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Estimation of kinetic model parameters in ball mill using MODSIM© simulator

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Abstract: Using a phenomenological grinding kinetic theory based on the pace of the process as described by the selection function (S_i) and breakage distribution function ($B_{i,j}$), the estimated grinding performance of a mill can be approximated. This method is now widely accepted and has been thoroughly explored by renowned scholars such as L.G. Austin. Despite wide acceptance of this method, insufficient studies were conducted on the kinetic model for fine sieve sizes. Since there is no extensive investigation on the fluctuation of model parameters over various sieve size groups, this paper presents one. Simulation models for the design of ball mills are included in the software for the digital layout of mineral processing circuits. The *MODSIM*© simulator calculates nearly complete mass balances for each mineral processing plant and simulates integrated flow diagrams including grinding. The S_i and $B_{i,j}$ equations were derived using the particle size distributions at varied grinding times and with model parameters for coarse and fine particle size groups. Experimentally derived data were statistically compared to the *MODSIM*© simulator data using model parameters.

Keywords: grinding, ball mill, kinetic model, MODSIM©

1. Introduction

Fine and ultra-fine grinding are desirable in a variety of industries, including fillers for paper, pigments or plastics, metals, and metallic compounds for electronics, medicine, and other applications, to name a few. According to Bel Fadhel et al. (1999), there are no hard and fast rules for either the top size of the ground material or the narrow size distributions.

Grinding uses up to 4% of the world's electrical energy and the typical energy consumption in a grinding circuit is estimated to be around 6700 kWh per kilo ton of mineral or ore. Ball mills are highly efficient grinding machines that yield extremely fine material (Ipek et al., 2005a). Consequently, numerous studies have been conducted to improve the efficiency of the ball milling process, evaluate the influence of operating parameters, and minimize energy consumption (Petrakis and Komnitsas, 2021).

Numerous scientific studies on grinding efficiency utilize various modeling approaches. In mineral processing, the primary objectives for modeling are typically related to either the optimization of processes or the investigation of mechanisms (Wołosiewicz-Głąb et al., 2019).

The grinding in mineral processing can be divided into three categories based on material size: coarse grinding, fine grinding and mechanical activation. Coarse grinding is done to reduce the size of the particles, while mechanical activation is done to alter the physical structure of particles and increase their reactivity (Boldyrev et al., 1996). Between coarse grinding and mechanical activation comes the process of fine grinding, which is a subset of the mechanical activation category. It is known that both physical and chemical changes occur due to the tremendous energy exerted by the balls in the mill on the particles during fine grinding, that is, due to the strong mechanical action occurring on the solid surface. These changes are referred to as "*physicochemical effects*". It is known that reducing the size of the solid, i.e. grinding it very finely, causes these changes. Mechanochemical effects are physicochemical

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effects that are triggered in particles by the action of mechanical forces (Kapur and Agarwal, 1970; Venkataraman and Narayanan, 1998).

In recent years, researchers have concentrated on evaluating size reduction in ball mills using the ideas of particular rates of breaking and main daughter fragment distributions. Austin and co-workers reviewed the benefits of this strategy and demonstrated that laboratory data can be scaled to industrial mills in several studies (Austin et al., 1981; 1984).

As shown by several different evaluations of individual fragmentation rates, the fundamental assumption of first-order kinetics in ball mills is advantageous for simulation model development. However, as several investigators have shown via their experiments, perfect first-order kinetics is more often the exception than the rule. As stated in a recent piece of research, the fluctuation in particle strength that occurs inside a size fraction is responsible for the estimation that all particle sizes will exhibit some degree of deviation from the first-order breaking kinetics. According to Austin and co-workers (1984), the model is predicated on the notion that the load at which a particle breaks is directly proportional to the rate at which the particle breaks.

This last premise may be challenged on first-principles grounds. On the other hand, it was indirectly validated by comparing the projected population of particles remaining after a specific grinding interval to the actual population of particles remaining, with the average strength growing as grinding progressed. An investigation on the kinetics of non-first-order breaking of coarse particle sizes in a ball mill was carried out using a spectrum of grinding medium forces as the variable of interest. These concepts have been used in several studies (Austin et al., 1984) to quantitatively explain coarse particle size breakage in laboratory ball mills.

