

Assessment of the Functionality of Selection and Breakage Rate Functions in Grinding Systems

M C Williams¹ and T P Meloy¹

ABSTRACT

Several important, fundamental aspects of the grinding behaviour of mineral systems are addressed. The Levenberg-Marquardt algorithm for systems of constrained non-linear equations was used to solve the steady-state and dynamic population balance model (PBM) grinding equations to obtain the mill matrices and grinding selection and breakage rate functions, respectively. The fact that the PBM model equation Inverse Problem is degenerate or underspecified is demonstrated. Multiple solutions to the same PBM equations are provided. It is shown that there is no unique solution to the Inverse Problem unless additional constraints are provided or assumptions are made such as the Arbiter-Bhrany normalisation assumption. The severity of the non-uniqueness problem for steady state grinding is demonstrated in several examples using typical feed distributions and mill matrices. In addition, it is also demonstrated that when higher than single powers are used in steady-state mill matrix expressions during simulation or calculation (or iterative procedures are used during numerical simulation) and four or more size intervals are used considerable amount of error is propagated throughout any calculation. Each solution to a PBM, while giving the same prediction during a single mill pass, gives different solutions or predictions for mill composition upon subsequent passes. In addition, it is shown that there is a problem with building up a grinding mill knowledge base with PBMs. A similar analysis was done for the dynamic or kinetic PBM equations. The fact that the dynamic PBM Problem is degenerate or underspecified is also demonstrated. Multiple solutions to the same dynamic PBM equations are provided. Again, it is shown that there is no unique solution to the Inverse Problem unless additional constraints are provided or assumptions are made such as the normalisation assumption. Each solution to a dynamic PBM, while giving the same prediction for a given grinding time interval, gives different solutions or predictions for mill composition for other grinding times. Actual experimental grinding data was assessed to determine the functionality of mill selection and breakage functions. The functionalities obtained through constraints were compared with those obtained with the normalisation assumption of Arbiter-Bhrany which relates breakage functions to particle size distribution. The capability of the population balance model to predict grinding behavior over time in various mineral grinding systems was assessed. The required functionality of selection and breakage functions for effective prediction of grinding behavior in mineral systems is discussed.

INTRODUCTION

The PBM for simulating comminution in grinding mills has been solved assuming linearity using matrix methods (Broadbent and Calcott, 1960; Meloy and Gaudin, 1962; Agar and Charles, 1962; Meloy and Bergstrom, 1964; Reid, 1965; Mika, 1970; Herbst and Mika, 1970; Klimpel and Austin, 1970; Austin, 1971; Kapur, 1972; Malgan and Fuerstenau, 1976; Herbst *et al.*, 1971; Fuerstenau *et al.*, 1984; Meloy and Williams, 1992 a and b).

Selection and breakage functions are lumped into a steady-state mill matrix. This steady-state mill matrix is multiplied (on the right side) by the feed matrix which describes the particle size distribution entering the mill. This multiplication yields the mill product matrix which describes the size distribution of the particles exiting the mill. In practice one creates the mill matrix by measuring the size distribution of the feed and product, then calculating the mill matrix by various methods. This is referred to as solving the Inverse Problem.

The dynamic (time-variant) PBM for simulating comminution in grinding mills has also been solved assuming linearity

(Fuerstenau *et al.*, 1984; Herbst and Fuerstenau, 1980; Klimpel, 1970; Klimpel, 1991; Kapur, 1972). Considerable effort has been expended in also normalisation of the selection and breakage rate functions (Arbiter and Bhrany, 1960).

The selection and breakage functions are not lumped together as in the steady-state mill matrix. The dynamic PBM introduces more unknowns than the steady-state PBM, that is, the kinetic terms or breakage rate functions.

PBM MODELS: DEVELOPMENT AND NUMERICAL SOLUTION

Steady-state PBM model

In simulating a wet ball milling operation for design or control purposes, today, most people use the PBM method. Even when the plot of the product from a mill is a straight line, the method of solution is to use matrix algebra to find the mill matrix, M , from idealised feed, F , and mill product, P , matrices, that is, solve the Inverse Problem. The relationship between M , F and P is:

$$MF = P \quad (1)$$

M is a sparse, square, n by n , steady-state, probabilistic (stochastic) matrix; n is the number of particle size classes into which the particle feed has been arbitrarily divided. The top particle size is designated one and the bottom size is designated size n . F and P are n by one, column matrices. The elements of M , the m_{ij} of row i and column j , are all fractions, less than one. The value of m_{ij} is the probability of a particle in the j -th particle size class being broken into the i -th particle class. For transient analysis the m_{ij} are Laplace-transformed differential equations. In the absence of any agglomeration phenomenon, m_{ij} is zero for all $j > i$. In addition, conservation of mass requires that:

$$\sum_{i=1}^n m_{ij} = 1.0 \quad \text{for each } j \quad (2)$$

Hence, m_{nn} must be one.

