Discretization Procedure for the Breakage Equation

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Fragmentation processes are important for several engineering applications, such as floc disintegration, drop breakage, and comminution of particulate solids. The continuous population balance equation that describes such processes is (Randolph and Larson, 1988)

$$\frac{dn(v,t)}{dt} = \int_v^\infty b(v,w)s(w)n(w,t)\,dw - s(v)n(v,t), \quad (1)$$

where $n(v,t)$ is the particle density function, that is, $n(v,t)\,dv$ is the number concentration of particles with mass in the range $[v, v+dv]$; the term $s(v)n(v)$ is the rate of breakage of particles v, and $s(v)$ is the breakage rate coefficient; $b(v,w)$ is the fragment distribution function, and $b(v,w)\,dv$ represents the number of particles with mass between v and $v+dv$ produced upon fragmentation of one particle of mass w. When the particles are formed by lumps of monomers with approximately the same size, as in the case of aggregates, Eq. 1 can be restated in discrete form:

$$\frac{dn_i(t)}{dt} = \sum_{j=i+1}^{\infty} b_{i,j}s_j n_j(t) - s_i n_i(t) \quad i = 1,2,3,\ldots, \quad (2)$$

where now $n_i(t)$ is the number concentration of particles made by i monomers.

In this note a sectional representation for Eqs. 1 and 2 is proposed in order to simplify the solution of the fragmentation problem. For the sake of simplicity the derivation reported below considers the continuous form of the population balance only. The extension to the discrete case is summarized in the Appendix.

The method proposed here is a modification of that developed by Hill and Ng (1995). The considered size range is divided into m arbitrary sections: $[v_{h-1}, v_h]$, $h = 1, 2, \ldots, m$. The number concentration of the particles belonging to a section is calculated according to the following expression:

$$N_h(t) = \int_{v_{h-1}}^{v_h} n(v,t)\,dv. \quad (3)$$

In each section h, a representative particle is chosen with mass v_h^* $(v_{h-1} \le v_h^* \le v_h)$, and it is assumed that every particle in the section behaves as such a particle. Moreover it is supposed that the particle density function, $n(v,t)$, is a constant in the section, equal to $n(v_h^*, t)$. Therefore,

$$N_h(t) = (v_h - v_{h-1}) \cdot n(v_h^*, t). \quad (4)$$

Now it is postulated that the balance equation of N_h assumes a form similar to Eq. 2:

$$\frac{dN_h(t)}{dt} = \sum_{k=h+1}^{m} C_k^{(1)} B_{h,k} S_k N_k(t) - C_h^{(2)} S_h N_h(t) \quad h = 1,2,\ldots,m, \quad (5)$$

where S_h is the breakage rate coefficient evaluated in v_h^*:

$$S_h = s(v_h^*), \quad (6)$$

$B_{h,k}$, the new fragment distribution function, is the number of child particles that fall in interval h from the rupture of the representative particle of interval k:

$$B_{h,k} = \int_{v_{h-1}}^{v_h} b(v, v_k^*)\,dv, \quad (7)$$

and the constants $C_h^{(1)}$ and $C_h^{(2)}$ are correction terms, whose scope is to reduce the two sources of errors in the sectional balance. If these constants were set to 1, the fragment distribution function, as defined by Eq. 7, would introduce some loss or gain of mass, depending on the choice of v_k^*. Moreover, the death term $(-S_h N_h)$ in Eq. 5 would not consider the possibility of a fragment remaining in the same section as its parent particle.