The departure from first-order breakage kinetics is affected by the size range of the relevant sieve size fractions. When relatively smaller size fractions are used in the grinding process, it has a lower coefficient of variation than the standard particle strength. The degree to which the selection function (S_i) and the breakage function ($B_{i,j}$) deviate from first-order kinetics is affected by the size range of the sieve size fraction in a manner that is proportional to the parameter values of these functions (Austin et al., 1984).

In the milling process modeling, it is generally assumed that the specific breakage rate for a given particle depends on its size, material properties, and the stressing conditions, but not on the presence of dissimilar-sized particles in the milling environment. An abundance of experimental evidence contradicts this assumption finding that the milling environment characterized by the instantaneous PSD may affect particle breakage behavior (Capece et al., 2015).

Many models have been widely used in mineral processing plant operations since the 1970s. Some were developed for general mineral processing, while others were developed for specific company needs. Today, the mineral processing industry relies heavily on simulator-based work such as JKSimMet (Bilgili et al., 2006), and *MODSIM* (King, 2001) and their variants.

Mineral processing consists of several types of unit operations, the most important of which are size reduction (which can be accomplished by crushing and grinding), particle classification, concentration methods, and solid-liquid separations. The efficiency of specific mineral processing units can be significantly affected by microscopic particle attributes such as shape and surface properties. Any mineral or coal processing plant can benefit from the *MODSIM*, a mass balance simulator, which supports all of these characteristics of particle systems. In addition, the *MODSIM* simulator provides an in-depth analysis of the most commonly used models for the above-mentioned tasks (King, 2001; Umucu et al., 2012).

Changes in kinetic model parameters for particles of fine size are the most important topics to examine. Researchers have not proved how model parameters alter when fine particle size decreases. Before this, researchers (Deniz, 2003; Deniz et al., 2011; Deniz, 2013; Cleary and Morrison, 2011; Capece et al., 2015; Petrakis et al., 2017) determined the breakage rate and distribution for the -3.35 mm and 0.106 mm coarse-size groups. However, few investigators (Tangsathitkulchai, 2002; Bilgili et al., 2006; Umucu and Deniz, 2015) worked on fine particle size groups (such as -0.106+0.045).

This study used coarse (-1.00+0.106 mm) and fine (-0.106+0.045 mm) sieve size groups for grinding. The percentage quantities based on product sieve size distribution were computed in the *MODSIM* simulator using model parameters derived from grinding experiment data on breakage rate and time.

In order to investigate both sizes for the same material, the change in model parameters caused by different particle size distributions has been shown to affect the simulation. This research reveals that the grinding efficiency, with a particular fragmentation rate and cumulative distribution function, is connected to the grinding behavior of coarse and fine particles.

2. Theory

2.1. Kinetic modelling

Generally, when evaluating the comminution of materials in tumbling ball mills, it is assumed that the fragmentation of each narrow size fraction is of a first-order nature. In other words, the rate of size 1 disappearance due to breakage is proportional to the amount of size 1 of material that is stored in the mill hold-up (Austin and Luckie, 1972). Because the mill hold-up, *W*, does not change, this becomes:

$$dw_i = \frac{(t)}{dt} = -\mathrm{S}_1 w_1(t) \tag{1}$$

where S_1 is constant, and its unit of measurement is time^{-1}. In addition, taking the logarithm of both sides of Eq. (1);

$$\log[w_1(t)] = \log[w_1(0)] - \frac{S_1 t}{2.3} \tag{2}$$

where S_1 is the specific rate of breakage, $w_1(t)$ is the weight fraction of size 1 mill hold up at time t (Austin and Bagga,1981). On the other hand, Austin and co-workers (1972; 1984) proposed the following formula to describe the link between particle size and the specific rate of breaking (S_i):

$$S_i = a_T \left(\frac{X_i}{X_0}\right)^{\alpha} Q_i \tag{3}$$

where X_0 is 1 millimeter, X_i is the upper limit of the size interval indexed by i, and the a_T and a are model parameters that depend on the material's properties. Q_i is a correction factor that has a value of 1 for smaller sizes (normal breakage) but has a value of less than 1 (abnormal breakage) for particles that are too large to be nipped and broken appropriately by the ball size. In the zone of a typical breaking, each size behaves as though it is composed of a proportion of weak material and a greater proportion of material with high strength. In this location, the empirical description of Q_i values is supplied by using a mean value for S_i (Austin and Bhatia, 1972; Austin et al., 1984),

$$Q_i = \frac{1}{1+\left(\frac{X_i}{\mu}\right)^{\wedge}}, \quad \wedge \geq 0 \tag{4}$$

where μ, λ and $\wedge$ are model parameters. The $B_{i,j}$ is generally used to characterize the size distribution resulting from the fracture of the material into a narrow dimension. The weight fraction of material broken from size j that falls less than the upper size of size interval "i" is defined as this distribution (Austin et al., 1989).

