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LETTER TO THE EDITOR

# A class of solutions of the time-dependent reaction–diffusion equation for the processes $A + A \to A$ and $A + A \to \emptyset$

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**Abstract.** Consideration is given to the treatment of the nonlinear partial differential equation describing the diffusion of an assembly of particles which simultaneously coagulate or annihilate. It is shown how a class of solutions may be obtained in terms of the solutions of an ordinary differential equation and detailed application is made to the case of an initially localized particle distribution.

The purpose of the present work is to develop a class of solutions to a problem which occurs in two distinct but closely related physical systems. The first of these is the coagulation process $A + A \to A$ in which two particles coalesce to form a single particle. The original treatment of this by Smoluchowski [1] was confined to the time-dependent spatially homogeneous situation, but since then consideration has been given to spatially inhomogeneous problems in which particles simultaneously diffuse and coagulate. For the case of simple coagulation kernels $P$ (constant $P$, $P$ proportional to the sum of the interacting particle volumes), exact results have been obtained in this field by van Dongen [2], Simons [3, 4], Slemrod [5], ben-Avraham *et al* [6] and Doering and ben-Avraham [7]. The second system of interest is the annihilation process $A + A \to \emptyset$ in which two particles coalesce to yield an inert product, and the corresponding situation with particles both diffusing and annihilating has been considered by van Dongen [2], ben-Avraham *et al* [6], Doering and ben-Avraham [7], Kang and Redner [8, 9], Kraemer [10] and Clément *et al* [11].

In both of the systems described above (with $P$ constant for the coagulation case), the interaction term is of the form $PN^2$, where $N$ is the particle concentration, and thus both systems can be described by the same reaction–diffusion equation [12],

$$D\frac{\partial^2 N}{\partial x^2} - \frac{\partial N}{\partial t} = PN^2 \tag{1}$$

where $D$ is the diffusion coefficient. We non-dimensionalize this equation by defining

$$X = (P/D)^{1/2}x \qquad \tau = Pt \tag{2}$$

and hence obtain

$$\frac{\partial^2 N}{\partial X^2} - \frac{\partial N}{\partial \tau} = N^2 . \tag{3}$$

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To develop a solution of this, we first note that the equation is invariant if $X$ and $\tau$ are each changed by an arbitrary additive constant. It is also invariant under the transformation $X \to \lambda X$, $\tau \to \lambda^2 \tau$, $N \to N/\lambda^2$ for arbitrary constant $\lambda$, and these considerations suggest a solution of the form

$$N(X,\tau) = f(u)/(\tau+\alpha) \tag{4a}$$

where

$$u = (X+\beta)/(\tau+\alpha)^{1/2} \tag{4b}$$

with constants $\alpha$ and $\beta$. It is then readily shown that (4) yields a solution of (3) if $f(u)$ satisfies the ordinary differential equation

$$\frac{\mathrm{d}^2 f}{\mathrm{d}u^2} = f^2 - f - \frac{u}{2}\frac{\mathrm{d}f}{\mathrm{d}u} \tag{5}$$

and we require solutions of this equation which are non-negative for all relevant $u$. To specify suitable boundary conditions for (5), we make the point that we are looking for a solution for $N(X,\tau)$ with a clear well defined physical interpretation. Now, in the absence of coagulation it is known that there exists a solution of the diffusion equation (equation (3) with the right-hand side zero) of the form

$$N(X,\tau) = \tau^{-1/2}\exp(-X^2/4\tau)$$

which (for given $\tau$) corresponds to a localized distribution with a single maximum at $X = 0$, and decreasing monotonically and symmetrically to zero as $X \to \pm\infty$. It is to be expected, on physical grounds, that the introduction of coagulation or annihilation should not change this general picture, and that the possibility should therefore exist of obtaining a solution of (1) which *qualitatively* behaves in exactly the same way; it is this form of solution which we now wish to investigate. Bearing in mind that (5) is invariant for the transformation $u \to -u$, it follows that $N$ will be an even function of $X$ if we take $\beta = 0$ and make $f$ an even function of $u$ by choosing as our first boundary condition

$$f'(0) = 0\,. \tag{6a}$$

For our second boundary condition we take

$$f(0) = A \tag{6b}$$

and now proceed to consider what constraints there may be on the allowed values of $A$ for our solution to behave as required. Since we want the stationary value at $X = 0$ to be a maximum, it is necessary that $f''(0) < 0$, and it then follows from (5) that for this to be so $0 < A < 1$. (It is readily seen that for $A > 1$, $f \to \infty$ as $X \to \pm\infty$, while for $A = 1$, $f(u) = 1$ for all values of $u$ giving $N(X,\tau) = (\tau+\alpha)^{-1}$ which is the standard spatially homogeneous solution of the time-dependent coagulation or annihilation equation.) For the form of solution under current consideration it is readily shown from (5) that as $u \to \infty$, $f(u) \sim u^{-2}$ and hence that $\lim_{u\to\infty} uf(u) = 0$. On integrating (5) from 0 to $\infty$, we then obtain

$$\int_0^\infty [f(u)]^2\,\mathrm{d}u = \tfrac{1}{2}\int_0^\infty f(u)\,\mathrm{d}u \tag{7}$$

