Solution Approaches to the Dynamic, Population Balance Modeling of Grinding with Transport

M. C. Williams and T. P. Meloy
West Virginia University*

M. Tarshan
Visiting Fulbright Scholar, Assiut University**

Abstract

The solution of the dynamic population balance model (PBM) with transport is problematic. The fact that the dynamic PBM model equation solution to the Inverse Problem for grinding systems is degenerate or underspecified is demonstrated. Two numerical solution approaches to the Inverse Problem are used. These are: 1) providing additional constraints on breakage selection functions or 2) performing the Arbiter-Bhrany (or other) normalization of the selection functions. Actual experimental anthracite batch grinding data is used to demonstrate the non-unique functionality of the batch dynamic mill selection and breakage functions for a real physical system. The Levenberg-Marquardt algorithm for systems of constrained non-linear equations is used to solve the batch dynamic PBM grinding equations to obtain the grinding selection and breakage rate functions. Different solutions to the same PBM transport equations are provided. The mill was modeled as a CSTR operating at various retention times. Batch dynamic PBM data was used to provide the mill kinetic and breakage selection function data. Two different solutions were obtained depending on the numerical solution approach. The severity of the non-uniqueness problem for dynamic grinding is demonstrated. Each solution approach to a dynamic PBM with transport, while giving the same prediction for a single batch grinding time, gives different solutions or predictions for mill composition for other grinding times. This fact makes dynamic nodal analysis and control problematic. The fact that the constraint solution approach gives a solution may suggest that normalization is not necessary.

1. 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, Meloy and Bergstrom 1964, Reid 1965, Mika 1970, Austin and Malgan 1976, Herbst and Klimpel 1970, Malgan and Fuerstenau 1976, Klimpel and Austin 1970, Austin 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 with or without transport 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 normalization 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.

2. Dynamic PBM model

BATCH

The batch 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. In this paper the model is presented without the complication of transport. The \( k_i \) is the rate of breakage of particle size \( i \) in the mill, while the \( b_{ij} \) are the breakage selection functions for the breakage of particles from class \( j \) into class \( i \).

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

\[
\begin{align*}
p_1 &= f_1 + \int (p_1 (-k_1)) \, dt \\
p_2 &= f_2 + \int (p_1 k_1 b_{21}) \, dt - \int (k_2 p_2) \, dt \\
p_3 &= f_3 + \int (p_1 k_1 b_{31}) \, dt + \int (p_2 k_2 b_{32}) \, dt - \int (k_3 p_3) \, dt \\
p_4 &= f_4 + \int (p_1 k_1 b_{41}) \, dt + \int (p_2 k_2 b_{42}) \, dt + \int (p_3 k_3 b_{43}) \, dt - \int (k_4 p_4) \, dt \\
p_5 &= f_5 + \int (p_1 k_1 k_{51} + p_2 k_2 b_{52} + p_3 k_3 b_{53} + p_4 k_4 b_{54}) \, dt - \int (k_5 p_5) \, dt
\end{align*}
\]

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.

\[
\sum_{i=1}^{n} b_{ij} = 1.0 \quad \text{for each } j \tag{6}
\]

As with the steady-state PBM equation, the solution is degenerate or underspecified. For the Inverse Problem there are more unknowns than equations. In this paper two numerical solution approaches are compared. These are: 1) providing additional constraints on breakage selection functions or 2) performing the Arbiter-Bhhrany (or other) normalization of the selection functions. Assumptions such as the Arbiter-Bhhrany (1960) normalization equation regarding the \( b_{ij} \) and \( k_i \) may be used. However, additional constraints may be used. The dynamic PBM constraint equations are quiet logical and may be generated from:

\[
1 \geq b_{ij} \geq 0 \tag{7}
\]

**TRANSPORT**

With the addition of transport, mixing and dispersion phenomena are added to the PBM model. For the Continuous Stirred Reactor Model (CSTR) of transport where \( V \) is the mill volume, \( Q \) is the mill volumetric flowrate, and \( r \) (retention time) is \( V/Q \), one has the following equations for five particle classes:

\[
\begin{align*}
\frac{d(VM_1(t))}{dt} &= -k_1VM_1(t) - QM_1(t) + QM_{1F}(t) \\
\frac{d(VM_2(t))}{dt} &= -k_2VM_2(t) - QM_2(t) + QM_{2F}(t) + b_{12}k_1VM_1(t) \\
\frac{d(M_3(t))}{dt} &= -k_3M_3(t) - \tau M_3(t) + \tau M_{3F}(t) + b_{13}M_1(t) + b_{23}k_2M_2(t) \\
\frac{d(M_4(t))}{dt} &= -k_4M_4(t) - \tau M_4(t) + \tau M_{4F}(t) + b_{14}M_1(t) + b_{24}k_2M_2(t) + b_{34}k_3M_3 \\
\frac{d(M_5(t))}{dt} &= -k_5M_5(t) - \tau M_5(t) + \tau M_{5F}(t) + b_{15}M_1(t) + b_{25}k_2M_2(t) + b_{35}k_3M_3 + b_{45}k_4M_1(t)
\end{align*}
\]

In solving the transport PBM, the kinetic and breakage selection function data obtained from the batch dynamic PBM data is used in the above mill transport equations. The simultaneous, linear ordinary differential equations are solved with Laplace transform techniques. The Laplace transformed transfer functions for each particle class were developed. The inverse Laplace transform of the response was determined and the response in the time domain calculated.

