>
<td>256</td>
</tr>
<tr>
<td>Mill Power (Watts)</td>
<td>103083</td>
</tr>
</tbody>
</table>

* Assuming fracture behaviour to be according to Equation 4.3, only events greater than 800J can cause fracture to particles of this size.
The lower energy events increase with increased material stiffness while the trend is reversed for higher energy events. This suggests that increasing stiffness increases particle vibration without necessarily increasing the overall energy in the system. It is seen from the table and graph that the events that can cause fracture at the lowest stiffness are more than double those at the highest stiffness. It is thus likely that breakage will be over-predicted when lower stiffness is specified. It was however decided not to use stiffness values higher than the order of $10^7$ due to the time constraint. The effect of stiffness on simulation time shown in the figure below also indicates a change in the slope of the logarithmic plot as stiffness goes beyond $10^7$ i.e. simulation time increases by a larger ratio as stiffness is increased by 10.
6.6.2 Coefficient of friction

This study was conducted as discussed in the previous section: keeping all other variable constant, friction was varied as shown in the table below.

Table 6-2 Results of varying the Coefficient of friction on contact events and mill power

<table>
<thead>
<tr>
<th>Energy range of Event (J)</th>
<th>Ball and wall coefficient of friction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.1</td>
</tr>
<tr>
<td>0-50</td>
<td>71186</td>
</tr>
<tr>
<td>50-800</td>
<td>19881</td>
</tr>
<tr>
<td>&gt;800</td>
<td>47</td>
</tr>
<tr>
<td>Mill Power (Watts)</td>
<td>95377</td>
</tr>
</tbody>
</table>
Figure 6-11 The effect of varying friction on the contact events

It is seen from the figure that higher energy events (>800J) are less when the friction coefficient is low and thus under-specifying the friction coefficient could lead to under predicting breakage. The higher energy events are less when friction is low due the balls not being raised high enough. Very little change is observed in the trends when the coefficient exceeds 0.5, this behaviour is probably dependent on both the mill speed and liner design.

6.6.3 Coefficient of restitution

As in the above cases, only the coefficient of restitution was varied while the rest of the parameters were as summarised in section 6.6.1.
Table 6-3 Results of varying the Coefficient of Restitution on contact events and mill power

<table>
<thead>
<tr>
<th>Energy range of Event (J)</th>
<th>Ball and wall coefficient of restitution</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.3</td>
</tr>
<tr>
<td>0-50</td>
<td>67844</td>
</tr>
<tr>
<td>50-800</td>
<td>13202</td>
</tr>
<tr>
<td>&gt;800</td>
<td>115</td>
</tr>
</tbody>
</table>

| Mill Power (Watts)        | 105847| 105155| 103900| 102425| 100995| 95995| 89703|

Figure 6-12 Effect on varying the coefficient of restitution on the contact events

From the table it is seen that there are less number of events when the collisions become more elastic and this can be attributed to balls being projected in a wider space and thus minimising chances of collisions as seen in the PDPs in Figure 6.13. The corresponding increase in the number of high energy events can be attributed to balls having higher kinetic energies. On the contrary the balls with highest damping (lowest coefficient of restitution) also show a higher number of high energy events than the middle coefficient values, indicating that apart from
the kinetic energies of the approaching entities the rate of energy dissipation at contacts is also significant.

Figure 6-13 PDPs comparing the space of ball interaction when coefficient of restitution is 0.9 (left) and 0.1 (right)

It can be seen from the PDPs above that the load with a lower coefficient of restitution has a higher centre of gravity and thus this accounts for a higher power trend with the decreasing coefficient of restitution.

6.6.4 Particle shape consideration

For reasons discussed in Chapter 2, a sphere is preferred for particle shape representation. However as shown in Figures 3.1 and 3.2 an elliptical shape could have probably been more appropriate. Failure to implement the elliptical shape affected the dynamics of the particles as well as determination of the correct mass of a sphere with an equivalent behaviour.