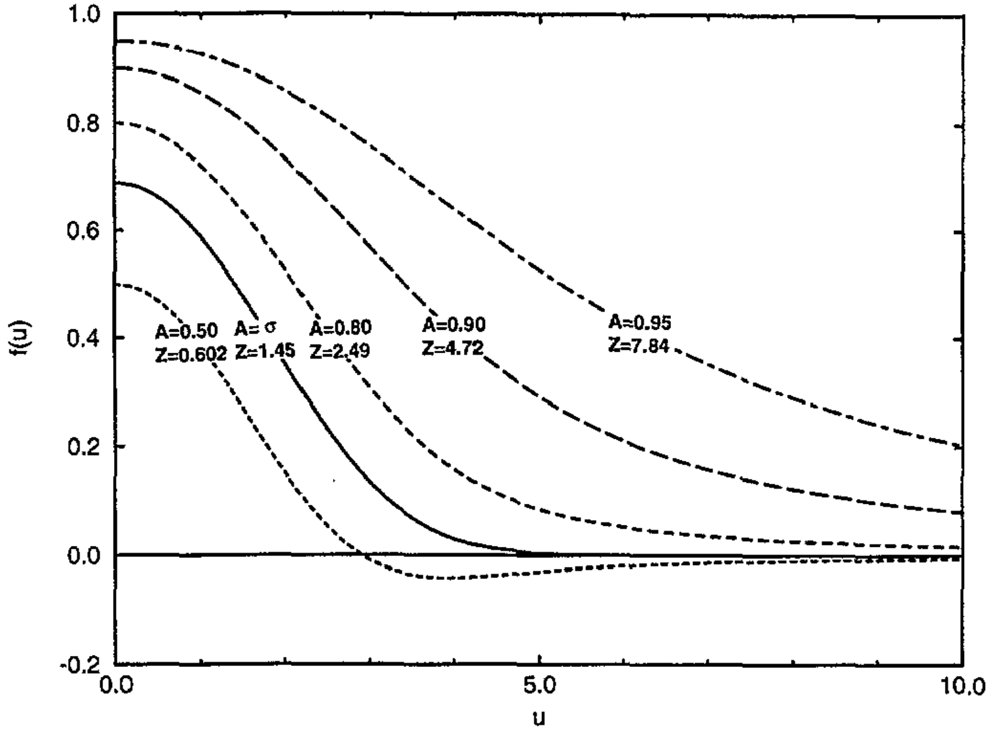


**Figure 1.** $f(u)$ for $0 < u < 10$, plotted for $A = 0.50$ (······), the critical value $\sigma$ (——), 0.80 (----), 0.90 (– – –) and 0.95 (— · —). The corresponding value of the integral $Z$ (equation 9(*b*)) is indicated against each curve.

(the above asymptotic form for $f(u)$ shows both of these integrals to be convergent), and this can only be satisfied with $f(u)$ positive everywhere and monotonically decreasing in the interval $[0, \infty]$ if $A > \frac{1}{2}$. Our analysis thus gives a necessary (but insufficient) condition $\frac{1}{2} < A < 1$ for our solution $f(u)$ to behave qualitatively as required.

To progress further, we employed the computer algebra system *Maple* [13] to confirm that there were no analytic solutions of (5) in terms of standard functions. We then used a standard Runge–Kutta–Fehlberg method [14] in order to calculate numerical solutions using the boundary conditions (6) with $A$ taking values lying within the interval $\left[\frac{1}{2}, 1\right]$. It transpired that there exists a critical value of $A$, which we denote here by $\sigma$, such that for $\sigma \leqslant A < 1$, $f(u)$ is positive everywhere and decreases monotonically to zero as $u$ increases from 0 to $\infty$, while for $A \leqslant \sigma - 10^{-9}$, $f(u)$ becomes negative throughout the interval $b \leqslant u < \infty$ where $b < 10$. We determined that $\sigma \simeq 0.689\,843\,611$. In figure 1, we show representative graphs of $f(u)$ for various values of $A$. For $A \geqslant \sigma$ these all have the same qualitative behaviour described earlier, but with the degree of localization increasing as $A$ decreases from unity down to the value $\sigma$.

