Communications in Information and Systems
Volume 13, Number 2, 183–200, 2013

Long-time behaviour of point islands under fixed rate deposition

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We discuss the asymptotic behaviour as as $t \to \infty$ of rate equations modelling submonolayer deposition for an arbitrary critical island size $i \geq 0$, generalising the results of da Costa, van Rössel and Wattis [7].

Keywords and phrases: Submonolayer deposition, asymptotic behaviour, similarity solutions.

1. Introduction

Among Marshall Slemrod's many important contributions to analysis and differential equations, his works on coagulation–fragmentation equations, and in particular on long-term behaviour in the Becker-Döring equations [12, 13] are very well known. In this paper we consider the dynamics of a related, much simpler, point island system, in which there also is a steady influx of monomers.

The context is of submonolayer deposition, i.e. of depositing atoms onto a surface, such that the deposited particles can then diffuse and coagulate into clusters. If in modelling this process we do not take the spatial structure into consideration, we are, broadly speaking, in the domain of **mean-field models**. If we furthermore assume that coagulation and fragmentation rates of clusters are not size-dependent, we are dealing with **point islands**. It makes sense to say that i is the **critical island size** if clusters of size $2 < j \leq i$ can fragment into monomers while clusters of size $j \geq n := i + 1$ cannot. If we assume that clusters of all sizes larger or equal to n are immobile, a point-island mean-field model would lead to Becker–Döring kinetics, i.e. stable clusters would be able to grow only by addition of monomers.

In [7], the authors consider such a mean-field point island deposition process with Becker–Döring kinetics and time-independent input of monomers with $i = 1$ (note that in the absence of diffusion the $i = 1$ case is equivalent to the $i = 0$ case). Using Poincaré compactification and centre manifold

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methods (see also [6] for a more elementary argument), they characterise long-term behaviour of solutions and then (see Theorem 4 of [7]) describe the convergence of solutions to a self-similar profile. This work has been further extended in [8] to allow for time-dependent input of monomers.

In the present paper we generalise the work of [7] to the case of submonolayer deposition with point islands of arbitrary critical size $i \geq 2$. There are roughly three ways of modelling this situation.

(a) We could allow all clusters of size $1 < j \leq i$ to fragment.

(b) We could assume that all clusters of size $1 < j \leq i$ are at equilibrium;

(c) We could assume that clusters of size $1 < j \leq i$ simply do not arise, i.e. that one needs the energy of a n-ary collision to create a stable cluster of size n.

(a) seems to us to be the most realistic approach. It has been adopted by [4, 11]; we will comment on the (formal) results of [4] below. However, the rigorous analysis of the resulting differential equations is prohibitively complicated, and we leave this approach to future work. (b) seems ad-hoc, and in this paper we analyse the scheme of (c). In fact, (c) is faithful to the physical mechanism that underlies Monte-Carlo simulations of submonolayer deposition with $i \geq 0$ [1].

As the qualitative methods of [6, 7] do not seem to work in this more general situation, we analyse the asymptotic behaviour of clusters from scratch, showing in particular that all the solutions of the reduced system (4) in the positive quadrant have the same asymptotics; in the Conclusions section we comment on the connections of this approach to the ones based on the Newton polygon, such as Bruno's power geometry and rivers.

2. The equations

In [7], the authors consider the system of equations

$$\begin{cases} \dot{c}_1 = \alpha - 2c_1^2 - c_1 \sum_{i=2}^{\infty} c_i, \\ \dot{c}_j = c_1 c_{j-1} - c_1 c_j, \quad j \geq 2, \end{cases} \tag{1}$$

where $c_j(t)$ is the concentration of a cluster of j monomers, and $\alpha \in \mathbb{R}_+$ is the monomer input rate.

In case (c), the system of equations in (1) becomes

$$\begin{cases} \dot{c}_1 = \alpha - nc_1^n - c_1 \sum_{j=n}^{\infty} c_j, \\ \dot{c}_n = c_1^n - c_1 c_n, \\ \dot{c}_j = c_1 c_{j-1} - c_1 c_j, \quad j > n. \end{cases} \tag{2}$$

The advantage of this formulation is that, as in (1), the analysis of the long-time behaviour of solutions reduces essentially to a study of a two-dimensional (2-D) system of ordinary differential equations (ODEs). It is convenient to use slightly different variables from the ones used in [7].

Let $Y(t) = c_1(t)$ and (formally) set $X(t) = \sum_{i=n}^{\infty} c_i(t)$. Then we have

$$\begin{cases} \dot{Y} = \alpha - nY^n - YX, \\ \dot{X} = Y^n, \\ \dot{c}_n = Y^n - Yc_n, \\ \dot{c}_j = Yc_{j-1} - Yc_j, \quad j > n. \end{cases} \tag{3}$$

Note that the first two equations decouple from the rest and that once behaviour of $Y(t)$ is known for large t, we can recover the long-time behaviour of c_j, $j \geq n$ by solving, one by one, linear equations.

As in [7], we have a theorem about the equivalence of solutions to (2) and (3):

Theorem 1. *If $\sum_{j=n}^{\infty} c_j(0) < \infty$, a solution of (3) also solves (2).*

The proof follows the lines of [7, Theorem 1].

To find the asymptotics of $c_i(t)$, $i = 1, 2, \ldots$, we therefore consider the first two equations of (3),

$$\begin{cases} \dot{X} = Y^n, \\ \dot{Y} = \alpha - nY^n - XY, \quad \mathrm{X(0),\ Y(0)>0}. \end{cases} \tag{4}$$

3. Asymptotics of (4)

Proposition 1. *For (4):*

(i) The first quadrant $(X, Y) \in \mathbb{R}_+^2$ is positively invariant.

