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LETTER TO THE EDITOR

Scaling theory for ballistic aggregation

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Abstract. We develop a Smoluchowski-type mean-field treatment for a recently introduced model of ballistic agglomeration. The predictions of this mean-field theory for the exponent characterizing typical cluster size are in agreement with earlier results for all dimensions. Nevertheless, the predicted monomer decay and particle size distribution are totally at variance with the numerical observations in one dimension. The reason for this discrepancy is found to be the fact that high velocity particles coalesce rapidly independently of their mass, which introduces correlations not taken into account by the mean-field treatment. This is likely to persist in all dimensions, so that the model has no upper critical dimension. The case where the initial velocity distribution function of the particles has a power-law tail is also examined. It is found that, at least in one dimension, the typical cluster size behaves in a way that depends on the specific velocity distribution function, whereas the monomer decay does not.

Irreversible aggregation phenomena have attracted a certain amount of attention recently: scaling theories [1], rate equations [2], numerical studies of explicit models [3–5] and exact solutions [6] have been developed. All this work has principally concentrated on the case of diffusive dynamics. Recently, the following model was proposed [7] to model aggregation phenomena with ballistic transport: particles of a given radius move with random (bounded) initial velocities in a d-dimensional space; upon two particles colliding, they join to form one larger particle of mass equal to the sum of the particle masses and with correspondingly larger radius. In the following, we shall always assume 'regular growth', i.e. the radius is assumed to grow so that the volume of the particle is proportional to its mass. The generalization to the case of fractal growth is straightforward. The velocity is determined by requiring the conservation of momentum. This model is viewed as an idealization for a large class of related, but far more complex phenomena, such as the coalescence of vortices in hydrodynamics [4] or the formation of planets by collision from smaller components [8]. We shall also consider the case where the initial distribution of velocities has a power-law tail, which may be relevant if the aggregating particles are carried by a turbulent fluid.

From the point of view of mean-field theory, such models can be described by a Smoluchowski equation [9] for the concentrations $c_i(t)$ of particles of mass i

$$\dot{c}_i = \tfrac{1}{2}\sum_{k=1}^{i-1} K(k, i-k) c_k c_{i-k} - c_i \sum_{k=1}^{\infty} K(i,k) c_k \tag{1}$$

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where $K(i,j)$ is the rate at which two particles of masses i and j respectively react. Once $K(i,j)$ is known, an extensive scaling theory [1, 2] exists that allows one to find the large-t and large-j behaviour of $c_j(t)$. One has in particular

$$c_j(t) \sim j^{-2}\Phi(j/s(t)) \qquad s(t) \sim t^z \qquad (t \to \infty) \tag{2}$$

where $s(t)$ is the typical cluster size and $\Phi(x)$ a scaling function. The behaviour of $\Phi(x)$ for small x can be of two different types: it can go as a power law in x, with the exponent traditionally called w/z, or it can be of the form $\exp(-x^{-\mu})$. In the first case, one then finds

$$\begin{aligned} &c_1(t) \sim t^{-w} \qquad (t \to \infty) \\ &c_j(t) \sim j^{-\tau} \qquad (1 \ll j \ll s(t)) \end{aligned} \tag{3}$$

where the scaling relation $(2-\tau)z = w$ determines [1] τ. This is commonly known as 'type I' behaviour. In the latter case, usually known as 'type III' behaviour, one has instead

$$c_1(t) \sim \exp(-t^{\mu z}) \qquad (t \to \infty) \tag{4}$$

and there is no power-law behaviour for the particle size distribution as in (3).

For ballistic transport, an ansatz for $K(i,j)$ is needed. The most natural is to take the product of the mutual cross section of the two particles and their relative velocity, i.e.

$$K(i,j) = (R(i) + R(j))^{d-1}|v(i) - v(j)| \tag{5}$$

where $R(i)$ is the (average) radius of a particle of mass i and $v(i)$ its average speed†. If we assume that the aggregates grow regularly, one finds $R(i) \sim i^{1/d}$. The scaling of $v(i)$ is obtained by noting [7] that the momentum of a particle of mass i is given by the sum of the momenta of its constituents, which are randomly distributed and of order one. From this follows that $v(i) \sim i^{-1/2}$. The degree of homogeneity λ of $K(i,j)$ is then $1/2 - 1/d$, so that the standard result from the scaling theory

$$z = \frac{1}{1-\lambda} = \frac{2d}{d+2} \tag{6}$$

is in agreement with the scaling result of [7].