Ellipsoids are provided for in PFC by allowing spheres of different sizes to be merged into required shapes. However this work is beyond the scope of this research and the parameters of the sphere were tuned to get the required behaviour.

6.6.5 Conclusion

From the discussion of the influence of parameters, it is seen that parameter values have a significant effect on the behaviour of balls in the mill. The task of
determining the correct parameters for simulating the experimental work discussed in Chapter 5 requires extensive data and cannot be dealt with exhaustively here. However important trends that can guide parameter choice have been observed.

6.7 Simulation work

6.7.1 Introduction

The main objective of these simulations was not to study grinding per se but to see how well the simulator could predict well-defined grinding experiments. An overview of the simulation results is considered here while in the next chapter an approach that uses the energy spectra to predict grinding rate will be developed.

6.7.2 Description of the simulation procedure

The setting up of the software for mill simulations has been discussed in detail already. The simulations that were conducted directly corresponded to the experimental work and were as listed below.

Set 1: Five simulations with -126 +106mm (20 spheres) as Media fraction, Mill fill at 20 % and speed at 78% (42rpm) and the fine feed fraction size used in each simulation is as follows:

(a) -8 +6.7mm (4080 spheres)
(b) -16 +13.2mm (556 spheres)
(c) -22.4 +19mm (195 spheres)
(d) -31.5 + 26.5mm (72 spheres)
(e) -45 +37.5mm (23 spheres)
Set 2: Three simulations with -16 +13.2mm as fine fraction

(a) 20% Mill fill running at 58.5% of Critical speed (32rpm) with -126 +106mm as Media fraction (20 spheres)
(b) 40% Mill fill running at 78% of Critical speed -126 +106mm as Media fraction (40 spheres)
(c) 20% Mill fill running at 78% of Critical speed with 106 – 89mm as Media fraction (33 spheres)

In all the above cases the fines fraction was always the same mass (3kg), while the media fraction was at 20% fill or at 40% fill.

The material parameters for both ball-ball and ball-wall were the same and were as follows:

- Stiffness (4 x 10^6 Normal and 3 x 10^6 Shear)
- Coefficient of Friction 0.3
- Coefficient of Restitution 0.6

The linear spring and dashpot model discussed in section 2.5.3 was used in all the simulations.

For all the simulations, the sampling of data commenced in the fifth revolution. The number of data sampling revolutions varied from 1 in Set 1 (a) to 20 in Set 1 (e). The considerations being the minimisation of simulation time on one hand and capturing enough interactive events on the other.

**6.7.3 Simulation results and discussion**

The discussions below are general survey of what the data is saying without attempting to explore any particular aspect in detail. The main purpose of this exploration is to establish principles that will be applied in Chapter 7, in the development of the Breakage rate prediction model.
### 6.7.4 Results of set 1 simulations

In Figures 6.14 (a) – (d), the energy spectra for the set 1 simulation series are shown. The simulation involving 8mm particles is excluded as the results showed a large discrepancy between mill input and dissipated energy and hence could not be relied upon. For the purpose of comparison, the results are plotted on one graph in Figure 6.15, in terms of events per particle per second.

![Energy Spectra Associated With 16 - 13.2mm Particles](image1)

Simulation period = 2 revs

(a)

![Energy Spectra Associated With 22.0 - 19.0mm Particles](image2)

Simulation period = 4 revs

(b)

![Energy Spectra Associated With 31.5 - 26.5mm Particles](image3)

Simulation period = 10 revs

(c)

![Energy Spectra Associated With 45.0 - 37.5mm Particles](image4)

Simulation period = 20 revs

(d)

Figure 6-14 Energy Spectra associated with the fine size fraction in each of the simulations involving Media (-126 +106mm) and a fine size fraction.
The general trend can be summarised in two points. Firstly, it can be seen that the total number of events per particle per second increases with decreasing particle size. Secondly, the frequency of the large energy events increases with particle size.

