A Simple Model of Particle Coalescence and Breakup

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ABSTRACT

A simple model of the evolution of particle size distributions by coalescence and spontaneous and binary disintegrations is formulated. Spontaneous disintegration involves single particles, while coalescence and binary disintegrations involve pairs of particles. Analytical solutions for the mean mass of the distribution and the equilibrium size distribution are obtained for the case of constant collection kernel and disintegration parameters. At equilibrium, the *forms* of the size distributions are identical under the action of coalescence and either or both disintegration processes; the particle concentration is proportional to the total mass concentration (M) and the mean mass of the distribution is independent of M when only coalescence and binary disintegrations are operative. At small values of M, the effects of spontaneous disintegrations dominate over those of binary disintegrations while the reverse is the case at large values of M. Some of the findings of the present simple model are in qualitative agreement with the results of numerical calculations of the evolution of raindrop size spectra with realistic formulations of drop coalescence and breakup.

1. Introduction

Coalescence and breakup are among the important processes governing the evolution of precipitation particle size spectra. Coalescence alone tends to increase the concentration of the larger particles, and decrease that of smaller particles. Particle breakup opposes this tendency of coalescence and it is conceivable that a combination of coalescence and breakup would produce stationary particle size distributions. Indeed this was found to be the case in a number of numerical studies of the evolution of particle size spectra. Srivastava (1971) found equilibrium size spectra resulting from the action of coalescence and spontaneous breakup of raindrops. Studies of coalescence and spontaneous and collisional breakup (e.g., Young, 1975; Srivastava, 1978; Gillespie and List, 1978) also showed the development of an equilibrium size distribution for raindrops. Furthermore, it was found that (i) the effect of collisional breakup dominates over that of spontaneous breakup at large particle concentrations, while the reverse is the case at small concentrations; and (ii) the equilibrium size distributions, resulting from coalescence and collisional breakup for different mass concentrations (M), are parallel to each other, or more explicitly, at equilibrium, the particle concentrations are proportional to M.

In this paper, we set up a simple formulation of particle coalescence and breakup which admits of analytical solutions. These solutions show explicitly the approach to equilibrium and the relative importance of spontaneous and collisional breakup in determining the particle size distributions. The solutions also reproduce qualitatively some of the results found in the numerical calculations cited above.

2. Model and equations

We consider a discrete size distribution, the particle masses being taken as the integers. The process of coalescence cannot produce particles of non-integral mass. The process of particle breakup will be formulated so that it too cannot produce particles of non-integral mass.

The usual formulation of particle coalescence will be adopted, that is, the rate at which particles of masses j and k combine to increase the concentration of particles of mass $(j + k)$ will be taken as $K(j, k)p_jp_k$, where p_j is the concentration of particles of mass j and $K(j, k)$ is the collection kernel.

Two modes of particle breakup will be considered. First, spontaneous breakup of particles of mass k will be assumed to occur at a rate αp_k, where α, the spontaneous disintegration parameter, can in general be a function of k. The second mode of particle breakup, involving a pair of particles, is similar to collisional breakup and will be referred to as binary breakup. Binary breakup involving particles of masses j and k will be assumed to proceed at a rate βp_jp_k, where the binary disintegration parameter β can in general be a (symmetrical) function of j and k. All fragments resulting from disintegrations will be assumed to be of unit size.

The time rate of change of particle concentration is given by

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$$\frac{dp_k}{dt} = \frac{1}{2}\sum_{j=1}^{k-1} K(j, k-j)p_{k-j}p_j - p_k \sum_{j=1}^{\infty} K(j, k)p_j$$

$$- \alpha(k)p_k - p_k \sum_{j=1}^{\infty} \beta(j, k)p_j, \quad k \geq 2, \quad \text{(1a)}$$

$$\frac{dp_1}{dt} = -\sum_{j=1}^{\infty} K(1, j)p_1p_j + \sum_{J=2}^{\infty} \alpha(j)jp_j + \frac{1}{2}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}$$

$$\times \beta(j, k)(j+k)p_jp_k - p_1 \sum_{j=1}^{\infty} \beta(1, j)p_j. \quad \text{(1b)}$$

For $k \geq 2$, the first two terms on the right-hand side of Eq. (1a) represent, respectively, the rates of gain and loss of particles of size k by coalescence, the third term represents the loss of particles by spontaneous disintegration, and the last term represents the rate of loss of particles by binary disintegrations. Eq. (1b) gives the rate of change of concentration of particles of unit size. The first term on the right-hand side of the equation represents the loss of particles by coalescence. The second term represents the gain in particle concentration by spontaneous breakup, while the third and fourth terms represent the gain by binary disintegrations.