(ii) Let $[0, t_0)$, $t_0 > 0$ be an interval of existence of the solution of the initial value problem (4) (such an interval exists by general ODE theorems). Then, on some interval (t_1, t_0) with $t_1 \in (0, t_0)$, Y is monotonic.

(iii) The solution of (4) exists for all $t > 0$.

(iv) $\exists \tau > 0\, s.t.\, \forall t > \tau$ Y is monotonically decreasing and X is monotonically increasing.

(v) As $t \to \infty$ we have $\lim_{t\to+\infty} Y(t) = 0, \lim_{t\to+\infty} X(t) = +\infty$.

(vi) $\lim_{t\to+\infty} X(t)Y(t) = \alpha$.

Theorem 2. *As $X \to \infty$ the function $Y(X)$ is well defined and has an asymptotic series of all orders in X of the form*

$$Y \sim \alpha X^{-1} - n\alpha^n X^{-n-1} + \alpha^{n+1} X^{-n-3} - n^3 \alpha^{2n-1} X^{-2n-1} + \cdots \tag{5}$$

where the subsequent terms in the expansion are unique (i.e. independent of $X(0)$, $Y(0)$; their relative order depends on the value of n).

Proof of Proposition 1. (i) The fact that $\dot{Y} = \alpha > 0$ means that the line $Y = 0$ can only be crossed from below. Similarly, $\dot{X} \geq 0$ implies that solutions cannot cross the line $X = 0$.

(ii) Indeed, assume first towards a contradiction that Y had infinitely many subintervals where it increases and infinitely many on which it is decreasing. Since Y is smooth, Y has infinitely many strict maxima and infinitely many strict minima. Let t_e be a minimum point. We have $\dot{Y}(t_e) = 0$ and thus

$$\ddot{Y}(t_e) = -\dot{X}(t_e)Y(t_e) = -Y(t_e)^{n+1} < 0, \tag{6}$$

a contradiction.

(iii) Since Y is monotonic on (t_1, t_0) bounded below by zero, $\lim_{t\to t_0} Y(t) = L_0 \in [0, +\infty]$ exists. If we had $L_0 = +\infty$, then for some t_2, we would have $nY^n > 2\alpha$ on (t_2, t_0), implying, by (4), that Y is strictly decreasing on (t_2, t_0) and thus $Y(t) < Y(t_2)$ on this interval, a contradiction. Therefore

$$\lim_{t\to t_0} Y(t) = L_0 \in [0, +\infty). \tag{7}$$

By (7), on $[0, t_0)$ we have $\dot{X} \in [0, L_0^n + a)$ for some $a > 0$ and X is increasing, with bounded derivative. Thus $\lim_{t\to t_0} X(t) = L_1$ exists and $L_1 \in [0, \infty)$. Then $\lim_{t\to t_0}(X(t), Y(t))$ exists, and by general ODE arguments, $(X(t), Y(t))$ extends beyond t_0, as claimed. Thus the solution $(X(t), Y(t))$ is global.

(iv) Assume that Y is not eventually monotonic. Then there would be infinitely many subintervals where it increases and infinitely many on which it is decreasing, and this is ruled out as in (ii). Thus Y is eventually monotonic and $\lim_{t\to\infty} Y(t) = L_2 \in [0, \infty]$. We claim that $L_2 = 0$. Indeed, if $L_2 > 0$ we get from $\dot{X} = Y^n$ that $X \to +\infty$ as $t \to \infty$. But then for sufficiently large t, we see from (4) that $\dot{Y} \to -\infty$ and thus for some t_3 and all $t > t_3$ we have $\dot{Y} < -1$ (say), and thus $Y \to -\infty$, contradicting the fact that the solution is confined to the first quadrant. Y being eventually monotonic implies that Y is eventually decreasing.

(v) By the proof of (iv), Y is eventually decreasing and we have

$$\lim_{t\to\infty} Y(t) = 0. \tag{8}$$

The fact that X is increasing is manifest in the first equation of (4), since $Y \geq 0$. Assume, again towards a contradiction that $\lim_{t\to\infty} X(t) = l < \infty$. Then, by (8) and the fact that X is bounded, we have $\dot{Y}(t) \to \alpha > 0$, and thus Y is eventually increasing, which is incompatible with (8).

(vi) We now look at the function $w(t) = X(t)Y(t)$. Note that

$$\dot{w} = \alpha X - nY^{n-1}w - Xw + Y^{n+1}.$$

Thus, if $\dot{w} = 0$, we have

$$w = \frac{\alpha X + Y^{n+1}}{X + nY^{n-1}}. \tag{9}$$

If there is an infinite sequence of intervals on which w is increasing and an infinite one in which it is decreasing, there are sequences of times, $\bar{t}^k \to \infty$ and $\underline{t}^k \to \infty$ of maxima and minima of w, respectively. Since $X \to \infty$ and $Y \to 0$, (9) implies that for any $\epsilon > 0$ there exists a $\tau > 0$ such that for all $\bar{t}^k, \underline{t}^k > \tau$, $w(\bar{t}^k) < \alpha + \epsilon$ and $w(\underline{t}^k) > \alpha - \epsilon$. Hence

$$\alpha - \epsilon < \inf_{t>\tau} w(t) \leq \sup_{t>\tau} w(t) < \alpha + \epsilon, \tag{10}$$