The first constraint needed to determine $C_h^{(1)}$ and $C_h^{(2)}$ is the condition of conservation of mass. According to Hill and

Ng, such a constraint leads to the following relationships:

$$C_1^{(2)} = 0$$

$$v_h^* C_h^{(2)} = C_h^{(1)} \sum_{k=1}^{h-1} v_k^* B_{k,h} \quad h = 2,3,\ldots,m. \tag{8}$$

The other condition imposes the correct evaluation of the death term. By comparing Eq. 5 and Eq. 1, the net rate at which particles are removed from section h must be given by

$$C_h^{(2)} S_h N_h(t) = \int_{v_{h-1}}^{v_h} s(v) n(v,t)\, dv - \left[\int_{v_{h-1}}^{v_h} \int_{v}^{v_h} b(v,w) s(w) n(w,t)\, dw \right] dv. \tag{9}$$

As shown by the right side of the equality, such rate is the difference between the total rate of death over the whole section and the rate of birth of child particles from parent particles belonging to the same section. Applying the assumption that the particle density and the breakage rate coefficient are constant in each section, Eqs. 4 and 6, one can obtain the required relationship:

$$C_h^{(2)} = 1 - \frac{1}{v_h - v_{h-1}} \int_{v_{h-1}}^{v_h} \left[\int_{v}^{v_h} b(v,w)\, dw \right] dv \quad h = 2,3,\ldots,m. \tag{10}$$

The procedure can be easily implemented in a computer code according to the following algorithm:

- Selection of section boundaries $v_0, v_1, v_2, \ldots, v_m$ and of representative section elements: $v_1^*, v_2^*, \ldots, v_m^*$.
- Evaluation of S_h and of $B_{h,k}$ from Eqs. 6 and 7.
- Evaluation of the initial conditions $N_h(0)$ from $n(v,0)$ by applying Eq. 3.
- Calculation of the constants $C_h^{(1)}$ and $C_h^{(2)}$ adopting Eqs. 8 and 10.
- Integration of the set of ordinary differential equations (Eq. 5).

For small values of h some types of fragment distribution function may give $B_{h,k} = 0$ for $k = 1, 2, \ldots, h-1$, and thus the summation of the righthand side of Eq. 8 vanishes, leaving $C_h^{(1)}$ indeterminate. In this case $C_h^{(1)}$ can be set to any finite value without affecting the correctness of the solution, since the corresponding birth term in Eq. 5, $C_h^{(1)} B_{k,h} S_h N_h(t)$, vanishes as well, as $B_{k,h} = 0$.

Results and Discussion

The procedure described here differs significantly from the method proposed by Hill and Ng (1995) only in the choice of the second set of constraints. While our method ensures the correct evaluation of the death term in the sectional balance, Hill and Ng imposed the correct prediction of the total number of particles (the zeroth moment of the distribution). Such a condition is likely to lead to solutions that are slightly more accurate, as will be shown later, but it may require complex analytical derivations that depend on the particular expressions used for the fragment distribution function and that cannot be executed automatically by a computer code. Hill and Ng made these derivations for three forms of the fragment distribution function only, considering exclusively the case in which $s = s_0 v^\alpha$ and the particle-size distribution is continuous. On the contrary, our model can be fully automated, provided that Eq. 10 is evaluated numerically, regardless of the form of the rate coefficient or of the breakage distribution function, and it can be applied both to continuous and to discrete distributions.

In order to evidence the properties of the method, two test cases are examined:

Continuous form: Uniform distribution of fragments

The following expressions for fragment distribution function, rate coefficient, and initial conditions have been adopted:

$$b(v,w) = \frac{2}{w} \qquad s(v) = s_0 v^2$$

$$n(v,0) = \begin{cases} 0 & 0 \le v < V_m \\ n_0 & V_m \le v < V_M \\ 0 & V_M \le v, \end{cases}$$

with $V_m = 0.6144 \times 10^{-11}$ kg; $V_M = 1.2288 \times 10^{-11}$ kg; $s_0 = 1 \times 10^{20}\ \text{s}^{-1}\ \text{kg}^{-2}$; $n_0 = 1 \times 10^6\ \text{m}^{-3}$. The analytical solution of this problem is (Prasher, 1987)

$$n(v,t) = \begin{cases} n_0 s_0 t \left(V_M^2 - V_m^2 \right) e^{-s_0 v^2 t} & 0 \le v < V_m \\ n_0 \left[1 + s_0 t \left(V_M^2 - v^2 \right) \right] e^{-s_0 v^2 t} & V_m \le v < V_M \\ 0 & V_M \le v. \end{cases}$$