A typical five by five mill matrix is:

$$M = \begin{matrix} m_{11} & m_{12} & m_{13} & m_{14} & m_{15} & & & & & \\ m_{21} & m_{22} & m_{23} & m_{24} & m_{25} & & & & & \\ m_{31} & m_{32} & m_{33} & m_{34} & m_{35} & & & & & \\ m_{41} & m_{42} & m_{43} & m_{44} & m_{45} & & & & & \\ m_{51} & m_{52} & m_{53} & m_{54} & m_{55} & & & & & \end{matrix} = \begin{matrix} 0.30 & 0 & 0 & 0 & 0 \\ 0.30 & 0.3 & 0 & 0 & 0 \\ 0.15 & 0.3 & 0.4 & 0 & 0 \\ 0.15 & 0.2 & 0.4 & 0.5 & 0 \\ 0.10 & 0.2 & 0.2 & 0.5 & 1.0 \end{matrix}$$

A typical feed distribution with slope of unity is given by:

$$F = \begin{matrix} f_1 & 0.516 \\ f_2 & 0.258 \\ f_3 & 0.129 \\ f_4 & 0.064 \\ f_5 & 0.033 \end{matrix}$$

For the case when M and F are known, the product matrix by matrix algebra is:

1. West Virginia University, Morgantown WV, 26505, USA.

$P_1 = 0.155$
 $P_2 = 0.232$
 $PF = MF = P_3 = 0.206$
 $P_4 = 0.213$
 $P_5 = 0.194$

Figure 1 shows the mill matrix operating on the feed five times in succession. Note that some product exits in the topline at all times. For the case that P and F are known, the problem (Inverse Problem) is to find M. For the case of wet grinding in a ball mill where all the top size is ground away during a small time interval, m_{11} and P_1 must both be zero. With these constraints, the number of unknowns in the mill matrix are reduced. The mill matrix becomes:

$$M = \begin{matrix} 0 & 0 & 0 & 0 & 0 \\ m_{21} & m_{22} & 0 & 0 & 0 \\ m_{31} & m_{32} & m_{33} & 0 & 0 \\ m_{41} & m_{42} & m_{43} & m_{44} & 0 \\ m_{51} & m_{52} & m_{53} & m_{54} & m_{55} \end{matrix}$$

In this example, there are 14 unknowns in the mill matrix. By performing the matrix multiplication of M and F, four equations relating the p_j to the m_{ij} and f_j can be developed. They can be generated from the following equation:

$$P_i = \sum_{j=1}^5 m_{ij} f_j \text{ for } 5 \geq i > 1 \tag{3}$$

From the conservation of mass described in Equation 2, the additional conservation equations can be generated from the following equation:

$$\sum_{i=1}^5 m_{ij} = 1.0 \text{ for } 5 \geq j \geq 1 \tag{4}$$

For the Inverse Problem there are 14 unknowns and only nine equations. Consequently, the solution is degenerate or underspecified. Normalisation or constraint equations need to be added to obtain a solution. The steady-state PBM constraint equations can be generated from:

$$1 \geq m_{ij} \geq 0 \tag{5}$$

Dynamic PBM model

The dynamic PBM model, also based on conservation of mass in the mill, uncouples the breakage rate and selection functions and introduces time as a variable. The k_i is the rate of breakage of particle size i in the mill, while the b_j are the breakage selection functions for the breakage of particles from class j into class i . The dynamic conservation of mass equations describing the

