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Solution of the breakage matrix reverse problem

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ABSTRACT

This paper is a complete overview of the reverse problem in the breakage matrix context. The procedure for calculating the input particle size distribution to a milling operation in order to obtain the desired output particle size distribution is given. The reverse problem was solved by the "precision" and "approximation" approaches. For the precision case, a detailed algorithm is presented, where in every step a precise range for the current output is provided. This approach is limited with a number of output size fractions that can be freely chosen. On the other hand, the approximation approach gives the best-fit solution which corresponds to the desired output particle size distribution. In this case the problem is solved by the orthogonal decomposition and non-negative least squares method and by semilogarithmic loss function. Applicability of the proposed methods was confirmed by examples related to wheat milling.

1. Introduction

Over the years, various modeling approaches (such as discrete element method, finite element method, population balance models, breakage matrix approach, etc.) were used for the analysis of particle breakage in the comminution processes. Population balance type of modeling (PBM) is probably most often used to mathematically describe the comminution process (for examples refer to [1–4]. PBMs are based on monitoring the evolution of particle size distribution (PSD) over time. Therefore, continual sampling within the process is required which is difficult or sometimes essentially impossible to achieve. The breakage matrix approach treats an entire process as a single breakage event. Although it is less informative than the population balance approach, it is more applicable to practical experiments [5]. The relationship between the input size vector (f) and the resulting output size vector (o) is described by the matrix equation:

$$B \cdot f = o, \qquad (1)$$

or in expanded form:

$$\begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ b_{21} & b_{22} & \cdots & b_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ b_{m1} & b_{m2} & \vdots & b_{mn} \end{bmatrix} \cdot \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix} = \begin{bmatrix} o_1 \\ o_2 \\ \vdots \\ o_m \end{bmatrix}, \qquad (2)$$

where f and o are column vectors of the PSD in the input and output material from a milling operation, and B is the breakage matrix. The breakage matrix approach is convenient for studies where PSDs are measured discretely using sieve analysis [6]. Elements of the breakage matrix B can be determined by milling narrow sized range fractions of inlet material and the obtained PSDs from the sieve analysis form the corresponding columns of the breakage matrix. Therefore, coefficients b_{ij} represent the weight fraction of the size range j of the output material obtained by milling the size range i of the input material. Since the elements of the breakage matrix, as well as the elements of input and output vectors, are weight fractions their values must be within the unit interval [0,1]. Moreover, the sum of the elements in every column equals 1.

The breakage matrix is associated with the PBM concept and it is effectively a combination of the selection function and the breakage function. The selection function is a mass fraction of particles that are selected and broken in time (during the process). The breakage function is a mass fraction of breakage products from size x that fall below size y, where $x \geq y$ [7]. The selection function is encompassed in diagonal elements of the breakage matrix, and the breakage function is in the off-diagonal elements [5].

Breakage matrix approach was first introduced by Broadbent and Callcot [8–10] to describe cone milling of coal, and later used to study milling of stone [11,12], coal [13] and wheat [6,14,15].

Broadbent and Callcott [8–10] used the same sieve sizes for both feed and product size distributions, giving a square breakage matrix (dimension N × N), where the above diagonal values are equal to zero.

The breakage matrix approach described in Eqs. (1)–(2) is appropriate for modeling comminution processes in once-through type of mills where retention time of the particles in the mill is short, such as roller mills or cone mills. One of the prime examples of roller mills application is wheat flour milling. Applicability of the breakage matrix approach for predicting the PSD on the first-break roller milling of wheat was confirmed by [14] and [6]. Retention time of wheat kernels in the roller

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mills grinding zone is very short. It is measured in m/sec, as it was shown by [16,17] using high-speed video system to observe wheat kernel breakage. Wheat flour milling is a gradual reduction process consisting of sequential and consecutive size reduction and separation with up to 16 roller milling operations (so called passages). After every grinding step the ground material is sieved and the undersize material removed before regrinding. This means that the grinding passages throughout the flour milling process differ in characteristics of the input material to the rolls, as well as in the set of roll parameters which are adjusted according to the characteristics of the input material. Although there is a number of grinding steps in the process, theoretically every step can be observed as once-through type of mill with very short retention time and therefore with its own breakage matrix.

Usually, the PSDs of the feed and milling output occur in different size ranges. Also, under the compressive crushing forces, it is entirely possible for a wheat kernel to break so as to produce flattened bran flake with dimensions larger than the kernel from which it came [16,17]. These facts are not accounted in square and triangular matrices of Broadbent and Callcott. Using different sized sieves and different number of sieves for inlet and outlet size distributions, the breakage matrices became non-square and non-triangular.

In a retention-type of mills multiple breakage events are likely to occur and PBM models are preferred [1,4]. The discrete linear PBM (DL-PBM) observe comminution process as series of elementary breakage events during the time. Then Eq. (1) is written as follows

$$B^k \cdot o^{(0)} = o^{(k)}, \tag{3}$$

where $o^{(0)}$ and $o^{(k)}$ are mass fraction frequency distribution at time $n = 0$ and $n = k$.