and this means that

$$\lim_{t\to\infty} w(t) = \alpha. \tag{11}$$

The other possibility is that w is eventually increasing or eventually decreasing. If w is eventually increasing, we see that it must be bounded above, or else we would have $\lim_{t\to\infty} X(t)Y(t) = +\infty$ implying from (4) and (v) above, that $\lim_{t\to\infty} \dot{Y}(t) = -\infty$ contradicting (v). Thus, whether increasing or decreasing, $\lim_{t\to\infty} w(t) = \lambda \in [0,\infty)$, in which case, from the first of (4),

$$\lim_{t\to\infty} \dot{Y} = \alpha - \lambda. \tag{12}$$

The only possibility consistent with (v) above is clearly $\lambda = \alpha$. □

Note 1. *Since Y is eventually decreasing and X is eventually increasing, the functions $Y(X)$ and $w(X)$ are well defined at least for large X and,* *since $\dot{X} \neq 0$, $Y(X)$ is smooth on (X_0, ∞) and decreasing. Furthermore, from Proposition 1 we have*

$$w(X) \sim \alpha,\ Y(X) \sim \alpha X^{-1}, \quad \text{as } X \to \infty. \tag{13}$$

Writing $w(X) = \alpha + \epsilon(X)$, by (13) we have $\epsilon(X) \to 0$ as $X \to \infty$. Straightforward algebra shows that

$$\frac{d\epsilon}{dX} = \frac{\alpha + \epsilon}{X} - \frac{\epsilon}{(\alpha + \epsilon)^n} X^{n+1} - nX. \tag{14}$$

Let $\beta = \frac{n}{n+2} \in (0, 1)$, $\xi = X^{n+2}$, and $\epsilon(X) = g(\xi)$. Denoting by "$'$" derivatives with respect to ξ, we get

$$g' = \frac{\alpha + g}{\xi(n+2)} - \frac{(\alpha + g)^{-n}}{2+n} g - \frac{\beta}{\xi^\beta}, \tag{15}$$

where we substitute $g(\xi) = \xi^{-\beta} h(\xi)$ to get

$$h' = -\beta + \frac{\alpha}{\xi^{1-\beta}(2+n)} - \frac{(\alpha + \xi^{-\beta} h)^{-n}}{2+n} h + \frac{h}{\xi}\left(\beta + \frac{1}{2+n}\right). \tag{16}$$

Theorem 3. *For all solutions in the first quadrant, $h(\xi)$ has an asymptotic behavior of the following form:*

$$h(\xi) \sim \sum_{l,m \geq 0} \frac{a_{l,m}}{\xi^{l(1-\beta)+m\beta}} = -n\alpha^n + \frac{\alpha^{n+1}}{\xi^{1-\beta}} - \frac{n^3 \alpha^{2n-1}}{\xi^\beta} + o(\xi^{-\beta}),$$

where $a_{l,m}$ can be calculated explicitly order by order by iterating (18).

Since $\epsilon(X) \to 0$, $g = \frac{h}{\xi^\beta} \to 0$ and thus $\lambda(\xi) = \frac{(\alpha + \xi^{-\beta} h)^{-n}}{2+n} \to \lambda := \alpha^{-n}(2+n)^{-1}$, so that

$$h' = -\beta + \frac{\alpha}{\xi^{1-\beta}(2+n)} + \frac{h\gamma}{\xi} - \lambda h - \delta(\xi, h), \tag{17}$$

where $\delta(\xi, h) = \lambda h((1 + \frac{h}{\alpha \xi^\beta})^{-n} - 1)$ and $\gamma = \frac{n+1}{n+2}$, and the solution of (17) must satisfy

$$h(\xi) = G(\xi) + e^{-\lambda\xi} \xi^\gamma \int_{\xi_0}^{\xi} \delta(s, h) e^{\lambda s} s^{-\gamma} ds, \tag{18}$$

where

$$G(\xi) = e^{-\lambda\xi}\xi^{\gamma}\Big[C + \int_{\xi_0}^{\xi}(-\beta + \frac{\alpha}{s^{1-\beta}(2+n)})e^{\lambda s}s^{-\gamma}ds\Big]. \tag{19}$$

Note 2. *By L'Hôpital's rule, (19) implies that $G(\xi) \to -\beta/\lambda$ as $\xi \to \infty$.*

Lemma 2. *$h(\xi)$ is bounded.*

Proof of Lemma 2. (18) can be rewritten in the following way:

$$g = \frac{h(\xi)}{\xi^{\beta}} = \frac{G(\xi)}{\xi^{\beta}} + e^{-\lambda\xi}\xi^{\gamma-\beta}\int_{\xi_0}^{\xi}\lambda\frac{h}{s^{\beta}}\Big((1+\frac{h}{\alpha s^{\beta}})^{-n} - 1\Big)e^{\lambda s}s^{-\gamma+\beta}ds.$$

Replacing h/s^{β} by g, taking maximum over $[\xi_0, \infty)$, and using the fact that

$$e^{-\lambda\xi}\xi^{\gamma-\beta}\int_{\xi_0}^{\xi}e^{\lambda s}s^{-\gamma+\beta}ds \to 1/\lambda \text{ as } \xi \to \infty,$$

we have

$$\begin{aligned} &\max_{[\xi_0,\infty)}|g| \le \frac{\max_{[\xi_0,\infty)}|G|}{\xi_0^{\beta}} + Const(n,\xi_0)(\max_{[\xi_0,\infty)}|g|)^2 \\ &\iff \max_{[\xi_0,\infty)}|g|(1 - Const(n,\xi_0)\max_{[\xi_0,\infty)}|g|) \le \frac{\max_{[\xi_0,\infty)}|G|}{\xi_0^{\beta}} \end{aligned} \tag{20}$$

for large enough ξ_0.