The $B_{i,j}$ are calculated using the *BII* method given in Eq. (5).

$$B_{i,j} = \phi_j \left(\frac{X_{i-1}}{X_j}\right)^{\gamma} + (1-\phi_j)\left(\frac{X_{i-1}}{X_j}\right)^{\beta} \qquad n \geq i > j \tag{5}$$

$$\text{where } \phi_j = \phi_1 \left[\frac{X_j}{X_1}\right]^{-\delta} \tag{6}$$

where δ, ϕ_j, γ and β are model parameters that rely on the characteristics of the material to determine their values. For normalized $B_{i,j}$ values, the δ value is 0. The intercept at $(X_{i-1}/X_j) = 1$ is denoted by the parameter ϕ_j; γ is the parameter denoting the slope of the lower segment of the $B_{i,j}$ curve, and β is the parameter denoting the slope of the steeper section of the $B_{i,j}$ curve (Ipek et al., 2005b; Deniz et al., 2011; Deniz, 2012; Deniz, 2013).

3. Materials and experimental methods

3.1. Materials

Due to the importance of barite as a raw material in the production of industrial dyes, barite mineral was used as the experimental material in this study. The specific gravity of the raw barite mineral used in the experiments is 4.5 and the standard Bond work index (W_i) is 7.03 kWh/t. The standard Bond test

approach was used to determine the Bond work index. In addition, the chemical analyzes whose results are given in Table 1 were performed with the Panalytical Zetium brand XRF device at Eskişehir Osmangazi University Research and Application Center. The chemical analysis results of the barite mineral used in the experiments are presented in Table 1.

Table 1. Chemical analysis results of barite mineral used in grinding experiments

Oxide	SiO_2	Al_2O_3	Fe_2O_3	CaO	MgO	Na_2O	SO_3	K_2O	$BaSO_4$	LOI
%	0.51	0.02	0.06	0.42	0.13	0.02	40.93	0.02	98.82	21.89

3.2. Grinding tests

To conduct the experiments defining the fracture parameters, the one-size-fraction approach suggested by Austin et al. (1984) was used. The two-dimensional fractions selected for the test were as follows; first group; -1.180+0.850, -0.850+0.600, -0.600+0.425, -0.300+0.212 and -0.150+0.106 mm; second group; -0.106+0.090, -0.090+0.075, -0.075+0.063 mm and -0.063+0.045 mm. The characteristics of the laboratory-type ball mill used in the experiments and the standard conditions for grinding used throughout the process are shown in Table 2. In addition, previous studies have determined that the interstitial filling ratio (U) for effective grinding is between 0.8 and 1.0 (Deniz, 2012). In this study, 0.8 was used as the U value.

Table 2. The laboratory ball mill characteristics and grinding test conditions

Mill	Diameter, D (mm)	200
	Length, L (mm)	200
	Volume (cm^3)	6283
	Mill speed Critical, Nc (rpm)	102
	Operational speed	77
Media (Balls)	Grinding Diameter, d (mm)	30
	Media (balls) Specific gravity	7.80
	Quality	Alloy steel
	Assumed porosity (%)	40
	Ball-filling volume fraction, J_b	0.30
Material	Specific gravity	4.5
	Powder-filling volume fraction, f_c	0.096
	Interstitial filling ratio, U	0.80

4. Results and discussion

4.1. Selection function (S_i)

According to the findings, the data indicate that the first-order relation is often followed by breaking and that S_i values may be calculated using the gradient of the straight line characterizing first-order plots. In addition, the relationship between S_i and short grinding time in the fraction of coarse (-1.180+0.106 mm) and fine (-0.106+0.045 mm) particle size for barite mineral is shown in Fig. 1.