It can be shown that Eqs. (1) ensure the conservation of total mass concentration

$$M = \sum_{k=1}^{\infty} kp_k \quad (2)$$

in the system, provided K and β are symmetric functions of their arguments.

A general solution of (1) is not possible. For the coalescence only ($\alpha = \beta = 0$) problem, analytical solutions were reported in the literature (e.g., Scott, 1968) for special forms of the collection kernel, namely, a constant kernel, a kernel proportional to the sum of particle masses, a kernel proportional to the product of particle masses, and a kernel which is a linear combination of the three foregoing kernels. In the following, we shall give an analytical solution of (1) for a constant collection kernel K and constant breakup parameters α and β. Other forms of K, and α and β will be briefly considered in Section 4.

3. Solution of equations and results

a. Constant kernel and breakup parameters

We introduce the generating function

$$G(z, t) = \sum_{k=1}^{\infty} p_k(t)z^k. \quad (3)$$

It can be shown that for constant $K(=c)$, α and β, the generating function satisfies

$$\partial G/\partial t + (cN + \beta N + \alpha)G = (c/2)G^2 + M(\alpha + \beta N)z, \quad (4)$$

where

$$N = N(t) = \sum_{k=1}^{\infty} p_k(t) = G(1, t) \quad (5)$$

is the total particle concentration. The following scaled variables will be used:

$$\left.\begin{aligned} \tau &= cMt \\ \alpha_* &= \alpha/cM \\ \beta_* &= \beta/c \\ P_k(t) &= p_k(t)/M \\ g(z, t) &= G(z, t)/M = \sum_{k=1}^{\infty} P_k(t)z^k \end{aligned}\right\}. \quad (6)$$

The mean mass of the distribution m is given by

$$m(t) = M/N(t) = 1/g(1, t). \quad (7)$$

If an equilibrium solution results, the equilibrium quantities will be distinguished by a subscript E. In terms of the scaled quantities, Eq. (4) may be rewritten as

$$\partial g/\partial\tau + (\alpha_* + \beta_*/m + 1/m)g = \tfrac{1}{2}g^2 + (\alpha_* + \beta_*/m)z. \quad (8)$$

We shall now consider the behavior of the mean mass and the equilibrium particle size distribution.

b. Mean mass

Putting $z = 1$ in Eq. (8), we have for the mean mass of the distribution

$$\frac{dm}{d\tau} = (\tfrac{1}{2} + \beta_*) + (\alpha_* - \beta_*)m - \alpha_* m^2. \quad (9)$$

First, we consider certain special cases. For the case of coalescence only, we have

$$m(\tau) = m(0) + \tfrac{1}{2}\tau. \quad (10)$$

Thus, the mean mass of the system increases linearly and the concentration tends to vanish with increasing time.

If coalescence and spontaneous breakup are considered, the solution of Eq. (9) is

$$y = \frac{(y_0 + \tanh x)}{(1 + y_0 \tanh x)}, \quad (11)$$

where y and x are related to m and τ by Eqs. (15) and (16), respectively, but with $\beta_* = 0$. The initial condition is $y = y_0$ at $\tau = 0$. It is seen from Eq. (11) that as $x \to \infty$, $y \to 1$; thus as $\tau \to \infty$, an equilibrium mean mass is approached which is given by

$$m_E = \tfrac{1}{2} + (\tfrac{1}{4} + \frac{1}{2\alpha_*})^{1/2}. \quad (12)$$

As might have been anticipated, the equilibrium mean mass decreases with increasing value of the scaled breakup parameter α_*. As $\alpha_* \rightarrow \infty$, $m_E \rightarrow 1$; i.e., all particles tend to be of unit size. Eq. (12) also implies that for fixed α/c, m_E increases with M. For M large, or more precisely, for

$$cN(0)/2\alpha \gg 1, \quad m_E \approx (c/2\alpha)^{1/2}M^{1/2}.$$

It can be shown that the approach to equilibrium takes place monotonically. An example is shown in Fig. 1. In this example $m_E = 215$. For an initial $m(0) = 450$, m_E is approached to within 10% at $\tau = 400$. Coalescence alone would have doubled the mean mass at $\tau = 200$. It can also be shown that the equilibrium is stable, that is, perturbations of m about its equilibrium value tend to return m to the equilibrium value.