In general, the solution $N(X, \tau)$ given by (4) will initially be set up at $t = 0$ by distributing a given total number of particles $n = \int_{-\infty}^{\infty} N(x, 0)\,\mathrm{d}x$ in accordance with this solution for a particular choice of the parameters $\alpha$ and $A$ which defines it. We rewrite our solution (4) in the form

$$N(x, t) = \frac{1}{P(t+\gamma)} f\left(\frac{x}{D^{1/2}(t+\gamma)^{1/2}}\right) \tag{8}$$

($\gamma = \alpha/P$) and note that the total number of particles at time $t$ in the $x$-interval $[-\infty, \infty]$ is given by

$$n(t) = \int_{-\infty}^{\infty} N(x,t)\,\mathrm{d}x = \frac{2ZD^{1/2}}{P(t+\gamma)^{1/2}} \tag{9a}$$

where

$$Z = \int_0^{\infty} f(u)\,\mathrm{d}u \tag{9b}$$

(values of $Z$ are shown against each of the graphs in figure 1). Corresponding to $n(0) = n$, we then have

$$n = 2Z(A)D^{1/2}/P\gamma^{1/2} \tag{10}$$

which for given $n$ specifies a relation between the hitherto arbitrary parameters $A$ and $\gamma$. We suppose $A$ to be given a value within the interval $[\sigma, 1]$ and eliminating $\gamma$ from (8) in favour of $n$ then yields

$$N(x,t) = \frac{C}{1+\nu t} f\left(\frac{x}{a(1+\nu t)^{1/2}}\right) \tag{11a}$$

where

$$C = \frac{Pn^2}{4Z^2D} \qquad \nu = PC \qquad a = \frac{2ZD}{Pn}. \tag{11b}$$

We note that for $\nu t \gg 1$, $N(x,t)$ takes the simpler form

$$N(x,t) = \frac{1}{Pt} f\left(\frac{x}{(Dt)^{1/2}}\right) \tag{12}$$

being independent of $n$. For given $n$, (11) give a class of solutions of (1), each being characterized by a particular value of $A$ in the interval $[\sigma, 1]$. The smaller the value chosen for $A$, the greater will be the initial localization of particles, firstly because the function $f(u)$ then decreases more rapidly for increasing $u$, and secondly because a given value of $x$ will then correspond to a greater value of $u$ as $Z$ will be less. Maximum localization will occur when $A = \sigma$, corresponding to $Z = 1.45$.

As regards the time variation of the total number of particles, we see from (9) and (10) that

$$n(t) = \frac{n}{(1+\nu t)^{1/2}} \tag{13a}$$

which takes the limiting form

$$n(t) = \frac{2ZD^{1/2}}{Pt^{1/2}} \tag{13b}$$

for $\nu t \gg 1$. We note that $n(t)$ decreases with increasing $t$, as would be expected due to the particle coagulation or annihilation, but that the rate of decrease is less rapid than in the spatially homogeneous situation where $n(t) = n/(1 + Pnt)$. This is due to the fact that in our situation, the effect of diffusion is to continually disperse the particles over a wider region and hence to continually decrease their average probability of interaction. It is also worth remarking that (13) show $n(t)$ to be less for smaller values of $Z$. This is readily understood as being due to the fact that smaller values of $Z$ correspond to smaller values of $A$, which as explained earlier imply a greater initial particle localization and hence greater subsequent particle coagulation or annihilation.

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## References


[1] Smoluchowksi M V 1916 *Phys. Z* **17** 557
[2] van Dongen P G J 1990 *J. Stat. Phys.* **58** 87
[3] Simons S 1991 *J. Phys. A: Math. Gen.* **24** 277
[4] Simons S 1992 *Phys. Lett.* **171A** 172
[5] Slemrod M 1990 *Physica* **46D** 351
[6] ben-Avraham D, Burschka M A and Doering C R 1990 *J. Stat. Phys.* **60** 695
[7] Doering C R and ben-Avraham D 1989 *Phys. Rev. Lett.* **62** 2563
[8] Kang K and Redner S 1984 *Phys. Rev. Lett.* **52** 955
[9] Kang K and Redner S 1985 *Phys. Rev.* A **32** 435
[10] Kraemer P J R 1991 *Physica* **173A** 548
[11] Clément E, Sander L M and Kopelman R 1989 *Phys. Rev.* A **39** 6472
[12] Friedlander S K 1977 *Smoke, Dust and Haze* (New York: Wiley)
[13] Char B W, Geddes K G, Gonnet G H, Leong B L, Monagan M B and Watt S M 1991 *Maple V Language Reference Manual* (New York: Springer)
[14] Press W H, Teukolsky S A, Vetterling W T and Flannery B P 1992 *Numerical Recipes in Fortran: The Art of Scientific Computing* (Cambridge: Cambridge University Press)