4.2. Breakage distribution functions ($B_{i,j}$)

The $B_{i,j}$ values were determined using the BII method to characterize the size distributions that occur from a certain size range to a smaller size for the shortest grinding times (15 or 30 seconds) as a result of material breakage (Austin, 1972; Austin et al., 1984). The values of $B_{i,j}$, that are produced from BII calculations are shown in Fig. 2 against the particle sizes that were calculated for each size fraction.

The selection (S_i) and breakage ($B_{i,j}$) functions are shown in Figs. 1 and 2, respectively, and these functions vary according to the mill conditions. These functions are the simplest model possible for a ball mill since it utilizes breakage and selection operations. It is considered that the mill only has a single

zone that is adequately blended. The S_i is the typical function, and the maximum value defines the degree to which the breakage rate decreases with increasing size.

The findings demonstrated a normalized behavior that is rather usual, in which the progeny distribution was unaffected by the feed particle size, and the δ parameter was set to zero. In addition, a full listing of the model's parameters is shown in Table 3.

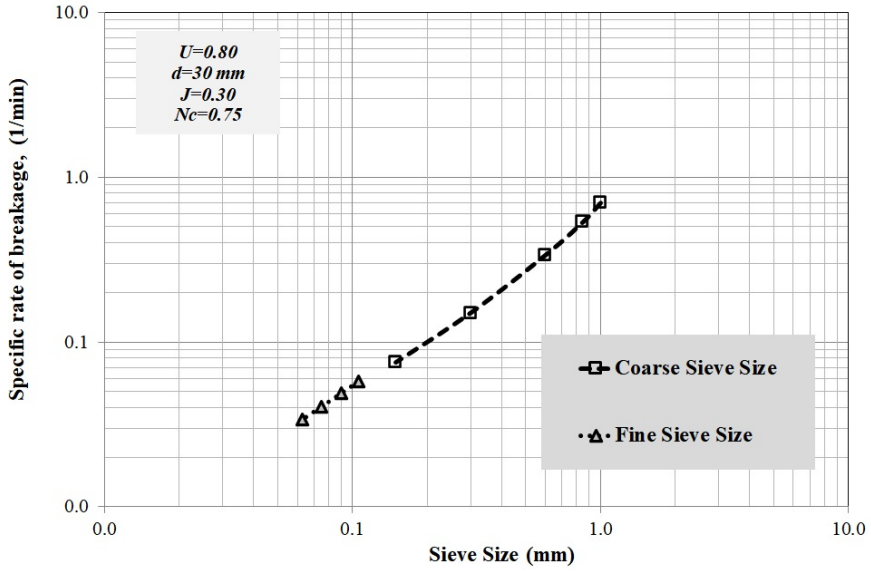

Fig. 1. Variations in the specific rates of breakage (S_i) values as a function of the mean particle size fractions

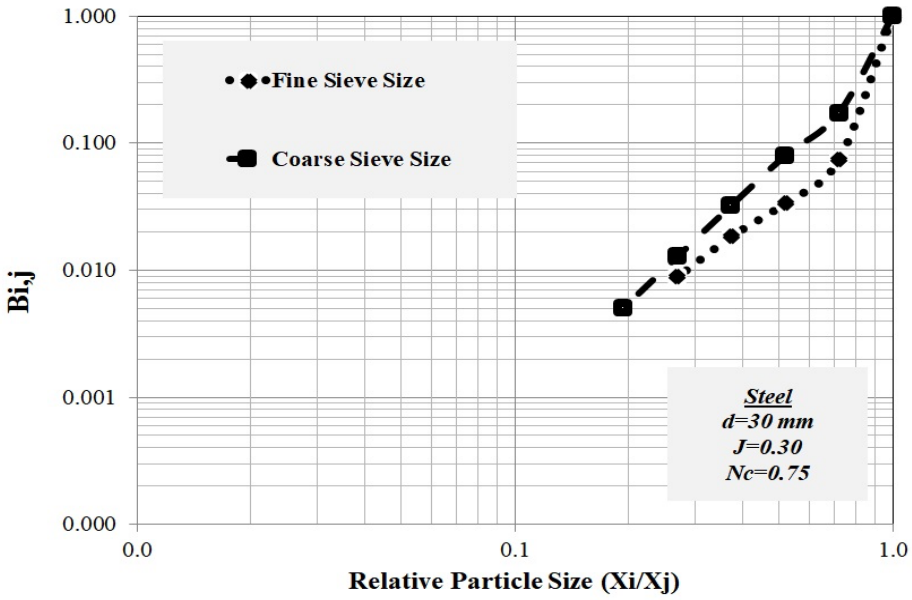

Fig. 2. The cumulative breakage distribution for short grinding time

Table 3. Breakage characteristics parameters of the various sieve size groups derived from the laboratory test