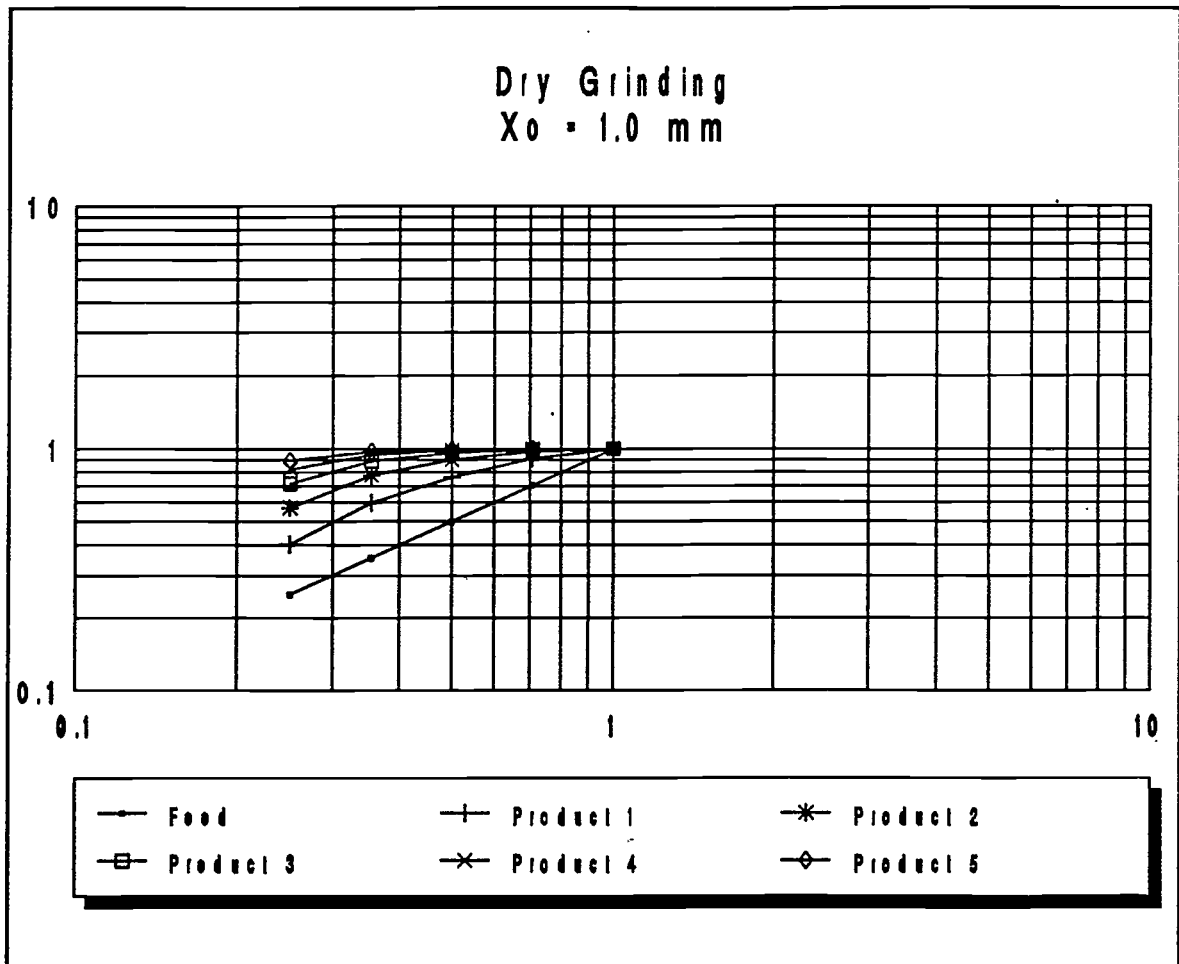


FIG 1 - Plot from a typical dry grinding mill showing the breakage at various times during which the topline in the mill does not change.

dynamic PBM model have been developed elsewhere (Herbst and Fuerstenau, 1980). The primary dynamic PBM conservation of mass equations for five particle sizes follow:

$$p_1 = f_1 + \int (p_1 * (-k_1)) dt \tag{6}$$

$$p_2 = f_2 + \int (p_1 * k_1 * b_{21}) dt - \int (k_2 * p_2) dt \tag{7}$$

$$p_3 = f_3 + \int (p_1 * k_1 * b_{31}) dt + \int (p_2 * k_2 * b_{32}) dt - \int (k_3 * p_3) dt \tag{8}$$

$$p_4 = f_4 + \int (p_1 * k_1 * b_{41}) dt + \int (p_2 * k_2 * b_{42}) dt + \int (p_3 * k_3 * b_{43}) dt - \int (k_4 * p_4) dt \tag{9}$$

$$p_5 = f_5 + \int (p_1 * k_1 * b_{51} + p_2 * k_2 * b_{52} + p_3 * k_3 * b_{53} + p_4 * k_4 * b_{54}) dt - \int (k_5 * p_5) dt \tag{10}$$

The integrals are all evaluated from time zero to the grinding time, t_m . In addition to Equations 6 - 10, the following conservation expression yields additional equations.

$$\sum_{i=1}^n b_{ij} = 1.0 \text{ for each } j \tag{11}$$

As with the steady-state PBM equation, the solution is degenerate or underspecified. For the Inverse Problem there are more unknowns than equations. Assumptions such as the Arbiter-Bhrany (1960) normalisation equation regarding the b_{ij} and k_i or additional constraints are required for solution. The dynamic PBM constraint equations can be generated from:

$$1 \geq b_{ij} \geq 0 \tag{12}$$

STEADY-STATE AND DYNAMIC PBM SOLUTION METHOD

The Levenberg-Marquardt (L-M) method was used to obtain both the steady-state and dynamic direct and Inverse Problem solutions to the PBM model (ANL, 1980; Levenberg, 1944; Marquardt, 1963). Solution of the steady-state equations involves the solution of a set of constrained or unconstrained algebraic linear or non-linear equations. The dynamic PBM solution involves the solution of a set of constrained or unconstrained linear or non-linear integral equations.

The L-M method is a quasi-Newton method which is a variation on the gradient method. The method involves finding the zeros of a vector of functions. In general, with these methods the simultaneous functions are approximated using a Taylor series. The equations are manipulated resulting in an explicit expression for new estimates of the x vector calculated from partial derivatives and the old x vector values. The procedure continues until there is no significant difference between estimated and old x vector values.