In spite of the advantages of the breakage matrix method, there are some limitations as the breakage matrix determined for one set of conditions cannot be used for another set of conditions [2]. Also, Eq. (1) presumes that particle breakage is independent of any inter-particle interactions (irrespective of the size distribution of surrounding particles). This assumption seems improbable in a retention-type of mill, especially in dense-phase systems, because it ignores multi-particle interactions during breakage. Some recent papers of [4,5,18,19] deal with the modified breakage matrix methodology in order to characterize multi-particle interactions during breakage. They include the influence of the multi-particle interactions among particles of different sizes during breakage. The problems of discrete non-linear PBM (DNL-PBM) and time-continuous non-linear PBM (TCNL-PBM) are introduced and studied in [3,4,18,20]. In particular, inverse problem and parameter estimation are studied in [18] which define breakage matrix methodology for characterization of multi-particle interactions in dense-phase systems.

Considering Eq. (1) the output PSD (vector o) can be altered by changing the breakage matrix (B) or by changing the input PSD (vector f). Usually, the most efficient way to influence the outlet PSD is by changing the process. In such way the desired outlet PSD is obtained by changing the breakage matrix (B). The significance of the forward problem and the inverse problem (parameter identification) is well-established in literature. The other possible approach, which has been addressed in this paper, is to identify the input PSD that would result in a desired output PSD. This approach implies that the breakage matrix (B) is constant and therefore it applies to the same set of milling conditions.

Examples given in the paper are related to roller milling of wheat. Therefore it is assumed that the particle breakage is independent of any inter-particle interactions. Also, it is presumed that the PSDs of the input and output occur in different size ranges. The study is carried out as a general case where a number of inputs and outputs could be different and the elements of the breakage matrix are arbitrary values between 0 and 1.

Fistes et al. [21] started the study of the reverse problem in the breakage matrix context in. This could be useful in milling operations where the possibility of controlling PSD of the input material exists. In that paper, the procedure for calculating the input PSD in a milling operation, in order to obtain the desired output PSD, is given. This is done by the transformation of the matrix Eq. (1) using standard Gaussian elimination techniques. Considering the number of input (n) and output (m) size fractions three different cases ($m = n$, $m > n$ and $m < n$) were studied. The case with more output than input size fractions ($m > n$) seems to be the most interesting case not only mathematically but also for its potential for practical application. In this case with the overdetermined set of linear equations, the values of $n - 1$ outputs are precisely defined, which then dictate the remaining $m - n$ output fractions. However, using this technique it is still possible to specify an output PSD that is unachievable with positive input values. To prevent that, the problem is interpreted as a system of linear inequalities and solved by a linear programming method. Acceptable outputs are the points in the interior of the convex polyhedron. Moreover, vertices of the polyhedron are the columns of the breakage matrix.

The other possible approach is to find a best-fit solution which corresponds to desired m output values. In the case of overdetermined set of linear equations associated by Eq. (1), the problem could be observed in the linear least square sense [22–27]. These problems are usually solved by orthogonal decomposition methods. For example, authors in [28] proposed that in their study on reconstruction of bubble size distributions from slices could be solved by singular value decomposition (SVD) method.

Thus, there are two possible ways for solving the reverse problem, namely "precision" and "approximation". Both of them have been extended and thoroughly discussed in this paper.

In the "precision" approach, instead of choosing $n - 1$ output simultaneously it is possible to set outputs one at the time, where in every step a precise range for the current output is provided [21]. The order of the outputs could be defined by the user's preferences. This approach leads to an algorithm (given in Section 2.); hence, the problem could easily be implemented. For dimension $n = 4$ a geometrical interpretation of the procedure is illustrated by an example.

In the "approximation" approach different numerical methods could be used such as: LU and Cholesky decomposition, modified Gram–Schmidt orthogonalization, SVD and QR decomposition with many modifications [22,23,25]. It should be noted that although the elements of the breakage matrix and chosen output PSD (weight fractions of output size fractions) are positive, the solution (weight fractions of input size fractions) obtained by the least square methods could be negative. Positive linear inverse problems are intensively investigated, usually in a strongly mathematical context, with many interesting applications [29–32]. Negative solutions could be avoided by imposing additional conditions or by using some other method instead of the least square. The first option is known as non-negative least squares problem (NNLS) with a well known algorithm [23]. Also, NNLS could be observed as a linear programming problem, where the least square estimate of error term is a function which is minimized. As another option, instead of least squares it is possible to use some other estimates of error in order to avoid negative solutions. In that case, positivity condition is integrated in the error approximation norm. For this purpose, semilogarithmic loss function [33] is used. In both cases (NNLS and semilogarithmic loss function) it is possible to add weighted coefficients to the minimization function and give different importance to the outputs. QR decomposition, NNLS and semilogarithmic loss function are used in the examples given in the paper which are related to wheat milling.

2. Theoretical part

Let us recall Eq. (1), by B is denoted the breakage matrix and by f and o are denoted input and output vectors, respectively. Then, the following conditions hold:

$$\sum_{j=1}^{n} f_j = 1, \quad \sum_{i=1}^{m} o_i = 1 \quad \text{and} \quad \sum_{i=1}^{m} b_{ij} = 1, j \in \{1, 2, \ldots, n\}. \tag{4}$$