Sieve size (mm)	Sieve size group	U (%)	a_T	a	Φ_j	γ	β	δ
-1.18+0.106	Coarse Sieve Sizes	0.80	0.68	1.32	0.520	2.83	9.90	0.00
-0.106+0.045	Fine Sieve Sizes	0.80	0.58	1.03	0.130	2.04	9.50	0.00

When barite samples were ground in a dry milling process across a range of sieve sizes, it was discovered that the different sieve sizes obeyed the first-order breakage rule and had consistent normalized primary breakage distributions. Also, the cumulative fracture threshold of the particle size distribution function is not considered into account when evaluating these samples.

According to Table 3, the model parameter values of different sieve size groups differ from the literature (Deniz, 2003; Deniz, 2012; Deniz, 2013) for coarse and fine sieve sizes. When examining Table 3, it was established that the coarse size group results in quicker grinding. The breakage rate of both the smaller and larger sizes reduced as sieve sizes became finer. This scenario was explained by the existence of macro-cracks and pores on the coarse sieve group.

4.3. Estimation of particle size distribution and kinetic breakage model parameters using the *MODSIM*© simulator for fine and coarse sieve sizes

The *MODSIM*© simulator framework is entirely modular, enabling the addition of models for unit operations. Consequently, the models used to simulate the operation of different unit activities may be developed and updated to fit the needs of each application and any operating state. This feature of the *MODSIM*© simulator also allows the user to include current research discoveries in the mathematical modelling of mineral processing unit operations. As users add new models, the system's model library continues to expand and any model is made available for the user (King, 2001). The process of adding parameters for mill feed material in the *MODSIM* simulator is shown in Figs. 3-5.

The unit models are fundamental to the *MODSIM*© simulator. The simulator cannot produce a believable depiction of the plant's behaviour if no model adequately explains the unit's functioning. For accurate work, models must be properly crafted and calibrated against sufficient experimental data (King, 2001).

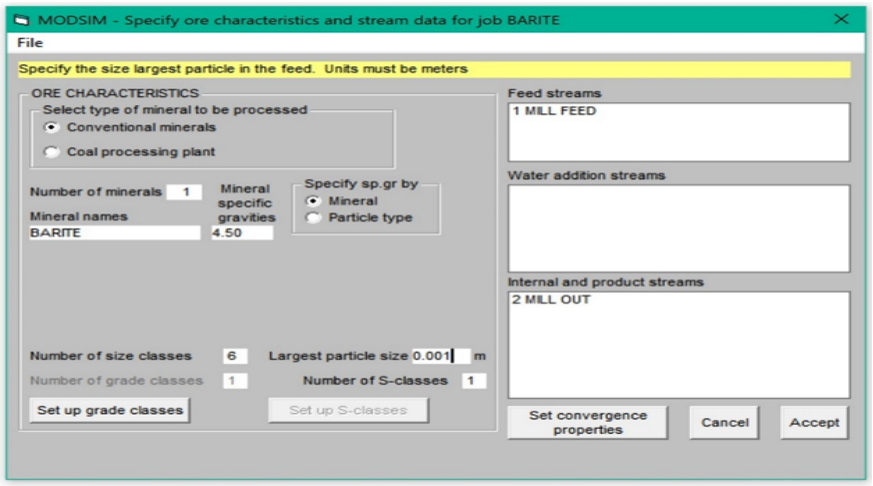

Fig. 3. The *MODSIM*© input format contains information about the particle size and distribution of mill feed and the material characteristics