At each step in the actual procedure an error function is generated. The first partial derivatives of the error function with respect to the variables to be solved are determined in order to create a Jacobian matrix. The matrix equation solved is:

$$J * s + f(x) = 0 \tag{13}$$

where J is the Jacobian matrix, s is the vector step to take to generate the next estimate of unknown variables, $f(x)$ is the error function vector, and x is the vector of current estimates for unknown variables. For the first step, x is the vector of initial guesses. Subsequent x vectors are the sum of the previous x vectors and the s vector for that step. Computation of s was done by inverting the Jacobian at each step. For the sake of brevity, the algorithmic details of the technique are presented elsewhere (ANL 1980).

DISCUSSION

Steady-state PBM

The degeneracy or underspecifity of the steady-state PBM solution is problematic. There is no unique solution to the Inverse Problem unless additional constraints are provided or further assumptions made.

The severity of the nonuniqueness problem is demonstrated in the following example. Consider a typical feed distribution given by:

f_1	0.400
f_2	0.300
$F = f_3$	= 0.200
f_4	0.050
f_5	0.050

Assume an initial mill matrix M1 is given by:

m_{11}	m_{12}	m_{13}	m_{14}	m_{15}	.125	.000	.000	.000	.000
m_{21}	m_{22}	m_{23}	m_{24}	m_{25}	.100	.033	.000	.000	.000
$M = m_{31}$	m_{32}	m_{33}	m_{34}	m_{35}	= .300	.250	.025	.000	.000
m_{41}	m_{42}	m_{43}	m_{44}	m_{45}	.430	.200	.340	.000	.000
m_{51}	m_{52}	m_{53}	m_{54}	m_{55}	.045	.517	.635	1.00	1.00

The product matrix by matrix algebra is:

P_1	0.05
P_2	0.05
$P = M F = P_3$	= 0.20
P_4	0.30
P_5	0.40

Now the coefficient m_{32} in M1 above can be varied from 0.25 to 0.10. The mill matrices become:

m_{11}	m_{12}	m_{13}	m_{14}	m_{15}	.125	.000	.000	.000	.000
m_{21}	m_{22}	m_{23}	m_{24}	m_{25}	.100	.033	.000	.000	.000
$M2 = m_{31}$	m_{32}	m_{33}	m_{34}	m_{35}	= .300	.200	.100	.000	.000
m_{41}	m_{42}	m_{43}	m_{44}	m_{45}	.430	.200	.340	.000	.000
m_{51}	m_{52}	m_{53}	m_{54}	m_{55}	.045	.567	.560	1.00	1.00

m_{11}	m_{12}	m_{13}	m_{14}	m_{15}	.125	.000	.000	.000	.000
m_{21}	m_{22}	m_{23}	m_{24}	m_{25}	.100	.033	.000	.000	.000
$M3 = m_{31}$	m_{32}	m_{33}	m_{34}	m_{35}	= .300	.150	.175	.000	.000
m_{41}	m_{42}	m_{43}	m_{44}	m_{45}	.430	.200	.340	.000	.000
m_{51}	m_{52}	m_{53}	m_{54}	m_{55}	.045	.617	.485	1.00	1.00

m_{11}	m_{12}	m_{13}	m_{14}	m_{15}	.125	.000	.000	.000	.000
m_{21}	m_{22}	m_{23}	m_{24}	m_{25}	.100	.033	.000	.000	.000
$M4 = m_{31}$	m_{32}	m_{33}	m_{34}	m_{35}	= .300	.100	.200	.000	.000
m_{41}	m_{42}	m_{43}	m_{44}	m_{45}	.430	.200	.340	.000	.000
m_{51}	m_{52}	m_{53}	m_{54}	m_{55}	.045	.667	.410	1.00	1.00

The reader can verify that the matrix product for each of these four M_i ($i = 1, 2, 3, 4$) with the same F matrix is indeed the same P matrix.

It is interesting to further note that if one multiplies the $M_i F$ matrix by M_i (for each i) again, one obtains the wide range of values shown in Figure 2 for the various M_i . Obviously, when higher order terms are used involving mill matrix expressions during simulation or calculation (or iterative procedures are used during numerical simulation) and four or more size intervals are used, considerable amount of difference exists among the various