### 3. 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:

$$ J \cdot s + f(x) = 0 \quad (13) $$

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).

In solving the transport PBM, the batch constants are used in the mill transport equations. The set simultaneous, linear ordinary differential mill transport equations are solved using Laplace transform techniques.

4. Discussion

BATCH

In order to assess the dynamic PBM, two examples were used. In the first example, actual grinding data was used (Klimpel 1970). Five particle classes experimentally representing standard sieve sizes were used. The following product $P(t_m = 6)$ and feed composition $F_a$ used was for anthracite coal being ground for six minutes:

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

In the first solution, inequality constraints were solved simultaneously with the conservation equations. The following solution was obtained for the batch PBM:

$$ k_1 = 0.250 \quad k_2 = 0.444 \quad k_3 = 0.462 \quad k_4 = 0.148 \quad k_5 = 0.000 $$

$$ B_n = b_{11} b_{12} b_{13} b_{14} b_{15} = 0.000 .000 .000 .000 .000 $$

$$ B_n = b_{21} b_{22} b_{23} b_{24} b_{25} = 0.443 .000 .000 .000 .000 $$

$$ B_n = b_{31} b_{32} b_{33} b_{34} b_{35} = 0.197 .404 .000 .000 .000 $$

$$ B_n = b_{41} b_{42} b_{43} b_{44} b_{45} = 0.000 .200 .449 .000 .000 $$

$$ B_n = b_{51} b_{52} b_{53} b_{54} b_{55} = 0.359 .396 .551 1.00 .000 $$

In the second solution, the selection functions were normalized. The normalization procedure eliminates enough unknowns to permit solution. The normalization equations are:

$$ b_{41} = b_{32} \quad (14) $$

$$ b_{42} = b_{33} \quad (15) $$

$$ b_{31} = b_{42} \quad (16) $$

$$ b_{32} = b_{43} \quad (17) $$

$$ b_{21} = b_{32} \quad (18) $$

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

$$ k_1 = 0.250 \quad k_2 = 0.428 \quad k_3 = 0.551 \quad k_4 = 0.237 \quad k_5 = 0.000 $$

$$ B_n = b_{11} b_{12} b_{13} b_{14} b_{15} = 0.000 .000 .000 .000 .000 $$

$$ B_n = b_{21} b_{22} b_{23} b_{24} b_{25} = 0.380 .000 .000 .000 .000 $$

$$ B_n = b_{31} b_{32} b_{33} b_{34} b_{35} = 0.620 .380 .000 .000 .000 $$

$$ B_n = b_{41} b_{42} b_{43} b_{44} b_{45} = 0.000 .620 .380 .000 .000 $$

$$ B_n = b_{51} b_{52} b_{53} b_{54} b_{55} = 0.000 .000 .620 1.00 .000 $$

The second physical example is similar.
In the first solution, inequality constraints were solved simultaneously with the conservation equations. The following solution was obtained:

\[
\begin{align*}
f_1 &= 0.100 \\
f_2 &= 0.300 \\
F(t_m = 6) &= f_3 = 0.100 \\
f_4 &= 0.300 \\
f_5 &= 0.200
\end{align*}
\]

In the second solution, the selection functions were normalized with the equations previously presented. The normalization procedure eliminates enough unknowns to permit solution. The following solution with the L-M algorithm was obtained:

\[
\begin{align*}
k_1 &= 0.250 \\
k_2 &= 0.428 \\
K_{ic} &= \begin{bmatrix} 
0.324 \\
0.013 \\
0.000 \\
\end{bmatrix} \\
b_{11} & b_{12} b_{13} b_{14} b_{15} .000 .000 .000 .000 .000 \\
b_{21} & b_{22} b_{23} b_{24} b_{25} .572 .000 .000 .000 .000 \\
B_c &= b_{31} b_{32} b_{33} b_{34} b_{35} = .132 .407 .000 .000 .000 \\
b_{41} & b_{42} b_{43} b_{44} b_{45} .008 .443 .437 .000 .000 \\
b_{51} & b_{52} b_{53} b_{54} b_{55} .289 .015 .563 1.00 .000
\end{align*}
\]

In the second solution, the selection functions were normalized with the equations previously presented. The normalization procedure eliminates enough unknowns to permit solution. The following solution with the L-M algorithm was obtained:

\[
\begin{align*}
k_1 &= 0.250 \\
k_2 &= 0.023 \\
K_{in} &= \begin{bmatrix} 
0.343 \\
0.000 \\
0.000 \\
\end{bmatrix} \\
b_{11} & b_{12} b_{13} b_{14} b_{15} .000 .000 .000 .000 .000 \\
b_{21} & b_{22} b_{23} b_{24} b_{25} .270 .000 .000 .000 .000 \\
B_n &= b_{31} b_{32} b_{33} b_{34} b_{35} = .730 .270 .000 .000 .000 \\
b_{41} & b_{42} b_{43} b_{44} b_{45} .000 .730 .270 .000 .000 \\
b_{51} & b_{52} b_{53} b_{54} b_{55} .000 .000 .730 1.00 .000
\end{align*}
\]

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, whether it may be impossible to build up any type of a breakage selection and rate function knowledge base, and whether or not normalization is required at all.