Since $Const(n,\xi_0)$ can stay the same for any bigger ξ_0, and $\max_{[\xi_0,\infty)}|g| \to 0$ as $\xi_0 \to \infty$, we can make $Const(n,\xi_0)\max_{[\xi_0,\infty)}|g| < 1/2$ by increasing ξ_0. Then from (20) we have

$$\max_{[\xi_0,\infty)}|g| \le \frac{2K}{\xi_0^{\beta}},$$

where $K := \max_{[\xi_0,\infty)}|G|$. (Since $G(\xi) \to -\beta/\lambda$, $|G(\xi)|$ is bounded.) Since

$$\frac{\max_{[\xi_0,2\xi_0]}|h|}{(2\xi_0)^{\beta}} \le \max_{[\xi_0,2\xi_0]}|g| \le \max_{[\xi_0,\infty)}|g| \le \frac{2K}{\xi_0^{\beta}},$$

we obtain $\max_{[\xi_0,2\xi_0]}|h| \le 2^{\beta+1}K$, and since ξ_0 can be any bigger number, the inequality can be extended to $\max_{[\xi_0,\infty)}|h| \le 2^{\beta+1}K$, proving that $|h|$ is bounded. $\square$

Lemma 3. *$G(\xi)$ has the following asymptotic form:*

$$G(\xi) \sim -\frac{\beta}{\lambda} + \frac{\alpha^{n+1}}{\xi^{1-\beta}} - \frac{\beta\gamma}{\lambda^2 \xi} + O(\xi^{-2+\beta}).$$

More precisely,

$$G(\xi) \sim \Big[-\frac{\beta}{\lambda} - \frac{\beta\gamma}{\lambda^2\xi} + \tilde{G}_1(\xi)\Big] + \xi^\beta \Big[\frac{\alpha^{n+1}}{\xi} + \tilde{G}_2(\xi)\Big],$$

where $\tilde{G}_1, \tilde{G}_2 = O(\xi^{-2}) \in \mathbb{C}[[1/\xi]]$.

Proof of Lemma 3. By integration by parts and L'Hôpital's rule, we have

$$e^{-\lambda\xi}\xi^a \int_{\xi_0}^{\xi} e^{\lambda s} s^b \, ds \sim \frac{1}{\lambda}\xi^{a+b} - \frac{b}{\lambda^2}\xi^{a+b-1} + \cdots, \text{ as } \xi \to \infty, \tag{21}$$

and so we get the above asymptotic form for $G(\xi)$. $\square$

Proof of Theorem 3. By Lemma 2, we can let $|h| < M$ for some M. Since

$$\Big| \Big(1 + \frac{h}{\alpha s^\beta}\Big)^{-n} - 1 \Big| \le C\frac{M}{s^\beta}$$

for $s > \xi_0$, we have

$$\begin{aligned} &\Big| e^{-\lambda\xi}\xi^\gamma \int_{\xi_0}^{\xi} \lambda h \Big((1 + \frac{h}{\alpha s^\beta})^{-n} - 1\Big) e^{\lambda s} s^{-\gamma} ds \Big| \\ &\le C\lambda M^2 e^{-\lambda\xi}\xi^\gamma \int_{\xi_0}^{\xi} e^{\lambda s} s^{-\gamma-\beta} ds \sim \frac{CM^2}{\xi^\beta} = O(\xi^{-\beta}), \end{aligned}$$

and so, by (18) we obtain

$$h = G(\xi) + O(\xi^{-\beta}) = -\frac{\beta}{\lambda} + \frac{\alpha^{n+1}}{\xi^{1-\beta}} + O(\xi^{-\beta}).$$

Now let

$$h(\xi) = -\frac{\beta}{\lambda} + \frac{\alpha^{n+1}}{\xi^{1-\beta}} + \frac{a}{\xi^\beta} + o(\xi^{-\beta}),$$

so that (18) becomes

$$
\begin{aligned}
(22)\qquad & -\frac{\beta}{\lambda}+\frac{\alpha^{n+1}}{\xi^{1-\beta}}+\frac{a}{\xi^{\beta}}+o(\xi^{-\beta})\\
&= G(\xi)+e^{-\lambda\xi}\xi^{\gamma}\int_{\xi_0}^{\xi}\lambda\Big(-\frac{\beta}{\lambda}+\frac{\alpha^{n+1}}{s^{1-\beta}}+\frac{a}{s^{\beta}}+o(s^{-\beta})\Big)\\
&\Big[-\frac{n}{\alpha s^{\beta}}\Big(-\frac{\beta}{\lambda}+\frac{\alpha^{n+1}}{s^{1-\beta}}+\frac{a}{s^{\beta}}+o(s^{-\beta})\Big)+O(s^{-2\beta})\Big]e^{\lambda s}s^{-\gamma}ds\\
&= -\frac{\beta}{\lambda}+\frac{\alpha^{n+1}}{\xi^{1-\beta}}-\frac{\beta\gamma}{\lambda^2\xi}+O(\xi^{-2+\beta})\\
&+e^{-\lambda\xi}\xi^{\gamma}\int_{\xi_0}^{\xi}\lambda\Big(-\frac{n\beta^2}{\lambda^2\alpha s^{\beta}}\frac{2n\beta\alpha^{n+1}}{\lambda\alpha s}+o(s^{-1})+O(s^{-2\beta})\Big)e^{\lambda s}s^{-\gamma}ds,
\end{aligned}
$$

and hence by (21) we get $a=-\frac{n\beta^2}{\lambda^2\alpha\xi^{\beta}}=-\frac{n^3\alpha^{2n-1}}{\xi^{\beta}}$. Replacing β/λ by $n\alpha^n$, we obtain:

$$
h(\xi)=-n\alpha^n+\frac{\alpha^{n+1}}{\xi^{1-\beta}}-\frac{n^3\alpha^{2n-1}}{\xi^{\beta}}+O(\xi^{-1})+O(\xi^{-2\beta}).
$$

Once n is given, the coefficients of the asymptotic series can be inductively calculated by iteration. Note that, without specifying the value of n, we cannot proceed explicitly any further for general n since the ordering of the subsequent terms depends on the concrete value of n.