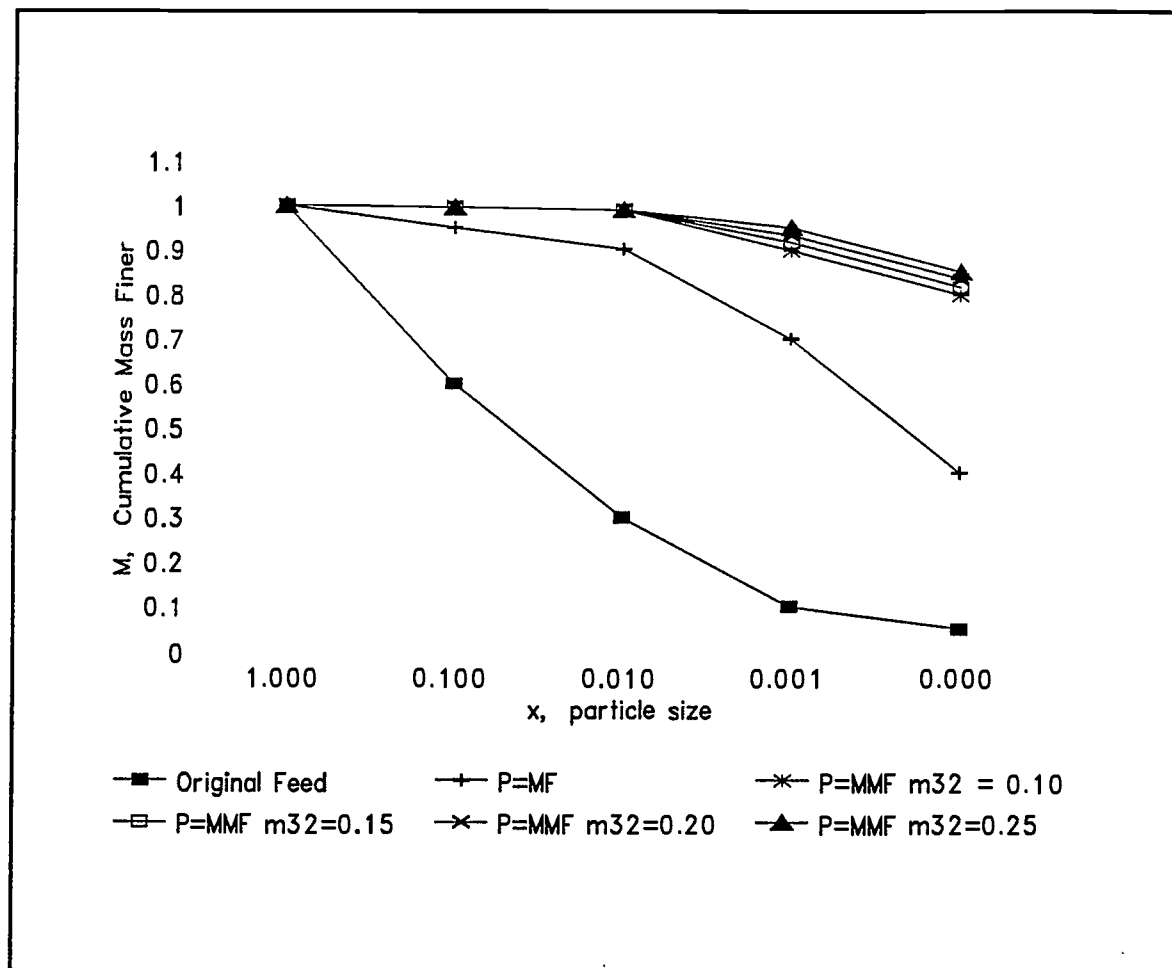


FIG 2 - The demonstration of the impact of nonuniqueness in PBM solutions involving higher order terms.

Inverse Solutions. This can result in a significant error propagation throughout any calculation. These errors could become significant when the grinding mills are placed into circuits or networks (Meloy, 1983; Williams and Meloy, 1983).

Underlying the numerical solution to the Inverse Problem is the assumption that the steady-state mill matrix is independent either of time or the size distribution of the feed, that is to say, both the selection and breakage matrices are time and particle size distribution invariant. As was shown by Meloy and Williams (1992 a and b) and Meloy *et al* (1990), for some wet grinding ball mill simulations, this assumption of linearity is not valid.

In wet grinding plots of the product from the mill (Fuerstenau and Sullivan, 1961; Coghill and Devany, 1937), when plotted as a log mass cumulative finer, $M(x)$, versus log particle size, x (Figure 3). It is in this case, when the plot of the mill product is a straight line, that the linearity assumption and the matrix methods are both mathematically and physically incorrect.

If, when sampling the product from a wet ball mill, there are two straight line plots for the product at two different grinding times, the larger size distribution of the earlier sampling time can be considered to be the feed for the smaller size product of the later sampling time. If one looks at the difference in the top size

particles between any two straight lines, one observes that all the particles in the top size range have been completely ground away - all the top size particles are gone. This means the probability of a particle in this largest top size fraction begins broken is identically one, not approximately one. No matter how close together the straight line plots for the mill product are (how short the grinding time), the probability that the largest particle will be broken is one. Put another way, the largest particle size is broken out of its class in an infinitely short time interval, that is, instantaneously. This is physically unrealistic.