If only coalescence and binary disintegration are considered, the solution of (9) is

$$m(\tau) = m(0)e^{-\beta_*\tau} + (1 + \frac{1}{2\beta_*})(1 - e^{-\beta_*\tau}). \quad (13)$$

As $\tau \rightarrow \infty$, the following equilibrium mean mass is approached:

$$m_E = 1 + \frac{1}{2\beta_*} = 1 + c/2\beta. \quad (14)$$

The equilibrium mean mass tends to 1 as $\beta_* \rightarrow \infty$. In contrast to the previous case, m_E is independent of the mass concentration. This suggests that at equilibrium, plots of the size distribution for different mass concentrations will be parallel to each other. This is verified later. It can also be shown that, as in the previous case, the approach to equilibrium is monotonic and the equilibrium is stable.

In the general case of coalescence and spontaneous and binary disintegrations, the solution of (9) is given by (11) where y and x are related to m and τ by

$$y = \left(m - \frac{\alpha_* - \beta_*}{2\alpha_*}\right)\left[\left(\frac{1}{2\alpha_*} + \beta_*/\alpha_*\right) + (\alpha_* - \beta_*)^2/(4\alpha_*^2)\right]^{-1/2}, \quad (15)$$

$$x = \tau\alpha_*\left[\left(\frac{1}{2\alpha_*} + \beta_*/\alpha_*\right) + (\alpha_* - \beta_*)^2/(4\alpha_*^2)\right]^{1/2}, \quad (16)$$

and y_0 is the initial value of y. As $\tau \rightarrow \infty$, an equilibrium mean mass is approached, i.e.,

$$m_E = (\alpha_* - \beta_*)/2\alpha_* + \left[\left(\frac{1}{2\alpha_*} + \beta_*/\alpha_*\right) + (\alpha_* - \beta_*)^2/(4\alpha_*^2)\right]^{1/2}. \quad (17)$$

It may be noted that (12) is a special case of (17), obtained by putting $\beta_* = 0$ in the latter. Also, the limit of (17) as $\alpha_* \rightarrow 0$ gives Eq. (14). Again, it can be shown that the approach to equilibrium is monotonic and the equilibrium is stable.

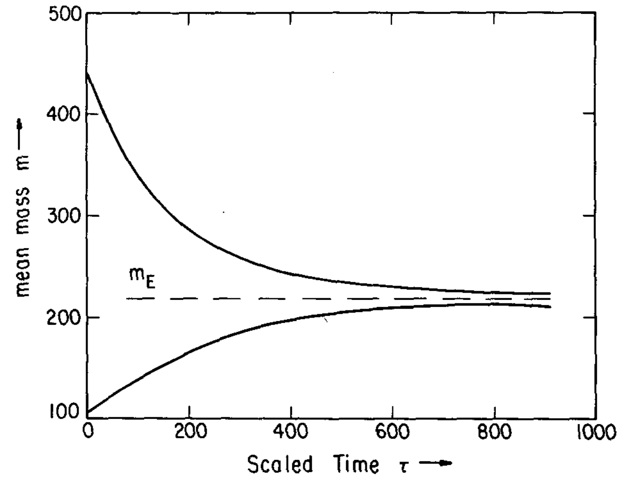

FIG. 1. Two examples of the variation of mean mass with scaled time for coalescence and spontaneous and binary breakup ($\alpha_* = 10^{-5}$, $\beta_* = 10^{-4}$).

The behavior of m_E is summarized in Fig. 2. The thin curves show the variation of m_E with α_* for selected β_*. The thick curve shows m_E as a function of β_* for $\alpha_* = 0$. It is seen that m_E decreases with increases in both α_* and β_*.