The problem has been solved using a geometric discretization with 28 sections ($v_{28} = V_M$) and $v_h / v_{h-1} = \sqrt{2}$. The mass of the representative section element, v_h^*, is the arithmetic mean of the two endpoints of the section. The system of ordinary differential equations (Eq. 5) has been integrated using the routine *lsode* from package ODEPACK (Hindmarsch, 1983), that implements a variable order−variable step predictor−corrector method.

Figure 1 reports the time evolution of the first four moments of the particle-size distribution, and compares the results of our procedure with the rigorous analytical solution and with the results of Hill and Ng's method (with the same set of discretization nodes). As already anticipated, the quality of our solution is slightly worse than that of Hill and Ng. Anyway, accuracy can be improved easily by increasing the number of nodes: if the number of adopted sections is doubled, the two sectional solutions become practically indistinguishable from the analytical result. Of course, doubling the number of nodes may lead to the unwanted effect of overdiscretizing, by creating a number of sections greater than that allowed by experimental data. In these cases, the procedure should include a final step in which the numerical results are regrouped into the larger intervals corresponding to the data. However, as an additional simulation with a double number of nodes provides a good estimate of the error of the method

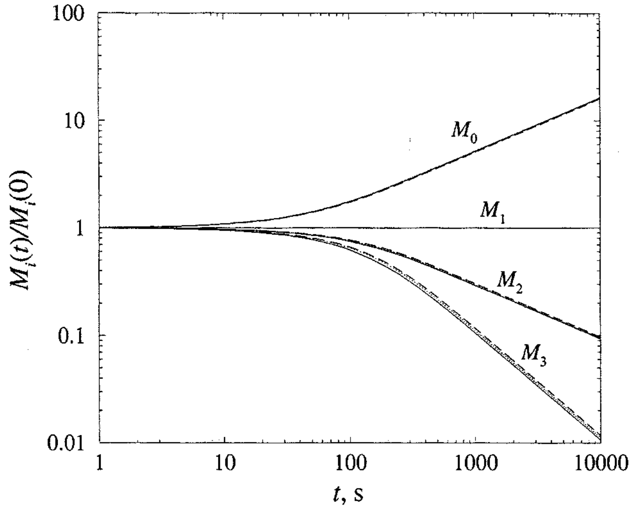

Figure 1. Predicted evolution of the first four moments of the particle mass distribution for uniform binary breakage according to analytical solution (——); Hill and Ng's sectional method (····); proposed sectional method (– – –).

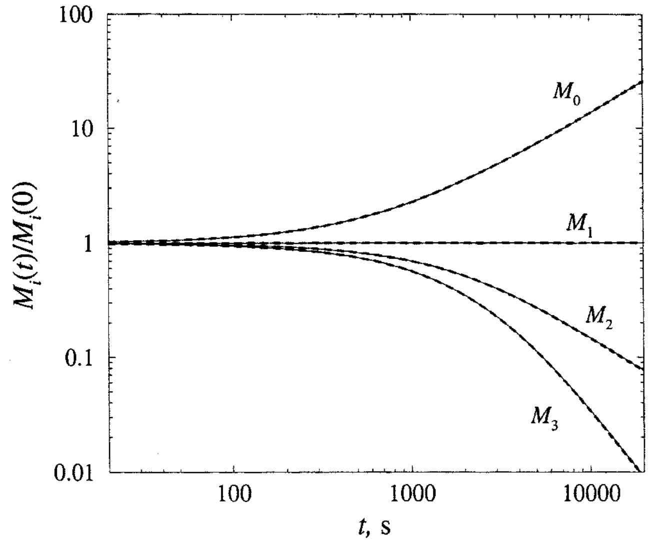

Figure 2. Rigorous solution (thick dashed line) vs. sectional approximation (thin solid line) in predicting moments of the particle mass distribution for breakage with formation of two fragments with mass ratio 1:4.