Finally, the authors often noted in solving the steady-state PBM equations with the L-M technique, that the assumptions of normalisation could result in physically impossible solutions. When the normalisation assumption was used rather than the constraint equations, negative m_{ij} values were sometimes obtained. No negative values were ever obtained using the constraint equations.

Dynamic PBM

In order to assess the dynamic PBM actual grinding data was used (Klimpel, 1970). The following product $P(t_m=6)$ and feed composition F_a used was for anthracite coal being ground for six minutes:

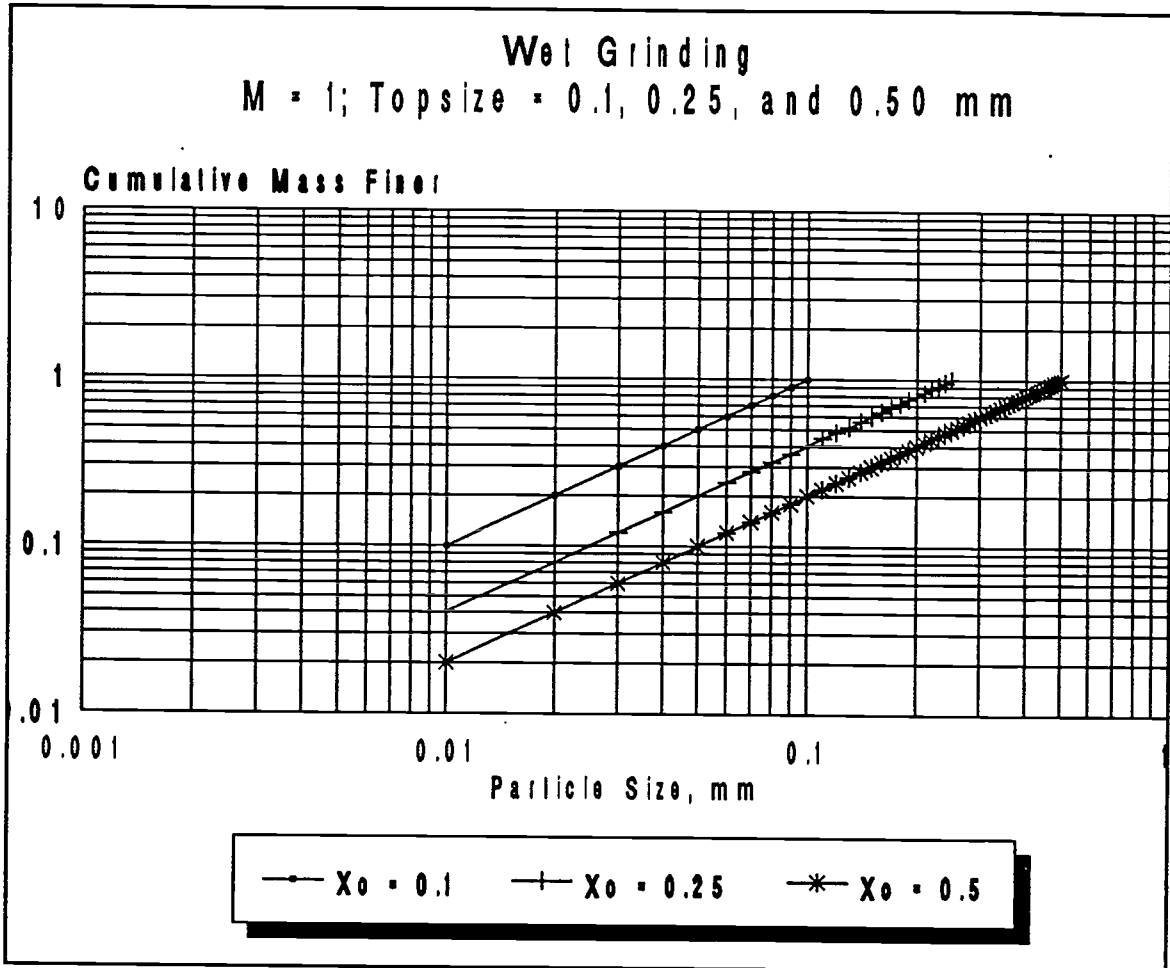


FIG 3 - Plot of product size distribution from a wet grinding mill showing the straight-line breakage at various times showing that the toptime (largest particle) in the mill changes (slope m is 1).