It may be recalled that the scaled spontaneous disintegration parameter α_* ($=\alpha_0/cM$) involves the mass concentration M. It is perhaps more instructive to consider the behavior of m_E with M for fixed α/c and β/c. This is done in Fig. 3. With coalescence and binary disintegration ($\alpha_* = 0$), m_E is independent of M (dashed curves). With coalescence and spontaneous disintegration ($\beta_* = 0$), m_E varies approximately as $M^{1/2}$. The curves for coalescence and both types of disintegrations approach the spontaneous breakup curve at small M and the binary disintegration curve at large M. Thus, at small M, the effect of spontaneous disintegration predominates over the effect of binary disintegrations; as M increases, however, the reverse is the case. A similar effect occurs for realistic formulations of collection and breakup of raindrops (Srivastava 1978).

c. *Equilibrium particle size distribution*

The scaled equilibrium generating function is found by putting $\partial/\partial\tau = 0$ in Eq. (8):

$$\tfrac{1}{2}g_E^2 - g_E(\alpha_* + \beta_*/m_E + 1/m_E) + (\alpha_* + \beta_*/m_E)z = 0. \quad (18)$$

Considering the coefficients of z in (18) we find

$$P_{1E} = \frac{(\alpha_* + \beta_*/m_E)}{(\alpha_* + \beta_*/m_E + 1/m_E)}, \quad (19)$$

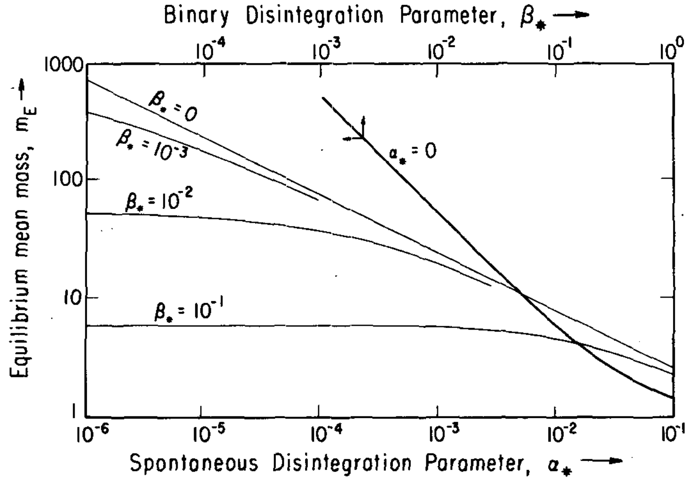

FIG. 2. Variation of the equilibrium mean mass with the spontaneous and binary disintegration parameters.

or, using Eq. (17),

$$P_{1E} = 1/(2m_E - 1). \quad (20)$$

Solving Eq. (18) for g_E, differentiating the result repeatedly with respect to z, and putting $z = 1$, we find the following recursion equation for P_{kE}

$$\frac{P_{kE}}{P_{k-1,E}} = \frac{2k - 3}{2k} \frac{m_E^2 - m_E}{(m_E - ½)^2}. \quad (21)$$

Eq. (21) can also be written as

$$P_{kE} = \frac{(2k-2)!}{k!(k-1)!} \frac{1}{2^{2k-1}} \frac{(m_E^2 - m_E)^{k-1}}{(m_E - ½)^{2k-1}}. \quad (22)$$

From Eq. (22) it is seen that the equilibrium size distribution depends explicitly only on m_E. The dependence on the parameters α_* and β_* is implicit through the dependence of m_E on those parameters. In other words, the *form* of the equilibrium size distribution is the same for (i) coalescence and spontaneous disintegration, (ii) coalescence and binary disintegration, and (iii) coalescence, spontaneous and binary disintegration. Consideration of the particular forms of m_E shows further that in case (ii), the equilibrium distributions for given β_* and different M are parallel to each other, the particle concentrations being proportional to M. This is not so in cases (i) and (iii). This result is understandable. In the case of coalescence and binary disintegration, all terms in the equation for the equilibrium distribution are proportional to the products of particle concentrations. Therefore, if one solution p_{kE} for a mass concentration M has been found, Ap_{kE} is a possible solution for a mass concentration AM where A is a constant.[1] In the case of coalescence and spontaneous breakup, however, the particle concentrations enter into the equation both linearly and quadratically and hence we do not anticipate size distributions which are parallel to each other. Gillespie and List (1978) and Srivastava (1978) found similar behavior with realistic formulations of coalescence and spontaneous and collisional breakup.