By collecting all the possible exponents of ξ and simple verification, similar to that of (22), we get the following asymptotic expansion for $h(\xi)$:

$$
(23)\qquad h(\xi)\sim\sum_{l,m\ge 0}\frac{a_{l,m}}{\xi^{l(1-\beta)+m\beta}}.
$$

(Note that (23) can be well ordered: since $\beta=\frac{n}{n+2}$ and $1-\beta=\frac{2}{n+2}$, for even $n=2k$, this sum can be expressed as $\sum_{m\ge1}a_m\xi^{-\frac{m}{k+1}}$, and for odd n, $\sum_{m\ge1}a_m\xi^{-\frac{m}{n+2}}$.) □

Proof of Theorem 2. Using (23) we get

$$
\begin{aligned}
w=XY=\alpha+\frac{h(\xi)}{\xi^{\beta}}=\alpha+\frac{h(X^{n+2})}{X^n}&\sim\alpha-n\alpha^nX^{-n}\\
&+\alpha^{n+1}X^{-n-2}-n^3\alpha^{2n-1}X^{-2n}+\cdots
\end{aligned}
$$

implying the result. □

Since $X' = Y^n$, we can calculate $X(t)$ and $Y(t)$ asymptotically, setting $w = f(X)$ and using

$$\int_{X(0)}^{X} \frac{X^n}{(f(X))^n}\, dX = \int_0^t dt, \quad Y(t) = \frac{f(X(t))}{X(t)},$$

to obtain

$$X(t) \sim [\alpha^n(n+1)]^{\frac{1}{n+1}} t^{\frac{1}{n+1}} - n^2\Big(\frac{\alpha}{n+1}\Big)^{\frac{n-1}{n+1}} t^{-\frac{n-1}{n+1}} + O(t^{-1}) \tag{24}$$

and

$$Y(t) \sim \Big[\frac{\alpha}{n+1}\Big]^{\frac{1}{n+1}} t^{-\frac{1}{n+1}} + \Big[\frac{n^2 - n\alpha}{\alpha(n+1)}\Big] t^{-1} + O(t^{-\frac{n+3}{n+1}}). \tag{25}$$

Note 3. *Since $X(t) \to \infty$ as $t \to \infty$, and we are interested in the asymptotic behavior as $t \to \infty$, for small initial value of X we choose a sufficiently large initial time t_0 so that $X(t_0)$ is also large.*

4. Similarity solutions

We expect the similarity solutions to be of the form

$$c_j(t) = Ct^{\gamma}\Psi(\zeta) \text{ as } t \to \infty,$$

where $\Psi(0) = 1$, and $\zeta = j/t^{\beta}$, $\beta > 0$. Since we know that

$$c_1(t) \sim \Big[\frac{\alpha}{n+1}\Big]^{1/(n+1)} t^{-1/(n+1)},$$

we have that

$$C = \Big[\frac{\alpha}{n+1}\Big]^{1/(n+1)} \text{ and } \gamma = -\frac{1}{n+1}.$$

The arguments in [14, p. 7832] imply that we should have $\beta = 1 + \gamma$ and

$$\Psi(\zeta) = \begin{cases} (1 - (1+\gamma)\eta/C)^{\gamma/(\gamma+1)} & \zeta < C/(1+\gamma) \\ 0 & \text{otherwise.} \end{cases} \tag{26}$$

The remainder of this section is devoted to formulating and proving this result rigorously.

First, we introduce a new timescale, $\tau(t) := \int_0^t Y(s)ds$, along with scaled variables, $\tilde{c}_j(\tau) := c_j(t(\tau))$. $\tau(t) > 0$ and is monotone increasing, and we denote by $t(\tau)$ the inverse function of $\tau(t)$. Note that $\tau(t) \to \infty$ as $t \to \infty$ by (25).

Using the new timescale, we have for $j > n$

$$\tilde{c}_j(\tau)' = \frac{dc_j}{dt}\frac{dt}{d\tau} = \tilde{c}_{j-1} - \tilde{c}_j.$$

By the variation of constants formula,

$$\tilde{c}_j = e^{-\tau}\int_0^\tau e^s \tilde{c}_{j-1}(s)ds + Ke^{-\tau} = \int_0^\tau e^{-s}\tilde{c}_{j-1}(\tau - s)ds + Ke^{-\tau},$$

where $K \equiv \tilde{c}_j(0)$. Note that c_n we have

$$\tilde{c}_n(\tau) = e^{-\tau}\tilde{c}_n(0) + \int_0^\tau e^{-(\tau-s)}[\tilde{c}_1(s)]^{n-1}ds.$$

Hence for all $j \geq n$,

$$\tilde{c}_j(\tau) = e^{-\tau}\sum_{k=n}^{j}\frac{\tau^{j-k}}{(j-k)!}\tilde{c}_k(0) + \frac{1}{(j-n)!}\int_0^\tau s^{j-n}e^{-s}[\tilde{c}_1(\tau - s)]^{n-1}ds. \tag{27}$$

From the results of Section 3, we have

Proposition 4. *As* $t, \tau \to \infty$

(i) $(\frac{n}{n+1})(\frac{n+1}{\alpha})^{1/(n+1)}t^{-n/(n+1)}\tau(t) \to 1$;
(ii) $(\frac{n\tau}{\alpha})^{1/n}\tilde{Y}(\tau) \to 1$;
(iii) $(\frac{n+1}{\alpha})^{1/(n+1)}t^{1/(n+1)}c_1 \to 1$;
(iv) $(\frac{(n+1)t}{\alpha})^{(n-1)/(n+1)}c_j \to 1, \ \forall j \geq n$.

