On the steady-state equation for particles undergoing simultaneous Brownian diffusion and coagulation

1996 J. Phys. A: Math. Gen. 29 303

(http://iopscience.iop.org/0305-4470/29/2/010)

J. Phys. A: Math. Gen. **29** (1996) 303–307. Printed in the UK

On the steady-state equation for particles undergoing simultaneous Brownian diffusion and coagulation

S Simons
School of Mathematical Sciences, Queen Mary and Westfield College, Mile End Road, London E1 4NS, UK

Received 7 April 1995, in final form 20 September 1995

Abstract. An earlier calculation of the solution of the time-independent equation for the diffusion of coagulating particles is modified to take into account the correct dependence of the Brownian diffusion coefficient on particle size. Explicit analytic results are obtained for the spatial dependence of the particle number density N and the volume fraction of particulate matter ϕ.

1. Introduction

Most work on the Smoluchowski coagulation equation has been concerned with the time-dependent spatially homogeneous situation. More recently, however, interest has been shown in problems exhibiting spatial dependence, and papers dealing with this include van Dongen (1989, 1990), Oshanin and Burlatsky (1989), Simons (1986, 1987, 1991, 1992), Simons and Simpson (1988) and Slemrod (1990). In Simons (1992), the problem tackled was that of calculating the particle number density $N(x)$ when a steady state had been attained as a result of primary particles being injected into the system at $x = 0$ and diffusing in the positive x direction up to $x = \infty$, whilst simultaneously coagulating. In order to complete this calculation without further approximation it was necessary to assume that both the coagulation kernel P and the diffusion coefficient D were constants, independent of particle size, and whilst this is known to be a good approximation for P in the case of coagulation due to Brownian motion (see, for example, Friedlander (1977)), it is, however, not a good approximation for the corresponding D which is known to exhibit a $v^{-1/3}$ variation, v being the particle volume. For the case of Brownian motion it is, therefore, clear that this assumption of constant D will give rise to quantitative errors in $N(x)$, but apart from this there will also exist a basic qualitative error in the approach. This is so because the constant D assumption implies that in the steady state the volume fraction of particulate matter $\phi(x)$ is a constant, independent of x, whilst with the true v-dependent D this will not be the case.

The above comments motivate us to consider, in the present paper, the same physical situation as that dealt with in Simons (1992), but with the consistent assumption that both coagulation and diffusion are due to Brownian motion of the particles. The above-mentioned v dependence of D then prevents us from carrying through an exact calculation as was done in Simons (1992). Rather, we follow the approach of Simons (1986, 1987) and Simons and Simpson (1988) whereby the spectrum of particle sizes is assumed to be that of a 'self-preserving' distribution (Friedlander and Wang 1966). This allows us to complete the calculation and obtain simple analytic forms for both $N(x)$ and $\phi(x)$.

0305-4470/96/020303+05$19.50

2. Basic formulation

Let $n(v, x, y, z)\,\mathrm{d}v$ be the number of particles per unit volume of space at position (x, y, z) whose own volumes lie between v and $v + \mathrm{d}v$. We shall suppose that the particles diffuse and coagulate within the half-space $x > 0$ with $n(v)$ being specified and independent of y and z on the plane $x = 0$. Then n will be independent of y and z for all x, and, following Friedlander (1977), will satisfy the equation

$$D(v)\frac{\partial^2 n}{\partial x^2} + \left(\frac{\partial n}{\partial t}\right)_{\mathrm{coag}} = 0. \tag{1}$$

Here $(\partial n/\partial t)_{\mathrm{coag}}$ is the rate of change of n due to coagulation, which is given by

$$\left(\frac{\partial n}{\partial t}\right)_{\mathrm{coag}} = \tfrac{1}{2}\int_0^v P(u, v-u)n(u)n(v-u)\,\mathrm{d}u - n(v)\int_0^\infty P(u, v)n(u)\,\mathrm{d}u \tag{2}$$

where $P(u, v)$ is the relevant coagulation kernel. For diffusion and coagulation due to Brownian motion