For large k, we can approximate P_{kE} in Eq. (22) by

$$P_{kE} = \frac{(m_E - ½)}{(m_E^2 - m_E)} \left[\frac{m_E^2 - m_E}{(m_E - ½)^2}\right]^k \frac{k^{-3/2}}{[2\pi]^{1/2}}. \quad (23)$$

Lushnikov and Piskunov (1977) considered the problem of coalescence and spontaneous disintegration and obtained equations similar to our Eqs. (21), (22) and (23). Here we have shown that these results are also valid for coalescence and binary disintegration and a combination of coalescence, spontaneous and binary disintegration processes provided the appropriate m_E is used in Eqs. (20)–(23).

Fig. 4 shows a plot of the equilibrium distribution for $m_E = 50$, computed from Eq. (22). Although indicated as a continuous curve, the distribution is discrete. On this figure, the asymptotic form (23) is indistinguishable from the exact solution for $k \geqslant 8$. For cloud physical purposes, it is perhaps more interesting to see the distributions plotted as log $\times (p_k k^{2/3})$ against $k^{1/3}$ (Fig. 5) which corresponds essentially to a plot of log$N(D)$ vs D, where D is the particle diameter and $N(D)$ the particle concentra-

[1] The result can be proved rigorously for the case of arbitrary coalescence kernel and binary breakup function. A somewhat more general result may be obtained for the time-dependent size distribution function by simple scaling of the governing equation [e.g., Eq. (2) in Srivastava (1978), with $m = 0$, $B_s = 0$, $A = 0$], *viz.*, it can be shown that if $f(m, t)$ is a solution of the governing equation then $cf(m, t/c)$ is also a solution for arbitrary coalescence kernel and binary breakup function, where f is the size distribution function, m the particle mass and c a constant.

tion density. In Fig. 5, the scaling has been removed and the equilibrium distributions for coalescence and spontaneous breakup ($\alpha/c = 0.1$, $\beta = 0$) have been shown for the indicated mass concentrations. Curves identical in *form* to those in Fig. 5 would be obtained for other cases provided the m_E are identical. As an example, we consider the $M = 2$ curve in Fig. 4. This curve has $m_E = 3.70$ [Eq. (12)]. Under the action of coalescence and binary breakup, the same m_E would be obtained for $\beta/c = 0.185$ [Eq. (14)]. Hence the $M = 2$ curve in Fig. 5 is also the equilibrium distribution for coalescence and collisional breakup for $\beta/c = 0.185$ and $M = 2$. However, if M is changed with β/c kept fixed, the equilibrium distribution will be displaced parallel to itself.

d. *Other forms of the collection kernel and breakup parameters*

Solutions have also been obtained for constant breakup parameters and (i) collection kernel proportional to the sum of particle masses and (ii) collection kernel proportional to the product of particle masses. A detailed discussion of these solutions will not be given here. Only certain new features which emerge in the behavior of the particle mean mass are summarized below.

As the power of the collection kernel increases, an equilibrium mean mass is not always possible. In case (i), an equilibrium mean mass is always obtained with coalescence and spontaneous breakup. With coalescence and binary breakup, however, an equilibrium m occurs only for $\beta_* > 1$ and the equilibrium value is independent of the mass content M. For $\beta_* < 1$, coalescence dominates, that is, $m \to \infty$ as $\tau \to \infty$.

In case (ii), m exhibits three distinct kinds of behavior. In a region of relatively large α_* and β_* an equilibrium m is always attained. In a region of small α_* and β_*, coalescence dominates in a finite time τ_c, i.e., $m \to \infty$ as $\tau \to \tau_c$. In a third region of small α_* but relatively large β_*, the behavior of m depends upon the initial condition. For small initial m an equilibrium m is attained while for large initial m, coalescence dominates. Moreover, two equilibrium values of m are possible. The smaller m is stable with respect to small perturbations, while the equilibrium point with the larger m is unstable. In the latter case, a small positive perturbation causes coalescence to dominate while a small negative perturbation causes the m to move to the stable equilibrium point. In this case also the equilibrium m is independent of M for coalescence and binary breakup.