Let us now look in more detail at the one-dimensional case. There, one has $K(i,j)$ equal to $|i^{1/2} - j^{-1/2}|$. Since $K(1,i) \gg K(i,i)$, it follows from standard results [2] that one has 'type III' behaviour with the exponents

$$\begin{aligned} &\Phi(x) \sim \exp(-|x|^{-1/2}) \qquad (x \to 0) \\ &c_1(t) \sim \exp(-t^{1/3}) \qquad (t \to \infty). \end{aligned} \tag{7}$$

† We take the absolute value of the difference in speed as an estimate of the average relative speed, that is, we implicitly perform the necessary averaging over orientation, which gives nothing but an irrelevant prefactor.

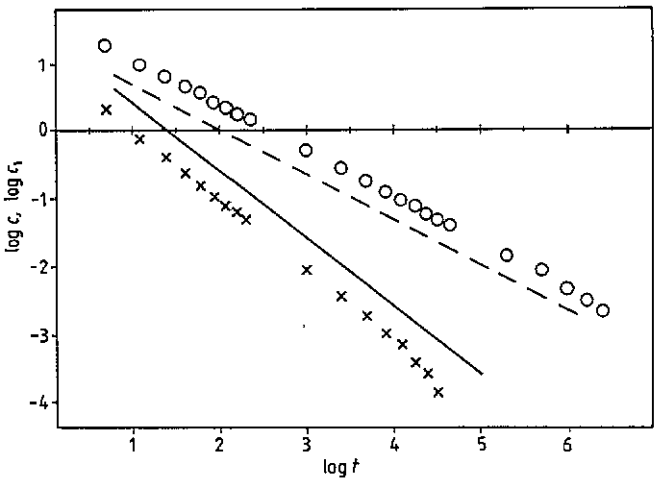

Figure 1. Double logarithmic plot of particle number c (circles) and monomer concentration c_1 (crosses) against time.

We have performed numerical simulations on this model, using 10^5 particles on a straight line with random initial velocities between -1 and 1 at $t = 0$. Free boundary conditions were used, except in the case of very low reaction rates, where it was necessary to use periodic boundary conditions. The initial particle configuration on the line was taken to be either random or uniform. The latter was used for simulations involving velocity distribution functions with power-law large velocity tails, as the short interparticle distances present in the random initial configuration induce long-lived transients.

The results of these simulations, shown in figure 1, indicate that $c_1(t)$ decays approximately as t^{-1}. In fact, it can be shown that t^{-1} is a lower bound on $c_1(t)$, as the following conjunction of three events is sufficient for a monomer to survive until time t without reacting:

(i) It has an initial velocity of the order $t^{-1/3}$ or less.
(ii) For all k of order $t^{2/3}$ or less, the sum of the initial momenta of the k particles to its right is positive.
(iii) A similar condition on the sum of the momenta of the particles to the left being negative.

That the particle at the origin then remains a monomer until time t follows from the remark that it cannot collide with the kth particle to the left or right, since then by conditions (ii) and (iii) the kth particle acquires a momentum away from the central particle before colliding with it. Values of k larger than $t^{2/3}$ can be disregarded, since $t^{2/3}$ corresponds to the maximal cluster size. All three events are mutually independent and each has probability $t^{-1/3}$. For event (i) this follows from the assumption that there is a finite probability density at zero velocity†, so that a

† Even if this is not the case, the exponents will be unaffected in the scaling sense. Thus, a distribution such as $v = \pm 1$ has pathologies, such as exponential decay of $c_1(t)$, but $c_2(t) \sim t^{-2/3}$, since condition (i) is vacuously fulfilled. It can be checked that $c_j(t) \sim 1/t$ for $1 \ll j \ll s(t)$, however, even in this peculiar case, so that $w = 1$ is true in the scaling limit.