$$D(v) = Av^{-1/3} \tag{3a}$$

and

$$P(u, v) = B(u^{1/3} + v^{1/3})(u^{-1/3} + v^{-1/3}) \tag{3b}$$

where $A = (2/3^{1/2}\pi)^{2/3}(kT/6\eta)$ and $B = 2kT/3\eta$, T and η being respectively the temperature and coefficient of viscosity of the gas (Simons 1986). Although equation (1) is conventionally used to describe the present situation, its derivation requires a little further consideration. The coagulation term (2) arises physically as the result of the particles diffusing and indeed its derivation involves the solution of a certain diffusion equation. This might suggest that for the present situation where there exists a superimposed variation of n in the x direction, such variation might effectively modify the coagulation term and hence necessitate the formulation of a single equation incorporating simultaneously the effects of diffusion in giving rise to both macroscopic transport and particle coagulation. In fact this is not necessary, since the diffusion involved in the calculation of the coagulation kernel occurs at scales of the order of the size of a typical particle, while for the diffusive term in equation (1) the relevant scale is of the order of the mean interparticle distance. Thus under normal circumstances, where the proportion of space filled by particulate material is much less than unity (typically $< 10^{-6}$), equation (1) may be used.

3. Development of solution

To tackle equation (1) we now assume that $n(v, x)$ follows the 'self-preserving' distribution which can be expressed in the form

$$n(v, x) = \frac{[N(x)]^2}{\phi(x)}\, g\left(\frac{N(x)v}{\phi(x)}\right) \tag{4}$$

for suitable spectral function $g(w)$. This assumption has been used extensively in the papers quoted earlier and also in various spatially homogeneous time-dependent problems. It is equivalent to assuming that, as regards its v dependence, the *shape* of $n(v, x)$ is independent of x, and while this will not hold exactly it would appear to be a reasonable approximation in our work where we are interested in calculating certain integrals over the distribution—$N(x)$ and $\phi(x)$, rather than the detailed v dependence of $n(v,x)$. We note that the relations

$$N(x) = \int_0^\infty n(v,x)\,\mathrm{d}v \qquad \phi(x) = \int_0^\infty vn(v,x)\,\mathrm{d}v \tag{5}$$

which define N and ϕ in terms of n, imply that $g(w)$ satisfies the constraints

$$\int_0^\infty g(w)\,\mathrm{d}w = \int_0^\infty wg(w)\,\mathrm{d}w = 1. \tag{6}$$

To obtain equations determining $N(x)$ and $\varphi(x)$ we now take the zeroth and first moments with respect to v of equation (1); that is, we consider the equation

$$\frac{\partial^2}{\partial x^2}\int_0^\infty v^\gamma D(v)n(v,x)\,\mathrm{d}v + \int_0^\infty v^\gamma \left(\frac{\partial n}{\partial t}\right)_{\mathrm{coag}} \mathrm{d}v = 0. \tag{7}$$

By letting γ take in turn the values 1 and 0, this will yield a pair of differential equations for $N(x)$ and $\varphi(x)$. Further, since $n(v,x)$ is specified on the plane $x = 0$, the values of $N(0)$ $(= N_0)$ and $\varphi(0)$ $(= \varphi_0)$ are known and may be used as boundary conditions for these differential equations. Now, for $\gamma = 1$ the second term in equation (7) is zero (since coagulation conserves the total volume of particulate material) and with the help of equations (3*a*) and (4) we thus obtain

$$\mathrm{d}(N^{1/3}\phi^{2/3})/\mathrm{d}x = \alpha \text{ (constant).} \tag{8}$$

Now, the total flux of particulate matter is given by

$$\begin{aligned} J &= -\int_0^\infty vD(v)(\partial n/\partial x)\,\mathrm{d}v \\ &= -A\int_0^\infty w^{2/3}g(w)\,\mathrm{d}w\,\mathrm{d}(N^{1/3}\phi^{2/3})/\mathrm{d}x \\ &= -\alpha A\int_0^\infty w^{2/3}g(w)\,\mathrm{d}w \end{aligned} \tag{9}$$

which is, as expected, constant in the steady state. Further, since particles are diffusing in the positive x direction from the source at $x = 0$, it follows that $J \geqslant 0$ and hence that $\alpha \leqslant 0$. Now, α cannot be negative since equation (8) would then imply that $N^{1/3}\phi^{2/3}$ becomes negative for some positive x, and hence we must take $\alpha = 0$ and

$$N^{1/3}\phi^{2/3} = \text{constant} = N_0^{1/3}\phi_0^{2/3}. \tag{10}$$

We now let $\gamma = 0$ in equation (7) from which it follows that

$$\frac{\mathrm{d}^2(N^{4/3}\varphi^{-1/3})}{\mathrm{d}x^2} = \nu N^2 \tag{11}$$

where

$$\nu = \frac{(6\pi^2)^{1/3}\int_0^\infty\int_0^\infty (w^{1/3}+w'^{1/3})(w^{-1/3}+w'^{-1/3})g(w)g(w')\,\mathrm{d}w\,\mathrm{d}w'}{\int_0^\infty w^{-1/3}g(w)\,\mathrm{d}w}. \tag{12}$$

