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Coagulation with fragmentation

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Abstract. An integro–differential equation is constructed which describes the evolution of a system of masses evolving by completely inelastic collisions and spontaneous fragmentations. The development of a characteristic size spectrum is demonstrated for a simple example.

1. Introduction

The coagulation equation predicts the time evolution of a spectrum of free masses which evolve by undergoing perfectly inelastic collisions. It has a wide sphere of application in the physical sciences and has been used in various situations where the asymptotic behaviour of a collection of merging objects is of interest. It was first written down in discrete forms by Smoluchowski (1916) and in an integral form, appropriate for the study of a continuous mass spectrum, by Schumann (1940) (see Chandrasekhar 1943). It has been used by astrophysicists to simulate star formation (Field and Saslaw 1965, Penston *et al* 1969, Silk 1980), galaxy formation (Silk and White 1978) and the size distribution of asteroids and planetesimals (Safranov 1969, Dohnanyi 1969, Zvyagina *et al* 1974, Pechernikova *et al* 1976, Wacker *et al* 1977, Simons *et al* 1978). Other important applications are found in colloid chemistry (Lushnikov 1973), aerosol science (Ramabhadran *et al* 1976), meteorology (Drake 1972) and haematology (Popel *et al* 1975).

Here we shall generalise the standard coagulation equation to include the effects of fragmentation and calculate the asymptotic form of the size spectrum predicted for a simple system of masses undergoing both coalescence and fragmentation.

2. Coagulation with fragmentation

The standard integral form of the coagulation (or scalar transport) equation describes the evolution of the quantity $n(m, t)$, the number of particles of size m existing at time t. Bodies lying in the mass interval $(m, m+\delta m)$ are formed by the binary coalescence of smaller bodies with masses $m-m'$ and m'. They are destroyed by any merger with a body of mass m. The evolution in time of a system undergoing these changes is given by an integro–differential equation for $n(m, t)$:

$$\frac{\partial n(m,t)}{\partial t}=\frac{1}{2}\int_0^m K(m'-m, m')n(m-m', t)n(m', t)\,\mathrm{d}m' - \int_0^\infty K(m, m')n(m, t)n(m', t)\,\mathrm{d}m'. \tag{2.1}$$

The symmetric kernel $K(x, y)$ is the coalescence rate between fragments of mass x and y. Its specific functional form will be dictated by the particular physical process that is being modeled.

We now augment (2.1) to include the possibility that masses of size $m+m'$ can fragment into pieces m and m' with rate given by a function $F(m, m')$. This consideration requires two additional terms in the transport equation (2.1): one accounting for the break-up of particles of mass $(m, m+\delta m)$ and another to monitor the number of this size that are created by the splitting of larger bodies. The addition of these two terms yields a coagulation–fragmentation equation:

$$\frac{\partial n(m,t)}{\partial t}=\frac{1}{2}\int_0^m K(m-m', m')n(m-m', t)n(m', t)\,\mathrm{d}m' - \int_0^\infty K(m, m')n(m, t)n(m', t)\,\mathrm{d}m' - \frac{1}{2}\int_0^m F(m', m)n(m+m', t)\,\mathrm{d}m' + \int_0^\infty F(m, m')n(m+m')\,\mathrm{d}m'. \tag{2.2}$$

In order to follow the evolution of $n(m, t)$ it is convenient to introduce some additional quantities: the total number of particles at time t, $N(t)$, is

$$N(t)\equiv\int_0^\infty n(m, t)\,\mathrm{d}m \qquad N(0)\equiv N_0. \tag{2.3}$$

If we integrate (2.2) over all masses we see that $N(t)$ satisfies an ordinary differential equation:

$$\dot{N}(t)=-\frac{1}{2}\int_0^\infty\int_0^\infty K(m, m')n(m, t)n(m', t)-F(m, m')n(m+m', t)\,\mathrm{d}m\,\mathrm{d}m'. \tag{2.4}$$