velocity of order $t^{-1/3}$ has a probability of the same order. Event (ii) corresponds to the probability that a random walk starting at the origin remains positive for $t^{2/3}$ steps, which has probability [10] $t^{-1/3}$, so that

$$c_1(t) \geqslant \text{constant} \times t^{-1}. \tag{8}$$

Some thought will show that these conditions are also, in essence, necessary, so that $c_1(t) \sim t^{-1}$ as indicated by our simulations.

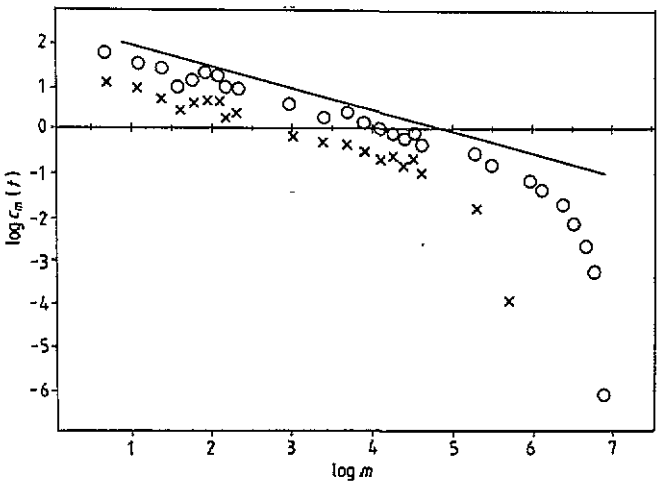

Figure 2. Double logarithmic plot of $c_m(t)$ versus m at $t = 1000$ (crosses) and $t = 5000$ (circles). The slope of the best fit line is approximately $-1/2$, as predicted by the theory.

From the above and the scaling relations of (3) it follows that $c_j(t)$ goes as $j^{-\tau}$ with $\tau = 1/2$ for $1 \ll j \ll s(t)$. We check that this is indeed correct (figure 2). Again, this is strongly at variance with the mean-field prediction, that the particle size distribution should be 'bell-shaped', that is, peaked around the typical size and decaying sharply for both large and small particle sizes (so-called 'type III' behaviour [2]). It is not quite clear to us at this stage how our results compare with those of [7]. They do not explicitly report numerical values for the exponents w and τ, but they do claim to have observed a certain scaling relationship, however this does not seem to coincide with the results obtained here. Specifically, it appears to predict a τ exponent of 0 instead of 1/2.

Such a complete failure of mean-field theory is rather surprising: indeed, since ballistic trajectories become transparent above one dimension, it is natural to think of $d = 1$ as the upper critical dimension for processes involving ballistic transport, as occurs with $d = 2$ in the case of diffusive aggregation [3, 11]. To find the explanation, we looked at the mass dependence of $v(i)$. In order to derive (4) from the expression in (3) for the reaction rate, we had assumed that $v(i)$ goes as $i^{-1/2}$. While this is true for the typical velocity of a cluster of typical mass, we find in our simulations that *at fixed time* the velocity is essentially independent of mass. In one dimension this can be explained by noting that any particle with an exceptionally high velocity would quickly disappear by reacting with one of its neighbours. Such is not the case,

however, if the reaction rate $K \ll 1$. In this case, one expects that a regime of mean-field behaviour will be found for intermediate times. We have performed simulations to verify this hypothesis. In these simulations, whenever two particles collide, they react with probability K to form a larger particle and pass through one another with no change in velocity with probability $1-K$. (This latter case may not appear very realistic, but it is a way to eliminate correlations and thus check whether our mean-field treatment is indeed the appropriate one.) The results are shown in figure 3 for the case of the reaction rate K equal to 0.05. The monomer concentration is found to decay approximately as $\exp(-Ct^{1/3})$ over a time range extending from 10 to 100, which then crosses over to the expected t^{-1} decay. A plot of $v(i)$ against i also reveals the expected behaviour of $i^{-1/2}$ at intermediate times. It should be pointed out that the usual t^{-1} behaviour is always recovered in the long-time limit. This allows one to reject the suggestion that the discrepancy with mean-field theory is due to the pathological feature that particles cannot avoid each other in one dimension.