We will also need the long time behaviour of $\tilde{c}_j(\tau)$:

Proposition 5. *As* $\tau \to \infty$,

$$\left(\frac{n\tau}{\alpha}\right)^{(n-1)/n}\tilde{c}_j(\tau) \to 1 \ \textit{as}\ \tau \to \infty, \ j \geq n, \tag{28}$$

The proof of Propositions 4 and 5 is analogous to the argument in [7, p. 381–383].

Let $\eta = j/\tau$. The objective is to find a function $\Phi_1(\eta)$, $\eta \neq 1$ such that

$$\lim_{j,\tau\to\infty}\left[\frac{n\tau}{\alpha}\right]^{(n-1)/n}\tilde{c}_j(\tau) = \Phi_1(\eta),$$

where η is fixed. For that we will need (27) and the results of Proposition 4 as well as the Stirling formula approximation for the Gamma function, $\Gamma(x) = \sqrt{2\pi}x^{x-1/2}e^{-x}[1+\mathcal{O}(x^{-1})]$ as $x \to \infty$.

For monomeric initial data with $j \geq n$, we have

$$\left(\frac{n\tau}{\alpha}\right)^{(n-1)/n} \tilde{c}_j(\tau) = \frac{\left(\frac{n\tau}{\alpha}\right)^{(n-1)/n}}{(j-n)!} \int_0^\tau s^{j-n} e^{-s} [\tilde{c}_1(\tau - s)]^{n-1} ds. \tag{29}$$

Consider the function ϕ_1 defined on $[n, \infty) \times [0, \infty)$ by

$$\phi_1(x,\tau) = \frac{\left(\frac{n\tau}{\alpha}\right)^{(n-1)/n}}{\Gamma(x-n+1)} \int_0^\tau s^{x-n} e^{-s} [\tilde{c}_1(\tau - s)]^{n-1} ds. \tag{30}$$

Let $x = \eta\tau$. Then, from (30), we obtain

$$\phi_1(\eta\tau,\tau) = \frac{\left(\frac{n\tau}{\alpha}\right)^{(n-1)/n}}{\Gamma(\eta\tau-n+1)} \int_0^\tau s^{\eta\tau-n} e^{-s} [\tilde{c}_1(\tau - s)]^{n-1} ds.$$

The change of variable $s = y\tau$ now leads to

$$\phi_1(\eta\tau,\tau) = \frac{\eta^{n-1/2-\eta\tau}\tau^{1/2}}{\sqrt{2\pi}e^{n-2}}(1+\mathcal{O}(\tau^{-1})) \int_0^1 \frac{\psi(\tau(1-y))e^{\tau(\eta\log(y)-y+\eta)}}{y^n(1-y)^{(n-1)/n}}\, dy, \tag{31}$$

where $\psi(\tau) = \left(\frac{n\tau}{\alpha}\right)^{(n-1)/n} [\widetilde{c_1}(\tau)]^{n-1}$. Let

$$I_n(\eta,\tau) := \eta^{-\eta\tau}\tau^{1/2}e^{\eta\tau} \int_0^1 \frac{\psi(\tau(1-y))e^{\tau(\eta\log(y)-y)}}{y^n(1-y)^{(n-1)/n}}\, dy,$$

as $\tau \to \infty$. There are two cases to consider, $\eta > 1$ and $\eta \in (0,1)$.

Proposition 6. *If $\eta > 1$, then $\Phi_1(\eta) = 0$.*

Proof. In the integral, $y^{-n}e^{\tau(\eta\log(y)-y)} = e^{(\eta\tau-n)\log(y)-y\tau} = e^{g_1(y)}$, where $g_1(y) = (\eta\tau - n)\log(y) - y\tau$. For all $y \in (0,1]$ and $\tau > \frac{n}{\eta-1}$, $g_1' > 0$. For $y \in (0,1]$, we have $g_1(y) \leq g_1(1) = -\tau$. This leads to

$$\int_0^1 \psi(\tau(1-y))\frac{e^{\tau(\eta\log(y)-y)}}{y^n(1-y)^{(n-1)/n}}dy \leq M_\psi e^{-\tau} \int_0^1 \frac{dy}{(1-y)^{(n-1)/n}} = nM_\psi e^{-\tau}.$$

Thus, following [7, p. 385], for $\eta > 1$ we have $I_n(\eta,\tau) \to 0$ as $\tau \to \infty$. $\square$

Proposition 7. *If* $\eta \in (0,1)$, $\Phi_1(\eta) = (1-\eta)^{-(n-1)/n}$.