We now specialise to consider homogeneous coagulation kernels of the form (Trubnikov 1971)

$$K(m, m')=\alpha+\delta(m+m')+\gamma mm' \tag{2.5}$$

where α, δ and γ are constants. In addition, we shall assume the fragmentation kernel to be constant:

$$F(m, m')=\beta \qquad \dot{\beta}\equiv 0. \tag{2.6}$$

If we introduce the notation

$$f(\tau)\equiv N(\tau)/N_0 \qquad \text{where } \tau\equiv 0{\cdot}5N_0t \tag{2.7}$$

then (2.4)–(2.7) gives

$$\frac{df}{d\tau}=-\alpha f^2-2\delta f-\gamma+p^2 \qquad f(0)=1 \tag{2.8}$$

where

$$p^2=\beta m_0/N_0 \tag{2.9}$$

$$m_0\equiv V/N_0 \qquad \text{and} \qquad V=\int_0^\infty mn(m, t)\,\mathrm{d}m. \tag{2.10}$$

Integrating (2.8) we have

$$f(\tau)=\frac{\theta^{1/2}-(\delta+\gamma-p^2)\tanh(\theta^{1/2}\tau)}{\theta^{1/2}+(\delta+\alpha)\tanh(\theta^{1/2}\tau)} \tag{2.11}$$

where $\theta\equiv\delta^2-\alpha\gamma+\alpha p^2>0$.

The fragmentation terms contribute to the total particle number in a manner that is similar to the coagulation effects of the product portion of the kernel $K(m, m')\propto mm'$, but in the opposing sense. If $\alpha=\beta=\delta=0$ and the system only coagulates through the product kernel then (2.11) reveals that all the particles coalesce in a finite time (Trubnikov 1971). However, if $\beta\neq 0\neq\gamma$ and $p^2>\gamma$ the fragmentation occurs more efficiently than the coalescence and the number of particles increases linearly with time; the solution now exists for all future time:

$$f(\tau)=(p^2-\gamma)\tau+1 \qquad p^2>\gamma. \tag{2.12}$$

However, it is clear that no time-independent steady state will exist. If $\gamma=0$ then we see that the total number of particles approaches a constant limit:

$$\lim_{\tau\to\infty} f(\tau)=(m_0\beta/N_0\alpha)^{1/2}\equiv\Gamma. \tag{2.13}$$

If Γ exceeds unity, fragmentation predominates over coalescence and the number of bodies will increase monotonically with time. If Γ is less than unity the particle number falls steadily due to coalescence. If Γ equals unity, $f(\tau)$ remains constant.

3. Evolution of the size spectrum

In order to trace the development of the mass spectrum $n(m, t)$ we shall require its Laplace transform

$$L(s, t)=\int_0^\infty \mathrm{e}^{-sm} n(m, t)\,\mathrm{d}m. \tag{3.1}$$

Transforming (2.2) we obtain a partial differential equation for $L(s, t)$:

$$\frac{\partial L}{\partial t}=\alpha\left(\tfrac{1}{2}L^2-N(t)L\right)+\beta\left(\frac{1}{2}\frac{\partial L}{\partial s}+N(t)s^{-1}-Ls^{-1}\right)$$
$$+\delta\left(N(t)\frac{\partial L}{\partial s}-L\frac{\partial L}{\partial s}-VL\right)+\gamma\left[\frac{1}{2}\left(\frac{\partial L}{\partial s}\right)^2+V\frac{\partial L}{\partial s}\right]. \tag{3.2}$$

In practice one would like to know if the mass spectrum approaches a steady, time-independent form as $t\to\infty$. If such asymptotically steady spectra exist their Laplace transforms will satisfy (3.2) with $\dot{L}=0$ and $N(t)=N(\infty)$, yielding a first-order ordinary differential equation to be solved for $L(s)$. This can be solved either approximately, by series methods, or exactly and then inverted to give the steady-state spectrum $n(m,\infty)$. As an example we solve the case where the coagulation and fragmentation kernels are both constant ($\delta=\gamma=0$).