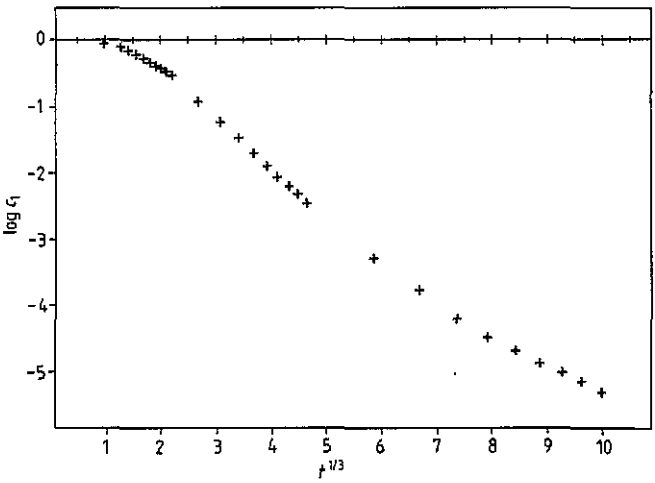

Figure 3. Plot of $\log c_1(t)$ against $t^{1/3}$ for the reaction rate K equal to 0.05. An approximate straight line regime corresponding to times less than 100 is seen. The later decay (not shown in this figure) can be checked to go as t^{-1}.

In all of the above, we assumed that the initial velocity distribution function (VDF) had finite variance, so that the central limit theorem could be invoked to yield $v(i) \sim i^{-1/2}$. An interesting generalization is the case where the initial VDF has a stable distribution of exponent α. One then has

$$v(i) \sim i^{(1-\alpha)/\alpha} \qquad \lambda = \frac{d-\alpha}{\alpha d} \qquad z = \frac{\alpha d}{\alpha d - d + \alpha} \tag{9}$$

as long as $\alpha > 1$, that is, as long as the average velocity is finite. The case of infinite average velocity is somewhat more involved and will be studied in a forthcoming publication [12]. In one dimension, we have confirmed these results both for $\alpha = 1$ and $\alpha = 3/2$ (see figure 4).

For the decay of monomers, we found numerically that the value of the exponent w was roughly equal to one independently of α. To understand this remarkable

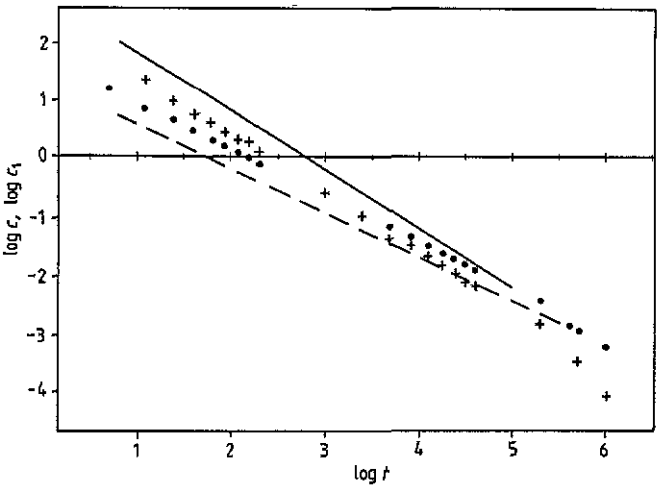

Figure 4. Double logarithmic plot of particle number c (crosses) and monomer concentration c_1 (circles) against time for an initial VDF with a power-law tail $P(v) \sim v^{-5/2}$ for large v. The full curves show the theoretical predictions.