To explain this we must note four kinds of contact events that a fine particle can experience:

- A particle in free flight collides with another particle, media rock or wall. The energy involved is moderately high but not likely sufficient for fracture.
- A particle bouncing or rolling on the surface of the wall or other particles. The energy involved is very minute but these events are the most frequent.
- A particle that is buried in the load and subjected to the pressure of the load above. These are long events but the
energy involved has been found to be only moderately high in most cases.

- A media particle hits a small particle that is resting on the wall or surface of another media rock or particles. These are usually high energy events, depending on the momentum of the media rock and are responsible for almost all the breakage.

The higher frequency of events experienced per particle by the finer particles can be explained by the increase in chances of interaction as the number of particles available for collision increase with decreasing particle size. Generally all particles tend to pack on the lifting side of the lifters as illustrated below. From Figure 6.16 below it is seen that any particle in case (a) has a higher chance of colliding with other particles than in case (b).

![Figure 6-16 Illustration of how particle size can influence the energy absorbed per particle](image)

The increase in the frequency of higher energy events with particle size can also be explained by referring to Figure 6.16 above. Assuming the two media rocks that have fallen on the bed of particles in both (a) and (b) had the same initial energy, the energy received per particle will be higher in case (b).

The relative increase in the frequency of higher energy events with increase in fine size can also be explained by referring to the PDPs. From the PDP pictures of the 16mm and the 45mm fraction shown in Figure 6.17 below (media is excluded), it is seen that the path of the 45mm fraction is more regular. The
behaviour of media is largely unaffected as shown by the PDP in Figure 6.19. If it is assumed that the impact zone is as indicated by the thick line then the fraction of the 45mm particles presented to the impact zone is higher. This is confirmed by the snap shot frames of the simulation shown in Figure 6.18. However it was observed from many simulations that mill speed, lifter configuration and coefficient of friction can easily influence the targeting of particles by the media and thus availability in the impact zone does not necessarily guarantee more collisions with the media.

Figure 6-17 Path of centres of the 16mm particles (left) and path of centres of the 45mm (right) for a mill running at 42rpm with 126mm media

Figure 6-18 Snapshot of the movement of particles and the media; 16mm particles (left) and 45 mm(right) for a mill running at 42rpm with 126mm media
6.7.5 Set 2 simulation results

6.7.5.1 The effect of mill speed
The strain energy spectrum for the mill running at 42rpm is compared with that at 32rpm in Figure 6-20 below. There is a slightly higher frequency of high-energy events for the mill running at 42rpm and the obvious explanation is the corresponding increased media kinetic energy with higher mill speed. This is confirmed by the dilation of the media charge kidney for the mill running at 42rpm shown by the PDPs in Figure 6-21.
CHAPTER 6 SIMULATION WORK

Figure 6-20 Comparison of the energy spectra affecting each particle at different mill speeds

Figure 6-21 The path of centres of the media of a mill running at 42rpm (left) and that of the mill running at 32rpm (right)
6.7.5.2 The effect of mill filling

The figure below shows a comparison of the energy spectra of the mill at 20% and 40% filling.

Figure 6-22 Comparison of the energy spectra affecting each particle at different mill fillings

There is evidence of reduction of impact events with higher mill filling. This is in accordance with expectations as with higher filling more media is to be found at the toe and thus particles are shielded from direct impacts. An interesting experiment that was omitted would have involved doubling the fine fraction to 6kg when J was increased to 40.

6.8 Conclusion

From the analysis and discussion of the Simulation results it has been seen that the DEM is a tool with a great potential for providing information that can be applied in a variety of ways. The flexibility of the tool allows many aspects of grinding to be studied at the desired level of detail. It has been shown that the movement pattern of the media is quite different from that of the fine particles, which has an effect on the grinding process. This qualitative information does
certainly give great insight into the grinding process but for the specific purpose of predicting the grinding rate in the mill a full chapter is devoted to this scheme.