Since $f\to\Gamma$ as $t\to\infty$ (from equation (2.13)), we have for the steady state $L(s)$:

$$\frac{\partial L}{\partial s}=-\frac{2}{s}+\frac{2L}{s}+\frac{2L}{\Gamma}-\frac{L^2}{\Gamma^2}. \tag{3.3}$$

This is a Riccati form and if any particular solution, $L_*(s)$, is known then the general solution is obtainable. A particular solution is

$$L_*(s)=\Gamma^2(\Gamma+s)^{-1} \tag{3.4}$$

and so the general solution will be

$$L(s)=L_*(s)+u(s) \tag{3.5}$$

where, by (3.3), (3.4) and (3.5),

$$u'(s)=-\Gamma^{-2}u^2+2u\Gamma^{-1}s^{-1}(s+\Gamma)^{-1}(s^2+\Gamma s+\Gamma^2) \tag{3.6}$$

so

$$u(s)=\frac{2\Gamma^2 s^2}{\Gamma(s^2-\Gamma^2)+2C(s+\Gamma)^2\exp(-2s\Gamma^{-1})} \tag{3.7}$$

with C constant. Although (3.4), (3.5) and (3.7) give the general solution for $L(s)$ we note that $u(s\to\infty)=2\Gamma$ and so this portion of the solution does not possess a smooth transform. The inverse of $L_*(s)$ yields a mass spectrum

$$n(m,t\to\infty)=\Gamma^2\,\mathrm{e}^{-\Gamma m} \tag{3.8}$$

whilst, when $C=0$, the portion $u(s)$ yields a mass spectrum which has a singularity at the origin. Thus, the asymptotic form for the mass spectrum of a system undergoing simultaneous coagulation and fragmentation is given by (3.8) where Γ is defined by (2.13). The behaviour of the solutions to the coagulation equation in the absence of fragmentation given by Trubnikov ($\Gamma=0=\beta$) indicates that in that case the steady-state size spectrum is of the form

$$n(m,t)\sim f^2(t)\,\mathrm{e}^{-mf(t)} \tag{3.9}$$

where

$$f(t)=(1+At)^{-1}. \tag{3.10}$$

Thus in the limit of large time the asymptotic form of the size spectrum is similar in form to the case where fragmentation is absent even when the fragmentation is strong ($\Gamma>1$).

It would be of interest to discover if this conclusion is sustained for a wider range of choices for the coagulation and fragmentation kernels. It is well known that, in the absence of fragmentation, coagulation with $\alpha=\gamma=0$ yields a characteristic size spectrum of the form $n(m)\sim m^{-1.5}\,\mathrm{e}^{-m}$, after long times. This is characteristic of various measured size spectra in astrophysical situations (Safronov 1969) and the persistence of this theoretical prediction under the influence of fragmentation processes would be of some interest.

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References

Chandrasekhar S 1943 *Rev. Mod. Phys.* **15** 1
Dohnanyi I S 1969 *J. Geophys. Res.* **74** 2531

Drake R L 1972 *J. Atmos. Sci.* **21** 537
Field B and Saslaw W 1965 *Astrophys. J.* **142** 568
Lushnikov A A 1973 *J. Coll. Interface Sci.* **45** 549
Pechernikova G V, Safronov V S and Zvyagina E V 1976 *Sov. Astron.* **20** 346
Penston M V, Munday V A, Strickland C J and Penston M J 1969 *Mon. Not. R. Astron. Soc.* **142** 355
Popel A S, Regirer S A and Shadrina N Kh 1975 *Prikl. Mat. Mech.* **39** 130
Ramabhadran T W, Poeterson T W and Seinfeld J H 1976 *AI Chem. Eng. J.* **22** 840
Safronov V S 1969 *Evolution of the Preplanetary Cloud and the Formation of the Earth and Planets* (Moscow: Nauka)
Schumann T 1940 *Q.J. R. Math. Soc.* **66** 195
Silk J 1980 *Star Formation* (Sauverny: Geneva Observatory) pp 131–222
Silk J and White S D M 1978 *Astrophys. J.* **223** L59
Simons S, Simpson I C and Williams I P 1978 *Astrophys. Space Sci.* **19** 399
Smoluchowski M 1916 *Phys. Zs.* **17** 557, 585
Trubnikov B A 1971 *Sov. Phys.-Dokl.* **16** 124
Wacker J F, Greenberg R, Hartman W K and Chapman C R 1977 *BAAS* **9** 544
Zvyagina E G, Pechernikova G V and Safronov V S 1974 *Sov. Astron.* **17** 793