Proof. The exponential term inside the integral $I_n(\eta,\tau)$ is $e^{f(y)}$ where

$$f(y) = \tau(\eta \log(y) - y)$$

so that $f'(y) = 0$ at $y = \eta$ and $f''(\eta) = -\frac{\tau}{\eta} < 0$. So the exponential term has a unique maximum at $y = \eta$. To seek the asymptotic behaviour of $I_n(\eta,\tau)$, we write

$$\begin{aligned} &I_n(\eta,\tau) \\ &\quad = \eta^{-\eta\tau}\tau^{1/2}e^{\eta\tau}\left(\int_0^{\epsilon} + \int_{\epsilon}^{1-\epsilon} + \int_{1-\epsilon}^{1}\right)\psi(\tau(1-y))\frac{e^{\tau(\eta\log(y)-y)}}{y^n(1-y)^{(n-1)/n}}dy \\ &\quad =: I_{n,1}(\eta,\tau) + I_{n,2}(\eta,\tau) + I_{n,3}(\eta,\tau). \end{aligned}$$

Consider $I_{n,1}(\eta,\tau)$ first. The calculation is similar to the case $\eta > 1$. Since we have $0 < y < \epsilon < \eta e^{-1}$, for all $\tau > \frac{n}{(1-e^{-1})\eta}$, we obtain $g_1(y) = (\eta\tau - n)\log(y) - y\tau$ and $g_1'(y) > 0$. Thus, $g_1(y) \le g_1(\epsilon) \le g_1(\eta e^{-1}) = (\eta\tau - n)\log(\eta) - (\eta\tau - n) - \tau\eta e^{-1}$. As in [7, p. 385], we have

$$I_{n,1}(\eta,\tau) \to 0 \quad \text{as } \tau \to \infty. \tag{32}$$

Next, consider the case $I_{n,3}(\eta,\tau)$. The exponential term is

$$e^{\tau(\eta\log(y)-y)}e^{\eta\tau}e^{-\eta\tau\log(\eta)} =: e^{-\tau g_3(y)},$$

where $g_3(y) = (\eta\log(\eta) - \eta) - (\eta\log(y) - y)$. As in [7, p. 18], we have

$$I_{n,3}(\eta,\tau) \to 0 \quad \text{as } \tau \to \infty \tag{33}$$

By (32) and (33), we have

$$I(\eta,\tau) = I_{n,2}(\eta,\tau) + o(1) \quad \text{as } \tau \to \infty. \tag{34}$$

To compute $I_{n,2}(\eta,\tau)$, we modify the arguments in [7]. Since $y < 1-\epsilon \Rightarrow \tau(1-y) > \tau\epsilon \to \infty$ as $\tau \to \infty$, then $\psi(\tau(1-y)) = 1 + o(1)$ for large τ as expected in the previous section. So, $\forall\delta > 0$, $\exists\ T(\delta) : \forall\tau > T(\delta)$, $\psi(\tau(1-y)) \in [1-\delta, 1+\delta]$ and with

$$J_n(\eta,\tau) := \int_{\epsilon}^{1-\epsilon}\frac{e^{-\tau\phi(y)}}{y^n(1-y)^{(n-1)/n}}dy \quad \text{and } \phi(y) = y - \eta\log(y) - \eta,$$

$$(1-\delta)\eta^{-\eta\tau}\tau^{1/2}J_n(\eta,\tau) \le I_{n,2}(\eta,\tau) \le (1+\delta)\eta^{-\eta\tau}\tau^{1/2}J_n(\eta,\tau). \tag{35}$$

Since $\phi(y)$ is smooth and has a unique minimum $y=\eta\in(\epsilon,1-\epsilon)$ with $\phi(\eta)=-\eta\log(\eta)$ and $\phi''(\eta)=\eta^{-1}$, we can use Laplace's method [15] to obtain

$$J(\eta,\tau) \approx \frac{e^{\eta\tau\log(\eta)}}{\eta^n(1-\eta)^{(n-1)/n}}\sqrt{\frac{2\pi}{\tau/\eta}} \tag{36}$$

By (31), (34), (35) and (36), we have

$$\phi_1(\eta\tau,\tau) = \frac{1}{(1-\eta)^{(n-1)/n}}(1+\mathcal{O}(\tau^{-1})). \qquad \square$$

Thus for monomeric initial data we have

Theorem 4.

$$\Phi_1(\eta) := \begin{cases} (1-\eta)^{-(n-1)/n} & \textit{if } 0<\eta<1, \\ 0 & \textit{if } \eta>1. \end{cases}$$

For non-monomeric initial data, we have

$$\left(\frac{n\tau}{\alpha}\right)^{(n-1)/n}\tilde{c}_j(\tau) = \phi_1(j,\tau) + \left(\frac{n\tau}{\alpha}\right)^{(n-1)/n} e^{-\tau}\sum_{k=n}^{j}\frac{\tau^{j-k}}{(j-k)!}\tilde{c}_k(0),$$

where $\phi_1(\eta)$ is defined in the previous subsection. Since we already have established that the term ϕ_1 is related to the term Φ_1 defined by Theorem 4, all that is required is to show that the second part of the non-monomeric initial data solution goes to zero. This will show that the asymptotic behaviour for monomeric initial conditions also holds for the non-monomeric case.

We define $v := \frac{1}{\eta}$, $\tau = jv$ and assume $\tilde{c}_k(0) \le \rho k^{-\mu}$. Then

$$\begin{aligned} &\left(\frac{n\tau}{\alpha}\right)^{(n-1)/n} e^{-\tau}\sum_{k=n}^{j}\frac{\tau^{j-k}}{(j-k)!}\tilde{c}_k(0) \\ &\le \rho\left(\frac{njv}{\alpha}\right)^{(n-1)/n} e^{-jv}\sum_{k=n}^{j}\frac{(jv)^{j-k}}{(j-k)!\;k^{\mu}} \\ &=: \rho\left(\frac{n}{\alpha}\right)^{(n-1)/n}\phi_2(v,j), \end{aligned}$$

where $\phi_2(v,j) = (jv)^{(n-1)/n} e^{-jv} \sum_{k=n}^{j} \frac{(jv)^{j-k}}{(j-k)!\ k^{\mu}}$. Note that $v \neq 1$ since $\eta \neq 1$.