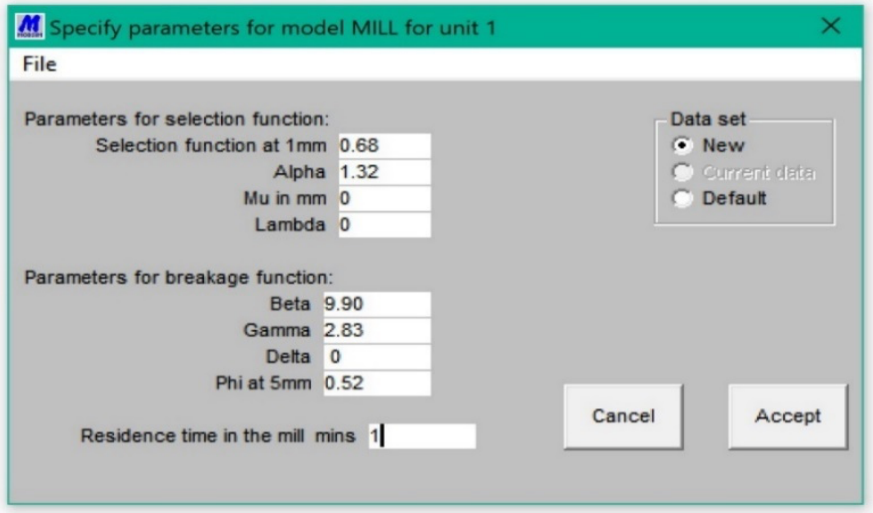

Fig. 4. The *MODSIM*© input format for the coarse size group, selection and breakage function parameter

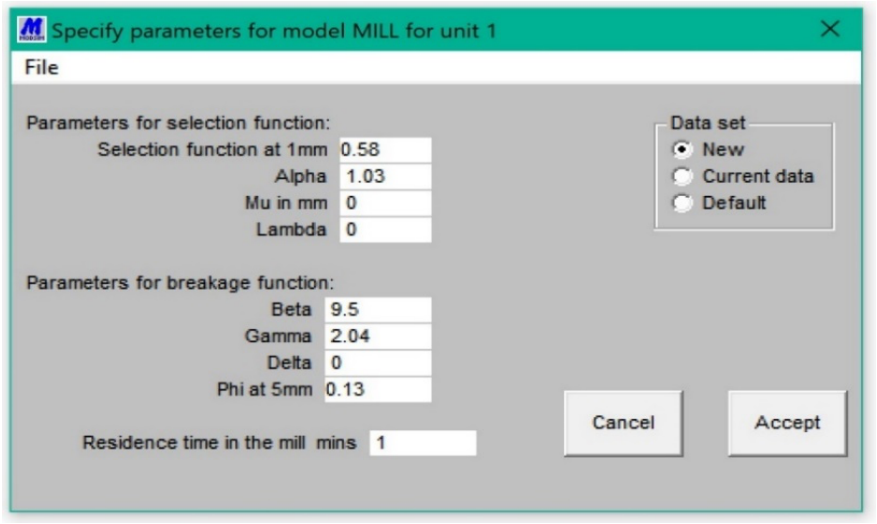

Fig. 5. The *MODSIM*© input format for the fine size group, selection and breakage function parameter

Firstly, the particle size distribution values obtained at different sieve sizes as a result of 60 seconds of grinding of a barite sample feed in a narrow size were determined. Then, using the *MODSIM*© simulator, the product particle size distribution was estimated using the parameters of the kinetic model at the same conditions.

The particle size distributions of the ground product predicted from the experimental and *MODSIM*© simulator are shown in Figs. 6 and 7.

In MODSIM simulation processes, the entire material was selected as -1.18+0.850 mm for coarse particle sizes and -106+90 microns for fine particle sizes and was ground for 60 seconds. The reason for selecting a narrow particle size feed is that it does not create a negative effect during the grinding of the material, such as bedding and fine particles during comminution.