'superuniversality', consider two typical neighbouring clusters at time t. Their constituent particles at $t = 0$ fill two adjacent intervals. If now an additional 'test' particle starts between these two intervals and if its initial velocity is sufficiently low to ensure that it is not likely to collide with either of its two neighbours before time t, this particle will survive as a monomer at time t. If we denote by $N(t)$ the total number of clusters and by $\overline{v}(t)$ the typical velocity at time t, one finds that the probability of a particle being between two such intervals is roughly $N(t)$ and the probability to start with a low enough velocity is about $\overline{v}(t)$. Thus one finds

$$c_1(t) \geqslant \text{constant} \times N(t)\overline{v}(t) \sim t^{-1}. \tag{10}$$

Again, it appears very likely that this lower bound is in fact exact.

Let us now consider higher dimensions. It is clearly important to know whether mean-field theory will eventually be correct in some upper critical dimension. We surmise that this will not happen. The ansatz (3) for the kernel $K(i,j)$ gives, in the terminology of [2], $\mu = -1/2$, and hence

$$\begin{aligned} \Phi(x) &\sim \exp(-|x|^{-1/2}) \qquad (x \to 0) \\ c_1(t) &\sim \exp(-t^{d/(d+2)}) \qquad (t \to \infty) \end{aligned} \tag{11}$$

which also imply that the particle size distribution is bell-shaped. These results have a rather simple physical interpretation: if $R(t)$ is the typical cluster radius, then the total reactive area of the system is roughly $N(t)R(t)^{d-1}$, which decays as $t^{-2/(d+2)}$. If one then assumes

$$\dot{c}_1 = -\text{constant} \times A(t)c_1 \tag{12}$$

one obtains exactly the above formulae.

These results, however, all rely upon the assumption that a VDF of the form $v(i) \sim i^{-1/2}$ is eventually established. In view of the one-dimensional results, this is highly questionable. Indeed, in higher dimensions, the conservation of the total volume fraction ϕ causes the mean free path of a cluster to be of the order of the typical cluster radius. This may well eventually eliminate high-velocity particles regardless of mass and lead to $v(i)$ being mass-independent, as in one dimension. In fact, we may repeat the preceding argument: let the constituent particles of distinct clusters at time t be labelled at $t = 0$ by the cluster they belong to at time t. Assume that particles with the same label are initially located in one regular (more or less spherical) domain of volume approximately $s(t)$, where $s(t)$ is the typical cluster size. Then the probability that an additional 'test particle' falls in the interstitial region between these domains is of the order of $s(t)^{-1/d}$. If this particle has in addition a velocity of the order of $\overline{v}(t)$ or less, it will survive as a monomer up to time t. This latter condition has a probability of $\overline{v}(t)^d$, as all components of the velocity must be small, so that

$$c_1(t) \geqslant \overline{v}(t)^d s(t)^{1/d} \approx t^{-(d^2+2)/(d+2)} \tag{13}$$

contradicting (11), which claims stretched exponential behaviour for $c_1(t)$. However, it should be borne in mind that, for many systems of practical interest, one has $\phi \ll 1$, so that the mean free path is infinite in practice. Mean-field theory would then be valid in much the same way as it is valid for low reaction rates in one dimension. Simulations in higher dimensions are clearly desirable, but they are, unfortunately, quite difficult to perform.

Summarizing, we find that the model of ballistic aggregation studied in [7] has the exponents $z = 2/3$ and $w = 1$ in one dimension. The latter is incorrectly predicted by mean-field theory to be a stretched exponential. The reason for this discrepancy lies in the fact that the VDF at large times is independent of mass. The case of initial VDFs obeying a stable law with finite mean velocity was also studied. Scaling arguments analogous to those used in the previous case were found to agree with numerical work. We found that the value of z changed continuously with the stable law exponent, whereas the value of one for the exponent w is unaffected by these variations, thus exhibiting a 'superuniversal' behaviour. We further speculate that these discrepancies will persist in higher dimensions, so that there is, strictly speaking, no upper critical dimension for this system. These effects may well be unobservable unless the volume fraction is sufficiently large, however, so that mean-field theory will presumably be excellent for a large variety of systems with small volume fractions.

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