$f_1 = 0.250$
 $f_2 = 0.300$
 $F_a = f_3 = 0.240$
 $f_4 = 0.200$
 $f_5 = 0.010$

$b_{11} b_{12} b_{13} b_{14} b_{15} = .000 .000 .000 .000 .000$
 $b_{21} b_{22} b_{23} b_{24} b_{25} = .443 .000 .000 .000 .000$
 $B_c = b_{31} b_{32} b_{33} b_{34} b_{35} = .197 .404 .000 .000 .000$
 $b_{41} b_{42} b_{43} b_{44} b_{45} = .000 .200 .449 .000 .000$
 $b_{51} b_{52} b_{53} b_{54} b_{55} = .359 .396 .551 1.00 .000$

$f_1 = 0.100$
 $f_2 = 0.100$
 $P(t_m=6) = f_3 = 0.100$
 $f_4 = 0.200$
 $f_5 = 0.500$

In the second example, the selection functions were normalised. The normalisation procedure eliminates enough unknowns to permit solution. The normalisation equations are:

$$b_{41} = b_{52} \tag{14}$$

$$b_{42} = b_{53} \tag{15}$$

$$b_{31} = b_{42} \tag{16}$$

$$b_{32} = b_{43} \tag{17}$$

$$b_{21} = b_{32} \tag{18}$$

The L-M algorithm was used to predict the performance of the mill at 18 and 30 minutes. In the first example, inequality constraints were solved simultaneously with the conservation equations. The following solution was obtained:

$k_1 = 0.250$
 $k_2 = 0.444$
 $K_{ic} = k_3 = 0.462$
 $k_4 = 0.148$
 $k_5 = 0.000$

The following solution with the L-M algorithm was obtained:

$k_1 = 0.250$
 $k_2 = 0.428$
 $K_{im} = k_3 = 0.551$
 $k_4 = 0.237$
 $k_5 = 0.000$

$b_{11} b_{12} b_{13} b_{14} b_{15} = .000 .000 .000 .000 .000$
 $b_{21} b_{22} b_{23} b_{24} b_{25} = .380 .000 .000 .000 .000$
 $B_n = b_{31} b_{32} b_{33} b_{34} b_{35} = .620 .380 .000 .000 .000$
 $b_{41} b_{42} b_{43} b_{44} b_{45} = .000 .620 .380 .000 .000$
 $b_{51} b_{52} b_{53} b_{54} b_{55} = .000 .000 .620 1.00 .000$

The existence of non-unique solutions to the dynamic PBM which was just illustrated is, of course, problematic for researchers and industry. A dilemma is created as to which solution is correct and whether it is impossible to build up any type of a breakage selection and rate function knowledge base.

When one compares the functionality of the kinetic and breakage rate functions obtained through the constrained and normalisation approaches, one sees immediately the problems possible with a force fit - the possible violation of conservation of mass constraints resulting in negative values. Examination of K and B indicate that most deviation occurs in the smallest sizes.

An interesting additional problem also arises during the course of dynamic mill simulation. Predictions of time-varying performance of mills using different solution of dynamic PBM models, leads to predictions which deviate at long grinding times especially for the smaller size fractions. When the two different dynamic solutions (normalised (n) and constrained (c)) above are used to predict the performance at 18 and 30 minutes, the predictions begin to diverge, particularly for the smaller sizes. This can be seen in Figure 4. The problem could be expected to be magnified in mill circuits.

It should be noted that if the normalisation constraints are used for the selection breakage functions (B), errors can be created in the kinetic parameters to accommodate force fits to normalisation assumptions.

Functionality of mill selection and breakage rate functions

The non-uniqueness observations previously discussed are not trivial and may have contributed to the difficulty experienced in developing a body of knowledge about selection and breakage functions that are transferable from mill to mill. Generalisable comminution information has not yet appeared in the literature and is indicative of the existence of the non-linear problems in the PBM.