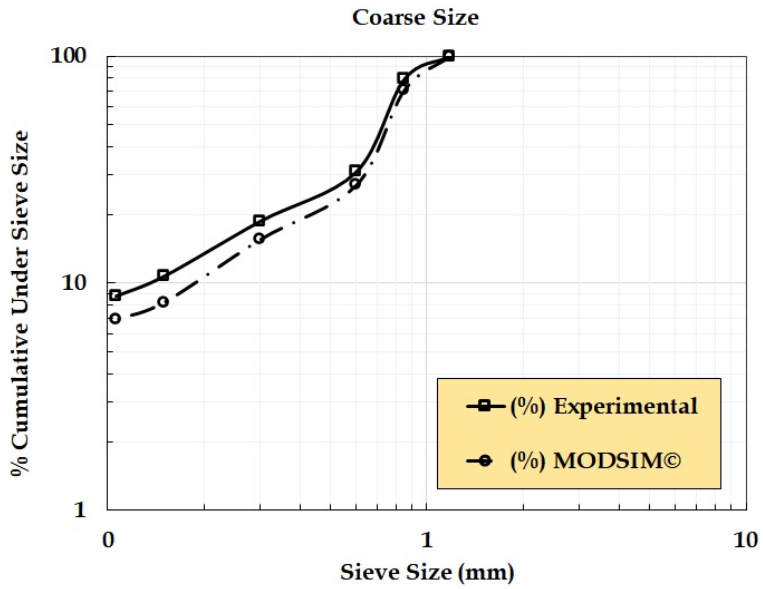

Fig. 6. Comparison of the *MODSIM*© simulator and experimental results for cumulative particle size distributions for the coarse sizes

4.4. Comparative analysis of the *MODSIM*© simulator and experimental data regarding product size distributions

To evaluate the agreement between the cumulative undersize distribution percentage data of the experimental and the *MODSIM*© simulator, Regression Constant (R^2), Mean Absolute Error (*MAE*), and Root Mean Squared Error (*RMSE*) are three metrics that are commonly used when attempting to

estimate the accuracy of data. While the *MAE* and *RMSE* are types of error indexes, and the closest and lowest value to 0 indicates the validity of the model, the R^2 value lies between 0 and 1, and a value of 1 represents fully matched data (Umucu et al., 2016; Deniz et al., 2022).

In this study, the R^2, *MAE*, and *RMSE* equations are given in Eqs. 6-8 were used to evaluate the effectiveness of the selected models.

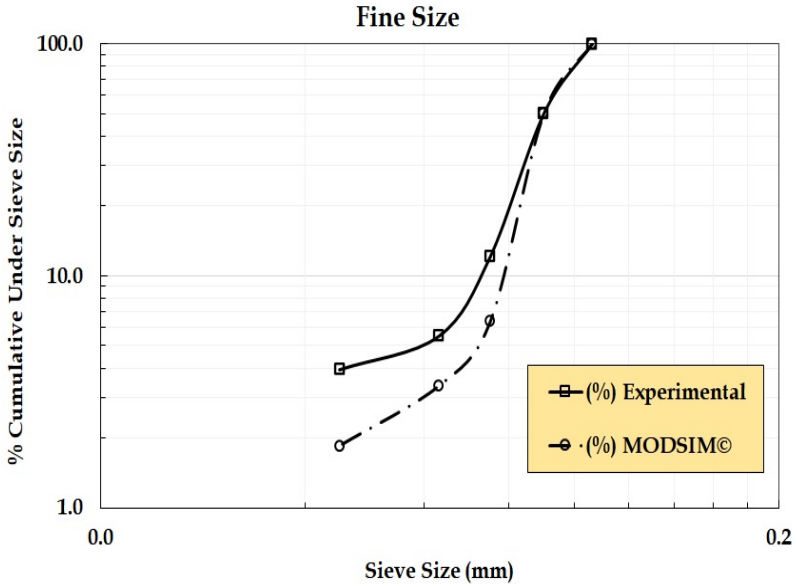

Fig. 7. Comparison of the *MODSIM*© simulator and experimental results for cumulative particle size distributions for the fine size

$$R^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2} \tag{6}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y - yi| \tag{7}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n}} \tag{8}$$

The y value represents the result of a measurement; n represents the total number of samples taken. The yi value is the estimated value and $\bar{y}$ is the mean of the experimental values (Deniz et al., 2022).

The relationships between the experimental results and the estimated particle size distribution values using the *MODSIM* simulator are shown in Fig. 8. Additionally, the performance of the *MODSIM*© simulator was evaluated according to the performance metrics given in Table 4.