On eliminating N between equations (10) and (11) we then obtain

$$\frac{\mathrm{d}^2\varphi^{-3}}{\mathrm{d}x^2} = \nu N_0^{2/3}\varphi_0^{4/3}\varphi^{-4} \tag{13}$$

combined with the boundary condition $\varphi(0) = \varphi_0$. To obtain a second boundary condition on φ we note that in the infinite time required for particles to diffuse to $x = \infty$ the mean particle volume $V = \varphi/N$ is known to increase to infinity. Since equation (10) gives

φ proportional to $V^{1/3}$ it follows that $\varphi(\infty) = \infty$, which is the required second boundary condition. It is then readily shown that the solution of equation (13) with the above boundary conditions is

$$\varphi(X) = (\varphi_0^{1/2} + N_0^{1/3}\varphi_0^{2/3}X)^2 \tag{14a}$$

where $X = (\nu/42)^{1/2}x$. Correspondingly

$$N(X) = (N_0^{-1/4} + N_0^{1/12}\varphi_0^{1/6}X)^{-4}. \tag{14b}$$

We note that as $x \to \infty$, φ increases monotonically to ∞ while N decreases monotonically to zero.

4. Discussion

Equations (14) are the main results of this work and should be contrasted with the corresponding results when D is a constant, independent of v. For that situation

$$\phi(x) = \phi_0 \tag{15a}$$

$$N(X) = [\sigma X + N_0^{-1/2}]^{-2} \tag{15b}$$

(σ a constant) (Simons 1992), and the difference in behaviour can be readily understood physically. In the steady state $K = \int_0^\infty vD(v)n(v,x)\,\mathrm{d}v$ is independent of x as pointed out earlier, and hence when D is independent of v, ϕ will be independent of x (see equation (5)). When, however, $D(v) = Av^{-1/3}$ we have

$$K \approx AV^{-1/3}\int_0^\infty vn(v,x)\,\mathrm{d}v \tag{16}$$

and hence constancy of K implies that $\phi(X) \propto V^{1/3}$. Now, since the particles coagulate as they diffuse in the positive X direction, $V(X)$ will increase with X and this gives rise to the increase in ϕ shown in equation (14*a*). Further, since $N = \phi/V$, the increase in V with X will lead in the constant D situation to the decrease in N given by equation (15*b*), while for $D \propto v^{-1/3}$ the increase in V with X will be more rapid, since larger particles will diffuse more slowly, and this accounts for the more rapid decrease of N with X in this case as shown in equation (14*b*).

Finally we consider the numerical value of ν defined in equation (12). Although its precise value will depend on the function $g(w)$, the conditions (6) act as powerful constraints and prevent large variations in the value of ν even when the shape of $g(w)$ varies substantially. This point was investigated in detail in the earlier papers quoted above, taking for $g(w)$ the standard gamma distribution $g(w) = Gw^q\exp(-Hw)$ which is known to give a reasonable representation of the particle size spectrum. The constants G and H were expressed in terms of q using equations (6) and the variation in the value of the expression (12) (albeit with a different value of γ) was examined as q varied. We now apply this approach to the expression (12) with the above-chosen value of $\gamma = 0$, and this suggests that as q increases from 0 to ∞ the variation in the value of ν is not expected to exceed about 10% of its mean value. We conclude that it is, therefore, reasonable to estimate ν by taking $q = \infty$, corresponding to $g(w) = \delta(w-1)$; this then yields $\nu \approx 16$.

Acknowledgment

I should like to express my thanks to the referees for their constructive comments and suggestions.

References

Friedlander S K 1977 *Smoke, Dust and Haze* (New York: Wiley)
Friedlander S K and Wang C S 1966 *J. Colloid. Interface Sci.* **22** 126–32
Oshanin G S and Burlatsky S F 1989 *J. Phys. A: Math. Gen.* **22** L973–6
Simons S 1986 *J. Phys. A: Math. Gen.* **19** 1413–27
——1987 *J. Phys. D: Appl. Phys.* **20** 75–81
——1991 *J. Phys. A: Math. Gen.* **24** 277–88
——1992 *Phys. Lett.* **171A** 172–4
Simons S and Simpson D R 1988 *J. Phys. A: Math. Gen.* **21** 3523–36
Slemrod M 1990 *Physica* **46D** 351–66
van Dongen P 1989 *J. Stat. Phys.* **54** 221–71
——1990 *J. Stat. Phys.* **58** 87–115