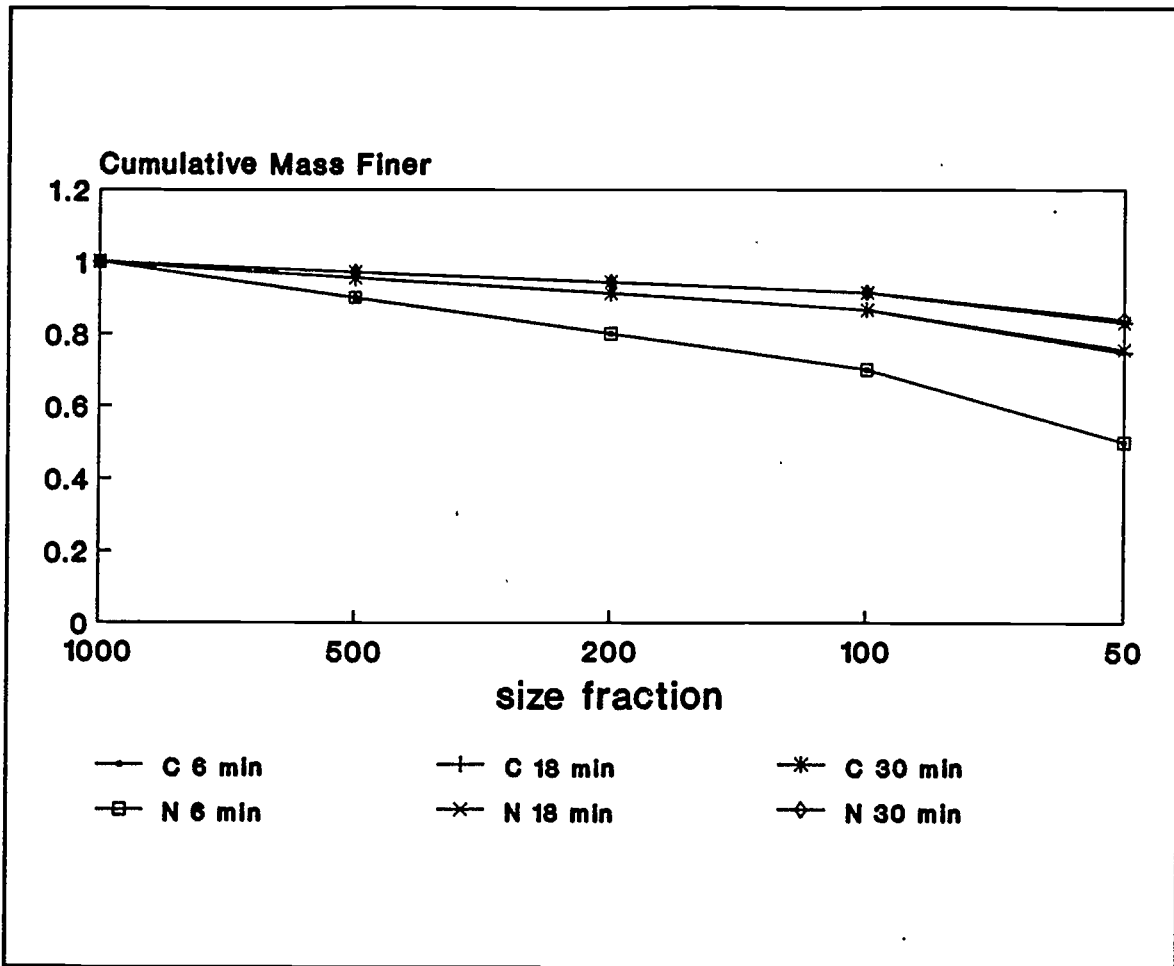


FIG 4 - The deviation of dynamic PBM model fits to experimental anthracite grinding data versus time.

The non-uniqueness of the solution, while a problem inherent in the solution of all PBMs wherever they are used, is not the only problem with PBMs. Another problem is the assumption that the elements of M or B are invariant with respect to time, composition (size distribution), rheology, temperature, slurry density, etc. The effect of these factors has been measured (Fuerstenau *et al.*, 1984; Klimpel, 1991; Klimpel, 1992).

In wet grinding Meloy and Williams (1992 a and b) have shown that the steady-state m_{ij} must be functions of the mill conditions such as mill loading and/or particle size distribution. A new mill matrix must be developed for each grinding time interval - or for each size distribution in the mill. The supposition of time variant M and B elements contradicts the basis linearity assumption used to justify the constancy and interrelatedness of the breakage and selectivity functions used to generate mill matrices. Thus, one cannot use the Arbiter-Bhrany (1960) or other such relationships, because they assume the matrix elements are constant over time.

Once the selection function becomes a function of the particle size distribution in the mill, then simulation using the PBM fails because the selectivity function is continuously varying. This means that even though two identical mills operate under nearly identical conditions, they will not have the same selectivity function.

Steady-state PBM mill matrices and the dynamic PBM selection and breakage rate functions are complex arrays composed of hundreds if not thousands of arbitrary constants which are arbitrarily chosen or curve fitted. With this number of arbitrary constants, a reasonable simulation of almost any phenomena can be made. It is, therefore, in surprise that pseudo mill matrices can be found to simulate a given wet mill for a given set of conditions, but this matrix is valid but for a fleeting instant in time. Unfortunately, these pseudo mill matrices are not transferable, they cannot be generalised, and thus they cannot be found in the literature.

CONCLUSIONS

An in depth review of the PBM used to simulate industrial wet grinding has found major flaws in the model showing:

1. There is no unique solution to the steady-state or dynamic PBM models. Several solutions were identified to yield the same product with the same feed matrix.
2. When steady-state mill matrix solutions were squared, significantly different product matrices were obtained.
3. Solution of dynamic PBM models using normalisation rather than mass balance constraints can lead to physically unrealistic solutions.
4. Predictions of time-varying performance of mills using different solution of dynamic PBM models, leads to predictions which deviate at long grinding times especially for the smaller size fractions.
5. Because of the non-uniqueness of PBM inverse solutions and the non-linearity of the mill matrices and selection and breakage rate functions for most commercial grinding circuits, no set of general mill selection functions and breakage rates have appeared or are likely to appear in the literature.
6. A useful line of comminution research would be to measure how the mill selection and breakage rates vary with the size distribution of the particles within the mill, as well as other mill conditions, such as slurry density, rheology, temperature etc.

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