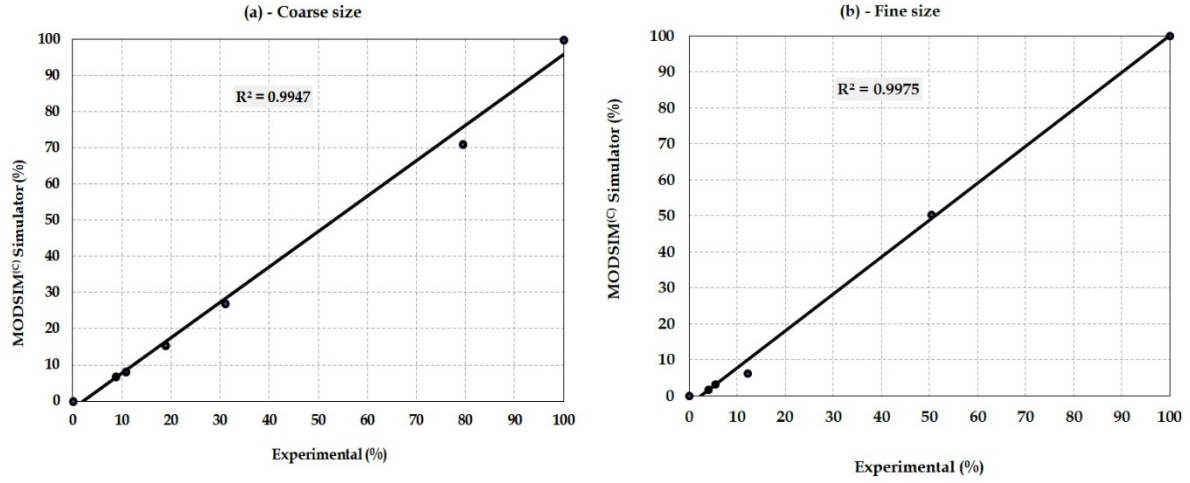

Fig.8. Relationships between experimental and *MODSIM*©simulator estimated cumulative particle size distribution values for coarse sieve sizes (a) and fine sieve sizes (b) of the barite sample

Table 4. Statistical evaluation between the *MODSIM*© and experimental data for fine and coarse sieve sizes

Rating	Coarse Sieve Size	Fine Sieve Size
R^2	0.9947	0.9975
MAE	3.34	2.01
RMSE	4.22	2.91

As seen in Table 4, the agreement between experimentally obtained results and *MODSIM* simulator estimates was quite good, as indicated by the R^2 values and statistical error analysis (*RMSE* and *MAE*). However, while the *RMSE* and *MAE* results obtained for coarse particle sizes were expected to be better, the R^2, *RMSE,* and *MAE* results obtained for fine particle sizes were better. This situation may have arisen due to the amount of data and calculation methods. Austin et al. developed a kinetic model in which studies were conducted on coarse particle sizes. However, studies on very fine particle sizes are very few. A similar trend was expected in simulation programs. On the other hand, due to the complexity of the grinding process, the estimation errors of the *MODSIM*© simulator for particle size distributions are at acceptable levels.

Consequently, it was decided that the grinding size analysis distribution obtained from the *MODSIM*© simulator gave estimation results close to the experimental grinding size analysis distributions.

5. Conclusions

An experimental investigation to understand the kinetics of grinding tests is not only time-consuming but also labor-intensive and subject to changing conditions. On the other hand, the grinding kinetics of any material can be used to determine the sieve size distribution of the ground product.

In this study, while the barite sample was effectively grinding for the coarse sieve size group, following the general comminution theory, a more difficult fracture situation emerged in the fine sieve sizes. When the model parameter changes were examined, different values were obtained for the sieve size groups. For the coarse sieve size, $a_T = 0.68$ and $\alpha = 1.32$, while for the fine sieve size group, $a_T = 0.58$ and $\alpha = 1.03$ were obtained. This situation emerged both from the experimental results and the estimation data made with the *MODSIM* simulator. These results indicate that the coarse particle size fraction breaks down significantly faster than the fine size fraction.

It is seen that the particle size distribution estimations made with the *MODSIM* simulator are compatible with the experimental results. While making the calculations in the *MODSIM* simulator, it has been revealed that the model parameters and values related to the different sieve sizes defined for the system do not play a large role in the calculation.

Since the model parameters for each sieve size group in the same sample are different, research needs to be done on various samples.

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