Proposition 8. *For $v \in (0,1)$ and $v > 1$, $\phi_2(v,j) \to 0$ as $j \to \infty$.*

The proof of Proposition 8 is analogous to the argument in [7, p. 387]. Hence, by Theorem 4 and Proposition 8,

Theorem 5. *With $\eta = \frac{j}{\tau}$ fixed and $\eta \neq 1$, we have*

$$\lim_{j,\tau\to\infty} \left(\frac{n\tau}{\alpha}\right)^{(n-1)/n} \tilde{c}_j(\tau) = \Phi_1(\eta),$$

where

$$\Phi_1(\eta) \ := \begin{cases} (1-\eta)^{-(n-1)/n} & \text{if } 0 < \eta < 1, \\ 0 & \text{if } \eta > 1. \end{cases}$$

Let us rephrase our results in terms of t. From Proposition 4, equations (24) and (27), for large t we have that

$$\text{(37)} \quad \langle j \rangle = \frac{\sum_{j=1}^{\infty} j c_j(t)}{\sum_{j=1}^{\infty} c_j(t)} \sim \frac{\alpha t}{[(n+1)\alpha^n t]^{1/(n+1)}} = \left(\frac{\alpha}{n+1}\right)^{1/(n+1)} t^{n/(n+1)}.$$

Therefore

$$\tau \sim \left(\frac{n+1}{n}\right) \left(\frac{\alpha}{n+1}\right)^{1/(n+1)} t^{n/(n+1)} \sim \left(\frac{n+1}{n}\right) \langle j \rangle.$$

This leads to the following main result:

Theorem 6. *As $t \to \infty$,*

$$c_j(t) \sim \begin{cases} \langle j \rangle^{-(n-1)/n} \Phi_1\left(\frac{n}{n+1}\frac{j}{\langle j \rangle}\right) & \text{if } \frac{n}{n+1}\frac{j}{\langle j \rangle} < 1, \\ 0 & \text{otherwise.} \end{cases}$$

5. Conclusions

We have described the large time behaviour of solution to (3) for the point-island case of general $i \geq 1$, generalising [7], who deal with the case of $i = 1$ ($n = 2$). We also prove the convergence to a self-similar profile $\Phi_1(\eta)$, with a discontinuity at $\eta = j/\tau = 1$.

Note that our results in Section 3 are consistent with the results in [4] in case (a) with $p = 0$ and the identifications $N_1(t) := Y(t)$, $M_0(t) :=$

$X(t)$, $m := i$ (see equations (19) and (20) in [4]). It is remarkable that the asymptotic behaviour is the same in case (a) and case (c), proving which requires further analytical work.

The model treated in this paper is closely related to the one studied by Bartelt and Evans in [2] for the point-island case $i = 1$. They have derived an equation for the scaled island size distribution (ISD) and obtain a discontinuity at $j/\langle j\rangle = 3/2$. Let us show that our analysis generalises this result. We have

$$\langle j\rangle = \frac{\sum_{j\geq n} jc_j(t)}{\sum_{j\geq n} c_j(t)} = \frac{\theta - \sum_{j=1}^{n-1} jc_j(t)}{\sum_{j\geq n} c_j(t)}, \quad \left(\theta = Ft = \sum_{j\geq 1} jc_j\right).$$

Now, recall that we simply do not allow clusters of size $1 < j \leq i$. This implies $c_k(t) = 0$ for $k = 2, 3, \ldots, n-1$. Then we have, with $\alpha = F$

$$\langle j\rangle = \frac{\alpha t - c_1(t)}{\sum_{j\geq n} c_j(t)}.$$

Since

$$\tau \sim \left(\frac{n+1}{n}\right)\left(\frac{\alpha}{n+1}\right)^{1/(n+1)} t^{n/(n+1)} \sim \left(\frac{n+1}{n}\right)\langle j\rangle.$$

The discontinuity (at $j/\tau = 1$) is in terms of $\langle j\rangle$, at

$$\frac{j}{\langle j\rangle} \sim \frac{n+1}{n},$$

confirms the result obtained by Bartelt and Evans for $i = 1, n = 2$.

Note that as explained in [2, p. 54] and [10, p. 89], there is no discontinuity in the similarity solution obtained from MC simulations. This raises by the question of formulating conditions on the coefficients of Smoluchowski coagulation equations which ensure a continuous scaling solution.

Finally, we would also like to comment on the connection of the calculations of Section 3, the work of Bruno [5], and the concept of a river [9]. In terms of rivers, it can be verified that (4) admits a unique locally Lyapunov stable river in the (positively invariant) first quadrant; our results prove that in this case uniqueness and local Lyapunov stability imply global Lyapunov stability in the positive quadrant. We leave a more extensive analysis of this implication for future work. Our results would also follow from the work of Bruno [5] once we establish that all solutions in the positive quadrant have the same order (see the definition in [5, p. 455]); this however seems equivalent to obtaining the leading order of the final results of that section, (24), (25).

Acknowledgements

MG and KPON would like to thank Drs. Wilson Lamb and P. Mulheran for their many substantive contributions to the work that led to this paper.

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Received September 15, 2013