(by comparing the original and the refined solution), overdiscretizing is always suggested in the real cases, in which the accuracy of the method cannot be verified by comparison with a rigorous simulation.

Discrete form: Two fragments with size ratio 1:4

A discrete system in which breakup gives rise to two fragments with size ratio 1:4 has been modeled as well. Such a situation was considered by Kusters et al. (1997) as representative of the breakage of aggregates. In this case, the rate coefficient has been assumed to be $s_i = 10^{-6} \cdot i \ \mathrm{s}^{-1}$ and the initial condition is

$$n_i(t) = \begin{cases} 0 & \mathrm{m}^{-3} \quad i = 1, 2, \ldots, 1{,}200 \\ 10^4 & \mathrm{m}^{-3} \quad i = 1{,}201, \ldots, 1{,}300 \\ 0 & \mathrm{m}^{-3} \quad i = 1{,}301, \ldots. \end{cases}$$

Figure 2 compares the first moments of the particle-size distribution as calculated by the rigorous discrete population balance, Eq. 2, and the proposed sectional method with uniform discretization in 26 classes and $v_h^* = (v_{h-1} + v_h)/2$. As before, the two differential systems have been integrated using the routine *lsode*. In this case, too, the prediction of the proposed sectional method is accurate, demonstrating its ability to simulate discrete systems and strongly discontinuous breakage distribution functions.

A final point concerns the choice of the representative section element, v_h^*, and the possibility of identifying an optimal location for it in order to reduce the error, since the only requirement of the method is $v_{h-1} \le v_h^* \le v_h$. This location is likely to depend on the particular configuration considered (i.e., breakage rate expression, fragment distribution function, initial size distribution), and it is not possible to obtain precise criteria for its determination in the general case. Nevertheless, it seems intuitive that one should not choose v_h^* near the endpoints of the interval, but rather take a mean value. Good results have been obtained adopting the arithmetic mean of the two endpoints (as was also done by Hill and Ng), and this choice seems slightly superior to other types of mean (geometric or arithmetic with a different weight factor). Although this is not the optimal selection of v_h^*, the gain in accuracy given by a better choice is not very high, especially in comparison to what can be obtained by increasing the number of sections.

Notation

$b_{i,j}$ = fragment distribution function in the discrete balance equations
s_i = breakage rate coefficient for the discrete balance equations, 1/s
t = time, s
v = mass of a particle, kg
v_h = mass of the particles at the upper boundary of section h, kg

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Appendix

In order to obtain a sectional representation for the discrete population balance equation, one must replace Eq. 3

with

$$N_h(t) = \sum_{i=i_{h-1}+1}^{i_h} n_i(t), \tag{A1}$$

where the section boundaries i_0, i_1, ..., i_m are expressed in terms of number of monomers. The representative particle is constituted by i_h^* monomers and therefore:

$$N_h(t) = (i_h - i_{h-1}) \cdot n_{i_h^*}(t) \tag{A2}$$

$$S_h = S_{i_h^*} \tag{A3}$$

$$B_{h,k} = \sum_{i=i_{h-1}+1}^{i_h} b_{i,i_k^*}. \tag{A4}$$

The sectional balance equation (Eq. 5) remains valid, but the expressions for the correction factors change to:

$$C_1^{(2)} = 0$$

$$C_h^{(2)} = 1 - \frac{1}{i_h - i_{h-1}} \sum_{i=i_{h-1}+1}^{i_h} \sum_{j=i+1}^{i_h} b_{i,j} \qquad h = 2,3,\ldots,m \tag{A5}$$

$$i_h^* C_h^{(2)} = C_h^{(1)} \sum_{k=1}^{h-1} i_k^* B_{k,h} \qquad h = 2,3,\ldots,m. \tag{A6}$$

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