When one compares the functionality of the kinetic and breakage rate functions obtained through the constrained and normalization 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 matrices K and B indicate that most deviation occurs in the smallest sizes.

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

The non-uniqueness of the solution, while a problem inherent in the solution approaches of PBMs wherever they are used, is a key problem with PBMs solution approaches.

Another related PBM issue 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, Tarshan 1992).

In wet grinding Melay and Williams (1992a 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 basic linearity assumption used to justify the constancy and interrelatedness of the breakage and selectivity functions used to generate mill matrices. Thus, one must question the use the Arbiter-Bhary (1960) or other such relationship, because the assume the matrix elements are constant over time.

TRANSPORT

When these two different dynamic batch solutions (normalized (n) and constrained (c)) above are used to predict the temporal of performance of an anthracite grinding network composed of one CSTR mill, the predictions diverge, particularly for the smaller sizes. The temporal plots of mass fraction of particle classes 1 and 2 are shown in Fig. 1 - 4. Two different retention times are shown for the first example in Fig. 1 through 4. This example is for a real anthracite system.

For the sake of brevity, only the dynamic transport equation solutions for the first two particle classes are reproduced here. These rather complicated equations were solved by forming the Laplace transforms of the simultaneous, linear PBM transport equations, solving the set of equations for the respective M_{ij}(s), and inverting the transformed equations to find the
response in the time domain.

The equations for $M_1(t)$ and $M_2(t)$ are as follows:

$$M_1(t) = \frac{M_{1F} \tau^{-1}}{(k_1 + \tau^{-1})} \left( 1 - e^{-(k_1 + \tau^{-1})t} \right)$$

(19)

$$M_2(t) = \frac{M_{2F} \tau^{-1}}{(k_2 + \tau^{-1})} \left( 1 - e^{-(k_2 + \tau^{-1})t} \right) + b_{12}k_1M_{1F} \tau^{-1} \frac{1}{(k_1 + \tau^{-1}) (k_2 + \tau^{-1})} + \frac{e^{-(k_1 + \tau^{-1})t}}{(k_1 - k_2)(k_1 + \tau)} - \frac{e^{-(k_2 + \tau^{-1})t}}{(k_1 - k_2)(k_2 + \tau^{-1})}$$

(20)

Obviously, examination of the figures reveals that predictions of time-varying performance of mills using different solution of dynamic PBM models leads to predictions which deviate at subsequent grinding times. This deviation is both startling and troublesome.

The effect of retention time in the mill is an important factor. At short retention times the mill contents raise quickly to their steady-state concentrations. At long retention times the temporal divergence is more prevalent and pronounced. Unfortunately different initial batch solutions lead to different steady-state concentrations in the mill.

Other approaches or data fitting techniques to batch data over different time intervals would expect to have the same inaccuracies. Other approaches include fitting the transport PBM equations to the first two time intervals of the transport experimental data, developing time and concentration dependent kinetic and selection breakage functions, and doing a global least squares type regression to batch or transport data over all time periods. It is the belief of the authors that this tantamount to just placing inaccuracies in other areas.

However, even though it is possible that the constrained solution approach may make up for the lack of determinacy in the PBM model, it is no substitute for a better quantifiable understanding of the dependencies of mill concentration on kinetics and breakage rate functions.

The temporal plots of mass fraction of particle classes 1 and 2 for the second physical example are shown in Fig. 5 - 8. Two different retention times...
are also shown for the example in Fig.5 through 8 for mill concentrations for the first two particle classes. Results and trends are similar for the other three particle classes whose figures are not shown for the sake of brevity. The results for the second physical example are quiet similar to the first even though the normalization assumptions appear less valid.

Unfortunately, the problem demonstrated in this problem could be expected to be magnified in mill networks. Network dynamic nodal analysis and control strategies would likely be different for each case.

An interesting additional problem also arises during the course of dynamic mill simulation which make dynamic nodal analysis and control problematic. Predictions of time-varying performance of mills using different solution of dynamic PBM models will lead to different control and operating strategies.

5. Conclusions

1 There is no unique solution to the batch dynamic PBM models. Different solutions were identified to yield the same product with the same feed matrix for actual anthracite grinding.

2 Solution of dynamic PBM models using normalization rather than mass balance constraints may not be necessary. In fact, normalization may lead to physically unrealistic solutions.

3 Predictions of the time-varying transport performances lead to predictions which deviate from other solution approaches to dynamic PBM transport models lead to predictions which deviate at other grinding times for all CSTR retention times.

4 Because of the differences in the constrained and normalization solution approaches, dynamic mill simulation, dynamic nodal analysis and control become problematic.

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