In addition to the above, it is also possible to obtain solutions for certain forms of variable breakup parameters. For example, we can consider

$$K(j, k) = cjk,$$

$$\alpha(k) = \alpha_0 k,$$

$$\beta(j, k) = \beta_0 jk,$$

where c, α_0 and β_0 are constants. A reference to Eqs. (1) will show that in this case, at equilibrium, the quantity jp_j obeys the same equation as the quantity p_j in the case of a constant kernel and breakup parameters. Hence the solution to this problem is immediate.

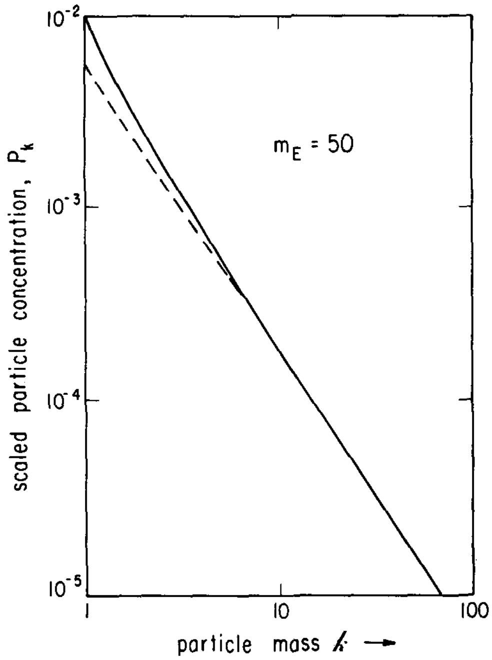

FIG. 4. Scaled equilibrium size distribution (full line) for an equilibrium mean mass $m_E = 50$ compared with the asymptotic solution (dashed line).

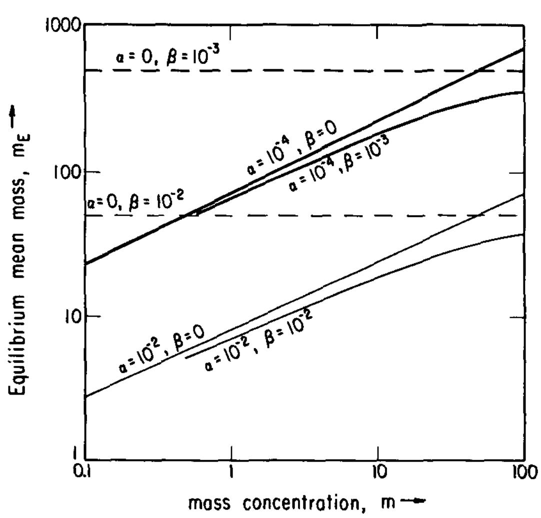

FIG. 3. Variation of mean mass with total mass concentration for selected values of the disintegration parameters.

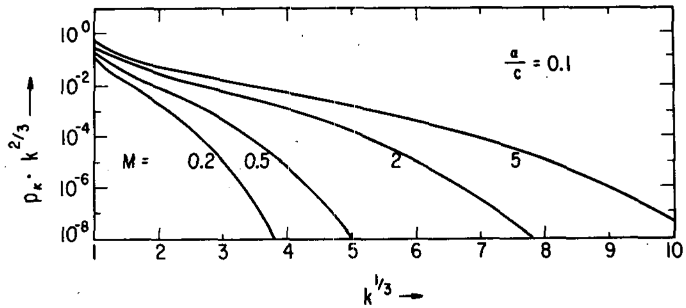

FIG. 5. Equilibrium size distribution, for selected mass concentrations, under the action of coalescence and spontaneous breakup.

4. Conclusions

The equations for a simple model of particle coalescence and breakup have been formulated. Analytical solutions of the equations have been obtained for a constant collection kernel and constant spontaneous and binary disintegration parameters. The behavior of the solutions is qualitatively similar to that of numerical solutions of the equations for the evolution of raindrop size distributions for realistic formulations of coalescence and breakup. An equilibrium particle size distribution is attained. For given breakup parameters, the effect of spontaneous disintegration dominates over that of binary disintegration at small mass contents M, while the reverse is the case at large M. With coalescence and only spontaneous disintegration, the equilibrium mean mass m_E increases with M while it is independent of M when coalescence and only binary disintegration are considered. In the latter case, the equilibrium particle size distributions for different M are parallel to each other.

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